Mon. Oct 29, 2018

Room1

Plenary Talk | Plenary Talk

[PL1] Plenary Talk 1
Chair: Ju Li(MIT, USA)
10:10 AM - 11:00 AM Room1

[PL1] Plenary Talk 1
○Christopher A. Schuh （Department of Materials Science and Engineering, MIT, USA）

Plenary Talk | Plenary Talk

[PL2] Plenary Talk 2
Chair: Alexey Lyulin(Technische Universiteit Eindhoven, The Netherlands)
11:00 AM - 11:50 AM Room1

[PL2] Plenary Talk 2
○Maenghyo Cho （School of Mechanical and Aerospace Engineering, Seoul National University, Korea）

Mon. Oct 29, 2018

Room1

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C1] Symposium C-1

Chair: Emmanuel Clouet(CEA Saclay, SRMP, France)
1:30 PM - 3:15 PM Room1

[SY-C1] Kinetic Monte Carlo model of screw dislocation-solute coevolution in W-Re alloys

Yue Zhao[1], Lucile Dezerald[3], ○Jaime Marian[1,2] （1.Dept. of Materials Science and Engineering, University of California Los Angeles, United States of America, 2.Dept. of Mechanical and Aerospace Engineering, University of California Los Angeles, United States of America, 3.Institut Jean Lamour, University of Lorraine, France）

[SY-C1] Thermally activated solute-drag strengthening by interstitial impurities in BCC Cr

○Christian Brandl （Karlsruhe Institute of Technology, Germany）

[SY-C1] Generalized yield criterion in BCC metals from first principles

○Antoine Kraych[1], Lucile Dezerald[2], Emmanuel Clouet[3], Lisa Ventelon[3], François Willaime[3], David Rodney[1] （1.Institut Lumière Matière, Université Lyon 1, France, 2.Institut Jean Lamour, Université de Lorraine, France, 3.DEN-Département des Matériaux pour le Nucléaire, CEA, Université Paris-Saclay, France）

[SY-C1] Dislocation Motion in High Entropy Alloys

○Luchan Zhang[1], Yang Xiang[2], Jian Han[3], David Srolovitz[3] （1.National University of Singapore, Singapore, 2.Hong Kong University of Science and Technology , Hong Kong, 3.University of Pennsylvania, United States of America）

[SY-C1] A random walk model of screw dislocation cross-slip in face-centered cubic solid solution alloys

○Wolfram Georg Noehring[1,2], William Arthur Curtin[2] （1. Department of Microsystems Engineering, University of Freiburg, Germany, 2. Institute of Mechanical Engineering, École Polytechnique Fédérale de Lausanne, Switzerland))

[SY-C1] Modeling the climb-assisted glide of edge dislocations through a random distribution of nanosized vacancy clusters

○Marie Landeiro Dos Reis[1], Laurent Proville[1], Maxime

Sauzay[2], Mihai Cosmin Marinica[1], Normand Mousseau[3] （1.SRMP-CEA Saclay, France, 2.SRMA-CEA Saclay, France, 3.Département de Physique, Université de Montréal , Canada）

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C2] Symposium C-2

Chair: Stefan Sandfeld(Chair of Micromechanical Materials Modelling, TU Bergakademie Freiberg, Germany)
3:45 PM - 5:30 PM Room1

[SY-C2] Finite deformation Mesoscale Field Dislocation Mechanics

Rajat Arora[1], Xiaohan Zhang[2], ○Amit Acharya[1] （1.Carnegie Mellon University, United States of America, 2.Stanford University, United States of America）

[SY-C2] Anisotropic and non-symmetric continuum dislocation dynamics

○Thomas Hochrainer （TU Graz, Austria）

[SY-C2] Numerical simulation of model problems in Plasticity based on Field Dislocation Mechanics

○Leo Morin[1,2], Renald Brenner[3], Pierre Suquet[2] （1.PIMM, Arts et Métiers-ParisTech, CNAM, CNRS, UMR 8006, 151 bd de l'Hopital, 75013 Paris, France, 2.Laboratoire de Mécanique et d'Acoustique, Aix-Marseille Univ, CNRS UMR 7031, Centrale Marseille, 4 impasse Nikola Tesla, CS 40006, 13453 Marseille Cedex 13, France, 3.Sorbonne Université, CNRS, UMR 7190, Institut Jean Le Rond d'Alembert, 75005 Paris, France）

[SY-C2] Direct computation of the stress field due to geometrically necessary dislocation densities

○Yichao Zhu[1], Yang Xiang[2] （1.Dalian University of Technology, China, 2.The Hong Kong University of Science and Technology, Hong Kong）

[SY-C2] Meshfree Analysis for Kink Band Formation in Mg-based LPSO Phase Based on Crystal Plasticity Cosserat Model Considering Disclination Density

○Yuichi Kimura[1], Yuichi Tadano[2], Kazuyuki Shizawa[3] （1.Grad. School of Science and Technology, Keio Univ., Japan, 2.Dept. of Mechanical Engineering, Saga Univ., Japan, 3.Dept. of Mechanical Engineering, Keio Univ., Japan）

[SY-C2] Dynamic recrystallization model for Mg/LPSO alloys coupling phase-field model and dislocation-based crystal plasticity model

○Sho KUJIRAI[1], Kazuyuki SHIZAWA[2] （1.Grad. School of Science and Technology, Keio Univ., Japan, 2.Dept. of Mechanical Engineering, Keio Univ., Japan）

Room2

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E1] Symposium E-1

Chairs: William A. Curtin(LAMMM, EPFL, Switzerland), Liang Qi(University of Michigan, United States of America)
1:30 PM - 3:15 PM Room2

[SY-E1] Mechanism of Enhanced Ductility in Mg Alloys
○W. Curtin[1], Z. Wu[2], R. Ahmad[1], B. Yin[1] （1.EPFL, Switzerland, 2.IHPC, Singapore）

[SY-E1] **Interaction of screw dislocations with interfaces during multiaxial loading: large scale 3D simulations**
○maxime Dupraz[1], S.I. Rao[2], Helena Van Swygenhoven[1,3] （1.PEM-LSC-PSD, Paul Scherrer Institute, Villigen, Switzerland, 2.Materials Directorate, Air Force Research Laboratory, WPAFB,, United States of America, 3.NXMM-IMX-STI, École Polytechnique Fédérale de Lausanne, Switzerland）

[SY-E1] **The Multiscale calculations on the behaviors of some nuclear fuels and cladding materials**
○shiyu du （Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, China）

[SY-E1] The connection between ideal strengths and deformation mechanisms in BCC Refractory Metals
○Liang Qi, Chaoming Yang （University of Michigan, United States of America）

[SY-E1] **Nanoscaled Matrix-Inclusions-Composites**
○Konrad Schneider[1], Swantje Bargmann[2] （1.Institute of Continuum and Material Mechanics, Hamburg University of Technology, Germany, 2.Chair of Solid Mechanics, University of Wuppertal, Germany）

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E2] Symposium E-2

Chairs: Ya-Fang Guo(Beijing Jiaotong University, China), Flemming JH Ehlers(University Paris Diderot, France)
3:45 PM - 5:30 PM Room2

[SY-E2] Using IM3D to simulate nano-beam and nano-target effects in ion radiation
○Ju Li （Massachusetts Institute of Technology, United States of America）

[SY-E2] First principles studies of H interaction with the face-centred cubic Al Σ5 [100] twist grain boundary during a uniaxial tensile test
Flemming JH Ehlers[2,1], Mahamadou Seydou[2], David Tingaud[1], Francois Maurel[2], Yann Charles[1], ○Sylvain Queyreau[1] （1.Universite Paris XIII, Sorbonne Paris Cite, Laboratoire des Sciences des Procedes et des Materiaux, LSPM UPR 3407, France, 2.University Paris Diderot, Sorbonne Paris Cite, ITODYS, UMR 7086, France）

[SY-E2] **Investigation of the {10-11} twin boundary migration in Magnesium**
Qun Zu[1], Xiao-Zhi Tang[2], ○Ya-Fang Guo[2] （1.School of Mechanical Engineering, Hebei University of Technology, China, 2.Institute of Engineering Mechanics, Beijing Jiaotong University, China）

[SY-E2] Effect of Twins on Mechanical Properties of Silicon Nanowires
○Zheng Qin （Tianjin Univ., China）

[SY-E2] Intrinsic Ductility of Alloys from Nonlinear Elasticity
○Ian Winter[1,2], Maarten de Jong[1,3], Daryl Chrzan[1,2] （1.University of California, Berkeley, United States of America, 2.Lawrence Berkeley National Laboratory, United States of America, 3.SpaceX, United States of America）

[SY-E2] **Tailoring the stability of {10-12} twin in magnesium with solute segregation at the twin boundary and strain path control**
Heyu Zhu, ○Ziran Liu （Dept. of Phyiscs, Hunan Normal University, Changsha, Hunan, China）

[SY-E2] Contribution of defects on the anisotropic diffusion behaviour of hydrogen in nickel single crystals
○Arnaud Metsue, Guillaume Hachet, Abdelali Oudriss, Xavier Feaugas （LaSIE UMR 7356 CNRS, France）

[SY-E2] Development of simplified model for one-sided mechanical joining of dissimilar materials
○Jaeho Kim, Heungjae Choi, Dongchoul Kim （Dept. of Mechanical Engineering, Sogang Univ, Korea）

Room3

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F1] Symposium F-1

Chair: Yunzhi Wang(The Ohio State University, United States of

America)
1:30 PM - 3:15 PM Room3

[SY-F1] **An Integrated Experimental and Computational Approach to Microstructure-Property Relationships in Structural Materials**

Longsheng Feng, Pengyang Zhao, Steve Niezgoda, Mike J Mills, ○Yunzhi Wang （The Ohio State University, United States of America)

[SY-F1] Development of a multiscale simulation system based on microstructure of fine-grained aluminum
○ATSUSHI SAGARA, YOSHITERU AOYAGI （Dept. of Finemechanics, Tohoku Univ., Japan)

[SY-F1] Image-based crystal plasticity analysis on the activities of slip systems in polycrystal alpha-Ti
○Yoshiki Kawano[1], Tetsuya Ohashi[1], Tsuyoshi Mayama[2], Masaki Tanaka[3], Yelm Okuyama[3], Michihiro Sato[1] （1.Kitami Institute of Technolgy, Japan, 2.Kumamoto University, Japan, 3.Kyushu University, Japan)

[SY-F1] Micro structure-based Crystal Plasticity Modeling of of Duplex Titanium Alloy During Hot Deformation
○Jun Zhang[1], Yang Wang[2], Yu Wang[2] （1.Institute of Systems Engineering,China Academy of Engineering Physics, China, 2.Department of Modern Mechanics, CAS Key Laboratory of Mechanical Behavior and Design of Materials, University of Science and Technology of China, China)

[SY-F1] Nonlocal multiscale modeling of deformation behavior of polycrystalline copper by second-order homogenization method
○makoto uchida, Akito Taniguchi, yosihisa kaneko （Osaka city Univ., Japan)

[SY-F1] Residual stress prediction for turning of Ti-6Al-4V considering the microstructure evolution
Zhipeng Pan[2], ○Donald S Shih[1], Hamid Garmestani[3], Elham Mirkoohi[2], Steven Y Liang[2] （1.Magnesium Research Center, Kumamoto University, Japan, 2.George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, United States of America, 3.School of Materials Science and Engineering, Georgia Institute of Technology, United States of America)

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F2] Symposium F-2
Chair: Selim Esedoglu(University of Michigan, United States of America)

3:45 PM - 5:30 PM Room3

[SY-F2] New algorithms for simulating grain boundary motion
○Selim Esedoglu （University of Michigan, United States of America)

[SY-F2] The Role of Grain Shape in Discrete Element Modeling of Snow Mechanics
○Carolin Willibald, Thiemo Theile, Martin Schneebeli （Institute for Snow and Avalanche Research (SLF, ETH), Switzerland)

[SY-F2] Experimental-Computational Analysis of Primary Static Recrystallizazion in DC04 Steel
○Martin Diehl, Markus Kühbach, Dierk Raabe （Max-Planck-Institut fuer Eisenforschung GmbH, Germany)

[SY-F2] Large scale phase-field simulations of solid state sintering
○Johannes Hoetzer[1,2], Marco Seiz[2], Michael Kellner[2], Wolfgang Rheinheimer[3], Hernik Hierl[1], Britta Nestler[2,1] （1.Karlsruhe University of Applied Sciences, Germany, 2.Karlsruhe Institute of Technology, Germany, 3.Purdue University, United States of America)

[SY-F2] Phase-field simulations of coupled dendritic-eutectic growth
○Marco Seiz[1], Michael Kellner[1,2], Johannes Hötzer[1,2], Philipp Steinmetz[3], Britta Nestler[1,2] （1.Institute of Applied Materials - Computational Materials Science, Karlsruhe Institute of Techology, Germany, 2.Institute of Digital Materials Science, Karlsruhe University of Applied Sciences, Germany, 3.Department of Materials Science and Engineering, University of Alabama at Birmingham, United States of America)

[SY-F2] The use of thermodynamic tensor models for phase-field simulations of spinodal decomposition in quaternary alloys coupled with CALPHAD data.
○Yuri Amorim Coutinho[1], Nico Vervliet[2], Lieven De Lathauwer[2,3], Nele Moelans[1] （1.Dept. of Materials Engineering, KU Leuven, Belgium, 2.Dept. of Electrical Engineering, KU Leuven, Belgium, 3.Group Science, Engineering and Technology, KU Leuven - Kulak, Belgium)

Room4

Symposium | M. Time- and History-Dependent Material Properties

[SY-M1] Symposium M-1
Chair: Thomas Voigtmann(German Aerospace Center, Cologne, Germany)

1:30 PM - 3:15 PM Room4

[SY-M1] Structure-property Relations in Sheared Dense Flocculated Suspensions

○Jan Vermant （ETH Zurich, Switzerland）

[SY-M1] Soft deformable colloids make strong liquids with stress-driven relaxation

Nicoletta Gnan, ○Emanuela Zaccarelli （CNR Institute for Complex Systems, Rome, Italy）

[SY-M1] Linear viscoelasticity on matter out of equilibrium

○Leticia Lopez-Flores[1], Magdaleno Medina-Noyola[1], Jose Manuel Olais-Govea[1,2], Martin Chavez-Paez[1] （1.Universidad Autonoma de San Luis Potosi, Mexico, 2.Instituto Tecnologico y de Estudios Superiores de Monterrey, Mexico）

[SY-M1] Memory effects in functional polymers: The interplay between entropic elasticity and kinetic arrest

○Fathollah Varnik, Elias M. Zirdehi （Ruhr-University Bochum, Germany）

[SY-M1] Modelling and Experimental Verified Coupled Visco hyper electro-elastic Behaviour of Dielectric Elastomer Circular Actuator

○ARPIT SRIVASTAVA, Sumit Basu （IIT KANPUR, INDIA - 208016, India）

Symposium | M. Time- and History-Dependent Material Properties

[SY-M2] Symposium M-2
Chair: Emanuela Zaccarelli(University of Rome I, Italy)
3:45 PM - 5:45 PM Room4

[SY-M2] MMM in aircraft industries: use cases for simulation of additive manufacturing

○Annett Seide[1], Thomas Goehler[1], Roman Sowa[2] （1.MTU Aero Engines AG, Germany, 2.MTU Aero Engines Polska Sp. z o. o., Poland）

[SY-M2] VISCOELASTIC BEHAVIOUR OF HETEROGENEOUS MATERIALS STUDIED THANKS TO AN EXTENSION OF CRAFT SOFTWARE IN HARMONIC REGIME

○Julien Boisse , Stéphane André, Laurent Farge （University of Lorraine, France, France）

[SY-M2] Multi-scale modelling of Zener Pinning during the solid solution treatment of a Nickel-based Superalloy

○Magnus Jack Anderson[1], Jonathan Benson[1], Christos Argyrakis[2], Jeffery William Brooks[1], Hector Christian Basoalto[1] （1.The University of Birmingham, UK, 2.Rolls-Royce plc, UK）

[SY-M2] Assessment of residual stresses in welds made of multiphase alloys

○Victor De rancourt[1], Sylvain Flouriot[1], Benjamin Sarre[2], Benoit Panicaud[2], Guillaume Geandier[3] （1.Commissariat a l'energie atomique, France, 2.Universite de Technologie de Troyes, France, 3.Universite de Lorraine - CNRS, France）

[SY-M2] Atomic analysis of crystalline nucleation and growth in the supercooled liquid of glass-forming binary alloy

○Masato Wakeda[1], Shigenobu Ogata[2,3] （1.Research Center for Structural Materials, National Institute for Materials Science, Japan, 2.Graduate school of engineering science, Osaka Univ., Japan, 3.Center for Elements Strategy Initiative for Structural Materials (ESISM), Kyoto Univ., Japan）

[SY-M2] Crystal growth in fluid flow: Nonlinear response effects

○Hailong Peng[1,2], Dieter Herlach[1], Thomas Voigtmann[1] （1.German Aerospace Center, Germany, 2.Central South University, China）

[SY-M2] **Time-dependent active microrheology in dilute colloidal suspensions**

Sebastian Leitmann[1], Suvendu Mandal[4,1], Matthias Fuchs[2], Antonio M. Puertas[3], ○Thomas Franosch[1] （1.Innsbruck Univ., Austria, 2.Konstanz Univ. , Germany, 3.University of Almeria, Spain, 4.Heinrich-Heine University Düsseldorf , Germany）

Room5

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O1] Symposium O-1
Chairs: Lars Pastewka(University of Freiburg, Germany), Izabela Szlufarska(University of Wisconsin, United States of America)
1:30 PM - 3:15 PM Room5

[SY-O1] A numerical insight into third body flow regimes within dry contacts

○Guilhem Mollon （INSA Lyon - LaMCoS, France）

[SY-O1] A novel multiscale framework for modeling of diamond tools wearA novel multiscale framework for modeling of diamond tools wear

○Adriana Quacquarelli[1], Nicolas Fillot[1], Guilhem Mollon[1], Thierry Commeau[2], Aurelie Nouveau[2] （1.Université de Lyon, LaMCoS, INSA-Lyon, CNRS

UMR5259, F-69621, France, 2.Umicore Specialty Powders France, France）

[SY-O1] **Thermodynamics of sliding contact: Joule-Thomson effect**

○Vera Deeva[1], Stepan Slobodyan[2] （1.Tomsk Polytechnic University, Russia, 2.Tver State Technical University, Russia）

[SY-O1] Molecular Simulation of adsorption process of anti-corrosion additives

○Kohei Nishikawa[1], Hirotoshi Akiyama[1], Kazuhiro Yagishita[2], Hitoshi Washizu[1] （1.University of Hyogo, Japan, 2.JX Nippon Oil &Energy Corporation, Japan）

[SY-O1] **The adhesive behavior of elastic contacts in the presence of interfacial shear stresses**

Nicola Menga[1,2], ○Giuseppe Carbone[1,2], Daniele Dini[2] （1.Department of Mechanics, Mathematics and Management - Polytechnic University of Bari, Italy, 2.Department of Mechanical Engineering, Imperial College London, UK）

[SY-O1] Soft Matter Mechanics: numerical and experimental methodologies for dry and lubricated tribological problems

○Carmine Putignano [1,2], Giuseppe Carbone[1,2] （1.Polytechnic University of Bari, Italy, 2.Imperial College London, UK）

[SY-O1] Two simple models for pull-off decay of self-affine rough surfaces

○Antonio Papangelo[1,2], Michele Ciavarella[1,2] （1.Politecnico di Bari, Italy, 2.Hamburg University of Technology, Germany）

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O2] Symposium O-2
Chairs: Mark Owen Robbins(Johns Hopkins University, United States of America), Tasuku Onodera(Hitachi, Ltd., Japan)
3:45 PM - 5:30 PM Room5

[SY-O2] Droplet Spreading on a Surface Exhibiting Solid-liquid Interfacial Premelting

○Yang Yang[1], Brian B Laird[2] （1.East China Normal University, China, 2.University of Kansas, United States of America）

[SY-O2] **Comparative Study on the Adsorption of Violate Organic Compounds on the Surfaces of Two-Dimensional Materials: Toward the Early Lung Cancer Detection**

○Van An Dinh[1,2] （1.Nanotechnology Program, Vietnam

Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan）

[SY-O2] Adsorption of the Volatile Organic Compounds on Graphene including Van de Waals Interaction

○Thi Viet Bac Phung[1], Trong Lam Pham[1], Yoji Shibutani[1,2], Van An Dinh[1,2] （1.Nanotechnology Program, Vietnam Japan University - Vietnam National University, Viet Nam, 2.Center for Atomic and Molecular Technologies, Graduate School of Engineering, Osaka University, Japan）

[SY-O2] **Diffusion of a Cu nanodroplet on an amorphous carbon surface**

Yong-Long Chen[1], ○Yu-Chen Chiu[1], Kai Chen[2], Yu-Chieh Lo[1] （1.National Chiao Tung University, Taiwan, 2.Xi'an Jiaotong University, China）

[SY-O2] First principal modeling of oxygen and carbon adsorption on Fe (110) surface with symmetrical tilt Sigma3(111) grain boundary

○Ivan Lobzenko, Yuki Uchiyama, Yoshinori Shiihara （Toyota Technological Institute, Japan）

[SY-O2] Theoretical study of the effects of boron doping on the electronic structure of $g\text{-}C_3N_4/TiO_2$(001) heterojunction

○Jianhong Dai, Yan Song （Harbin Institute of Technology at weihai, China）

[SY-O2] Atomistic Simulations that Reach Anthropological Timescale and Beyond

○Ju Li （Massachusetts Institute of Technology, United States of America）

Room6

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A1] Symposium A-1
Chair: Anton Van der Ven(University of California Santa Barbara, United States of America)
1:30 PM - 3:00 PM Room6

[SY-A1] Atomistic to continuum: coarse-graining in and out of equilibrium

○Celia Reina[1], Xiaoguai Li[1], Peter Embacher[2], Nicolas Dirr[2], Johannes Zimmer[3] （1.University of Pennsylvania, United States of America, 2.Cardiff University, UK, 3.University of Bath, UK）

[SY-A1] **Finite-temperature Localized Stress and Strain for Atomic Models**

○Ranganathan Parthasarathy[1], Anil Misra[2], Lizhi

Ouyang[1] （1.Tennessee State University, United States of America, 2.University of Kansas, United States of America）

[SY-A1] Uncertainty Quantification for Classical Effective Potentials

○Sarah Longbottom, Peter Brommer （School of Engineering, University of Warwick, UK）

[SY-A1] The role of null-lagrangians in the continuum interpolation of the linear chain with hyper-pre-stress

○Alexandre Danescu （Ecole Centrale de Lyon, France）

[SY-A1] Practical Time Averaging of nonlinear dynamics

Sabyasachi Chatterjee[1], ○Amit Acharya[1], Zvi Artstein[2] （1.Carnegie Mellon University, United States of America, 2.The Weizmann Institute of Science, Israel）

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A2] Symposium A-2
Chair: Kenjiro Sugio(Hiroshima Univ., Japan)
3:45 PM - 5:30 PM Room6

[SY-A2] Bridging the chasm between phenomenological theories and electronic structure

○Anton Van der Ven （University of California Santa Barbara, United States of America）

[SY-A2] Two-component Dirac-Kohn-Sham calculation for multiscale modeling of materials

○Koichi Nakamura[1,2] （1.Kyoto Univ., Japan, 2.E-JUST, Egypt）

[SY-A2] Combination of Kinetic Monte Carlo Method and First Principles Calculation to Explore Stable Structure of Solute Cluster in Al-Si Based Alloys

○Kenjiro Sugio, Hiroshi Mito, Yongbum Choi, Gen Sasaki （Hiroshima Univ., Japan）

[SY-A2] Electronic structure analysis of Fermi level instability in Fe-rich Si alloy

○Chen Ying[1], Arkapol Saengdeejing[1], Tetsuo Mohri[2] （1.School of Engineering, Tohoku University, Japan, 2.Institute for Materials Research, Tohoku University, Japan）

[SY-A2] **From first-principles defect chemistry to device damage models of radiation effects in III-V semiconductors**

○Peter A Schultz, Harold P Hjalmarson （Sandia National Laboratories, United States of America）

[SY-A2] How to model ordering processes in metallic

---

hydrides? A Tight-Binding Ising modeling proposal and its application to Zr-H

Paul Eymeoud[1], ○Fabienne Ribeiro[1], Remy Besson[3], Guy Tréglia[2] （1.Institut de Radioprotection et de Sûreté Nucléaire/PSN-RES/SEMIA/LPTM, France, 2.Centre Interdisciplinaire de Nanoscience de Marseille, CNRS, France, 3.Unité Matériaux Et Transformations (UMET), CNRS UMR 8207, Université de Lille, 59655 Villeneuve D'Ascq, France）

Room7

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I1] Symposium I-1
Chairs: David Sroloviz(University of Pennsylvania, USA), Enrique Martinez Saez(Los Alamos National Laboratory, USA)
1:30 PM - 3:15 PM Room7

[SY-I1] **Grain Growth at the Nanoscale: The Coupling of Stress and Grain Boundary Motion**

○Peter Voorhees[1], Kevin McReynolds[1,3], Akinori Yamanaka[2] （1.Northwestern University, United States of America, 2.Tokyo University of Agriculture and Technology, Japan, 3.National Institute for Standards and Technology, United States of America）

[SY-I1] Verification of grain growth models by time-resolved 3D experiments in pure iron

○Jin Zhang[1,2], Yubin Zhang[2], Wolfgang Ludwig[3], David Rowenhorst[4], Henning F Poulsen[2], Peter W Voorhees[1] （1.Northwestern University, United States of America, 2.Technical University of Denmark, Denmark, 3.European Synchrotron Radiation Facility, France, 4.The US Naval Research Laboratory, United States of America）

[SY-I1] Coarse-grained, three-dimensional modeling of defects at low-angle grain boundaries with the amplitude expansion of the phase field crystal model

○Marco Salvalaglio[1], Rainer Backofen[1], Ken R. Elder[2], Axel Voigt[1] （1.Institute of Scientific Computing, Technische Universität Dresden, 01062 Dresden , Germany, 2.Department of Physics, Oakland University, Rochester, 48309 Michigan , United States of America）

[SY-I1] **Estimation of Grain Boundary Anisotropy using Multi-phase-field Model based on the Ensemble Kalman Filter**

○Akinori Yamanaka, Yuri Maeda, Kengo Sasaki （Tokyo University of Agriculture and Technology, Japan）

[SY-I1] Multiscale Modelling of Graphene from Nano to Micron Scales

○Tapio Ala-Nissila （Aalto and Loughborough University, Finland）

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I2] Symposium I-2
Chair: Elizabeth Holm(Carnegie Mellon University, United States of America)
3:45 PM - 5:30 PM Room7

[SY-I2] Energy and dynamics of grain boundaries based on underlying mircrostructure

○Yang Xiang （Hong Kong University of Science and Technology, Hong Kong）

[SY-I2] **Grain growth in ultrafine-grained thin films: A 3D problem**

○Ahu Oencue[1], Thorsten Halle[2], Dana Zoellner[3] （1.Institute of Experimental Physics, Otto-von-Guericke University, Magdeburg, Germany, 2.Institute of Materials and Joining Technology, Otto-von-Guericke University, Magdeburg, Germany, 3.B CUBE Center for Molecular Bioengineering, TU Dresden, Dresden, Germany）

[SY-I2] The Kinetics of Ideal Grain Growth: A Large Scale Monte Carlo Simulation

○Xiangge Qin （School of Materials Science and Engineering, Jiamusi University, China）

[SY-I2] Understanding the energetics of grain boundary motion in terms of compatible transformations and optimal transport theory

○Ian W Chesser[1], Brandon Runnels[2], Elizabeth Holm[1] （1.Carnegie Mellon University, United States of America, 2.University of Colorado Colorado Springs, United States of America）

[SY-I2] **Microstructure Stabilization and the Herring Condition**

○Jeremy K Mason, Erdem Eren （University of California, Davis, United States of America）

Room8

Symposium | L. Structure, Statistics and Mechanics in Crystal Dislocation Plasticity

[SY-L1] Symposium L-1
Chairs: Jerome Weiss(CNRS/ University of Grenoble-Alpes, France), Yinan Cui(University of California, Los Angeles, United States of America)
1:30 PM - 3:15 PM Room8

[SY-L1] Flow and failure of (amorphous) materials - a nonequilibrium phase transition?

○Peter Schall （University of Amsterdam, Netherlands）

[SY-L1] Reversibility and Criticality in Amorphous and Crystalline Solids

○Charles Reichhardt （Los Alamos National Laboratory , United States of America）

[SY-L1] Exploring Crystal-plastic Constitutive Rules with the OOF Tool

○Andrew Reid[1], Stephen Langer[1], Shahiryar Keshavarz[1,2] （1.NIST, United States of America, 2.Theiss Research, United States of America）

[SY-L1] Objective fusion of multiscale experiments and multiscale models using Bayesian inference

○Surya Raju Kalidindi （Georgia Tech, United States of America）

Symposium | L. Structure, Statistics and Mechanics in Crystal Dislocation Plasticity

[SY-L2] Symposium L-2
Chairs: Charles Reichhardt(Los Alamos National Laboratory , United States of America), Peter Schall(University of Amsterdam, Netherlands)
3:45 PM - 5:45 PM Room8

[SY-L2] The role of system size, internal disorder, and dislocation patterning on the nature of plastic fluctuations

○Jerome Weiss （CNRS/University of Grenoble-Alpes, France）

[SY-L2] Dislocations associated with stick-slip friction of lubricants in boundary lubrication

Rong-Guang Xu[1,2], Hengxu Song[2], Stefanos Papanikolaou[2], ○Yongsheng Leng[1] （1.George Washington Univ, United States of America, 2.West Virginia Univ, United States of America）

[SY-L2] **Comparison of surface-indentation and pillar-compression at the nanoscale of FCC metals: Unification of size effects using 3D Discrete Dislocation Dynamics**

○Hengxu Song[1,2], Stefanos Papanikolaou[1,2] （1.west virginia university, United States of America, 2.johns hopkins university, United States of America）

[SY-L2] Statistical models for cross slip and reaction rate processes in continuum dislocation dynamics

○Vignesh Vivekanandan, Peng Lin, Anter El-Azab （Purdue University, United States of America）

[SY-L2] Designing Interfaces: a combinatorial approach to

geometrical manipulation of interfaces
○Hakan Yavas[1], Alberto Fraile[1], Tomas Polcar[1,2], Ondrej Man[3] （1.Czech Technical University, Czech Republic, 2.University of Southampton, UK, 3.CEITEC, Czech Republic）

Room10

Symposium | J. Multiscale Modeling of Heterogeneous Layered Media

[SY-J1] Symposium J-1

Chairs: Jinghong Fan(Alfred University, United States of America), Sinan Keten(Northwestern University, United States of America)
1:30 PM - 3:15 PM Room10

[SY-J1] **A multiscale failure analysis for layered composites with statistical account of manufacturing defects**
○Ramesh Talreja （Texas A&M University, United States of America）

[SY-J1] Multiscale Modeling of Fiber Reinforced Materials for Future Aerospace Structures
○Anthony M Waas （U. Washington, Seattle, WA 98195; also Univ. of Michigan, Aerospace Engineering, Ann Arbor, MI 48109, United States of America）

[SY-J1] **A-DiSC (Adaptive Discrete-Smeared Crack) Model for Multi-Scale Progressive Damage Analysis of Composite Structures**
○Tong-Earn Tay, Xin Lu, Vincent Beng-Chye Tan （National University of Singapore, Singapore）

[SY-J1] Analysis for the Plane Problem of Layered Magnetoelectric Composite with Collinear Interfacial Cracks
○Wenxiang Tian[1], Zheng Zhong[1,2] （1.School of Aerospace Engineering and Applied Mechanics,Tongji Univ, China, 2.School of Science, Harbin Institute of Technology, China）

Symposium | J. Multiscale Modeling of Heterogeneous Layered Media

[SY-J2] Symposium J-2

Chairs: Anthony M Waas(University of Washington, United States of America), Junqian Zhang(Shanghai University, China)
3:45 PM - 5:30 PM Room10

[SY-J2] Simulation-based Design of Bioinspired Impact-resistant Nanocellulose Films with Bouligand Microstructure
○Sinan Keten （Northwestern University, United States of America）

[SY-J2] **Amelogenesis: Nature's 3D printing system for multi-scale laminates**

○brian n cox （arachne consulting, United States of America）

[SY-J2] **Role of geometrical features on mechanical properties in bio-inspired staggered composites**
Aman Mahar, ○Siladitya Pal （Indian Institute of Technology Roorkee, India）

[SY-J2] Dynamic homogenization for acoustic metamaterials
○Celia Reina, Chenchen Liu （University of Pennsylvania, United States of America）

[SY-J2] **Cracking behavior of ferrite-pearlite pipeline steel with hierarchical and concurrent multiscale modeling schemes**
○Taolong Xu[1,2], Wei Wang[1], Xiaojiao Deng[1], Anlin Yao[1], Jinghong Fan[3,2] （1.Southwest Petroleum University of China, China, 2.International Institute of Material Multiscale Modeling, United States of America, 3.Alfred University, United States of America）

Mon. Oct 29, 2018

Poster Hall

Poster Session | A. Advances in Materials Theory for Multiscale Modeling

[PO-A1] Poster Session 1
5:45 PM - 8:00 PM Poster Hall

[P1-01] The Coadsorption Effect of Cl- and H_2O on the Various Defect Al_2O_3 Film Surface

○Chuan-Hui Zhang, Bao Chen, Peng Shi （University of Science and Technology Beijing, China）

[P1-02] Incorporation of double cross-slip in continuum dislocation dynamics

○Xingjian Zhou, Yichao Zhu （Faculty of vehicle Engineering and Mechanics, Dalian University of Technology, China）

[P1-03] **Effect of Defect on Structural and Optical Properties in Methyl-Ammonium Lead Iodide(MAPI) Perovskite via First Principles Calculations**

○Abdullah Al ASAD, Keiichi MITANI, Atsushi ISHIKAWA, Kenji TSURUTA （Dept. of Electrical and Electronic Engineering, Okayama University, Japan）

[P1-04] Isogeometric modeling and large-scale computation for stress field around lattice defects

○Shunsuke Kobayashi[1], Ryuichi Tarumi[2], Atsushi Suzuki[3], Masao Ogino[4], Yoji Shibutani[1] （1.Graduate School of Engineering, Osaka Univ., Japan, 2.Graduate School of Engineering Science, Osaka Univ., Japan, 3.Cybermedia Center, Osaka Univ., Japan, 4.Information Technology Center, Nagoya Univ., Japan）

[P1-05] **A local/nonlocal plasticity model for upscaling microstructural effects**

○John Mitchell （Sandia National Laboratories, United States of America）

[P1-06] **First-principles investigation of atomic hydrogen adsorption and diffusion on/into Mo-doped Nb (100) surface**

○Zhong-min Wang, Yang Wu, Qingrong Yao, Yan Zhong, Chaohao Hu, Huaiying Zhou （Guilin University of Electronic Technology, China）

[P1-07] **First-principles Study on Electronic Properties of Hybrid MA*BX*$_3$ perovskites (MA= $CH_3NH_3^+$; *B*= Pb, Sn, Ge; *X*= I, Br, Cl)**

○Narasak Pandech[1,2], Thanundon Kongnok[1], Sirichok Jungthawan[1], Sukit Limpijumnong[1], Walter R.L Lambrecht[2] （1.School of Physics and NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials, Suranaree University of Technology, NakhonRatchasima 30000, Thailand, Thailand, 2.Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106-7079, USA., United States of America）

Poster Session | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[PO-C1] Poster Session 1
5:45 PM - 8:00 PM Poster Hall

[P1-08] Pressure effects on dislocation core structures in Mg_2SiO_4 olivine: insights from atomic-scale modeling

○Philippe Carrez, Srinivasan Mahendran, Patrick Cordier （Lille University, Lab. UMET UMR-CNRS 8207, France）

[P1-09] Structural and magnetic properties of long-period stacking ordered (LPSO) structure of iron; A first-principles study

○Takao Tsumuraya[1], Ikumu Watanabe[2], Takahiro Sawaguchi[2] （1.Magnesium Research Center/POIE, Kumamoto Univ., Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan）

[P1-11] Dislocation transmission behaviors of bi-crystal BCC Tantalum with high and low angle symmetric tilt grain boundaries: Multiscale simulation study

○Moon Sunil, Kang Keonwook （Dept. of Mechanical Engineering, Yonsei Univ., Korea）

[P1-12] Ab Initio Dislocation Core Calculations using a Cluster Model

○Jonas Frafjord[1,3], Bjørn Holmedal[4], Jesper Friisj[2,3], Randi Holmestad[1,3], Ingeborg-Helene Svenum[2], Inga Gudem Ringdalen[2] （1.Dept. of Physics, Norwegian University of Science and Technology, Norway, 2.SINTEF Industry, Trondheim, Norway, 3.Centre for Advanced Structural Analysis, SIMLab, Norway, 4.Dept. of Materials Science and Engineering, Norwegian University of Science and Technology, Norway）

[P1-13] Anelastic recovery of a steel wire under pure shear strain with various magnetic treatments

○Shigeo Kotake, Takuro Murata （Dept. of Mechanical Engineering, Mie Univ., Japan）

[P1-14] Possible explanation of sudden stress drop at upper yield point in iron by magnetostriction and

unpinning dislocations with law of approach in residual magnetization

○Shigeo Kotake （Dept. of Mechanical Engineering, Mie Univ., Japan）

[P1-15] Investigation of dislocation core structure in Aluminum by using a generalized Peierls-Nabarro model

○Hideki MORI （College of Industrial Technology, Japan）

[P1-16] Crystal orientation evolution analysis during deformation using molecular dynamics

○Keisuke Kinoshita （Nippon Steel &Sumitomo Metal Corporation, Japan）

[P1-17] Nanoindentation of Nanoparticles -A Molecular Dynamics and Discrete Dislocation Dynamics Simulations Study

Roy Shyamal[1], Riccardo Gatti[2], Benoit Devincre[2], ○Dan Mordehai[1] （1.Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel, Israel, 2.LEM, UMR 104, CNRS-ONERA, 29 Av. de la Division Leclerc, 4 Chatillon, France, France）

[P1-18] Machine learning interatomic potentials for molecular dynamics simulations of dislocations

○Eyal Oren, Guy Makov （Dept. of Materials Engineering, Ben-Gurion University of the Negev, Israel）

Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E1] Poster Session 1
5:45 PM - 8:00 PM Poster Hall

[P1-21] Large-scale molecular dynamics simulations: coupling with dislocation dynamics

○Pavel A. Pokatashkin, Denis K. Ilnitsky, Alexei V. Yanilkin （Dukhov Research Institute of Automatics (VNIIA), Russia）

[P1-22] **Hydrogen embrittlement controlled by reaction of dislocation with grain boundary in alpha-iron polycrystals**

○Liang Wan[1,2], Wen Tong Geng[2,3], Akio Ishii[2], Jun-Ping Du[2,4], Nobuyuki Ishikawa[5], Hajime Kimizuka[2], Shigenobu Ogata[2,4] （1.Wuhan University, China, 2.Osaka University, Japan, 3.University of Science and Technology Beijing, China, 4.Kyoto University, Japan, 5.JFE Steel Corporation, Japan）

[P1-23] Study of solute effect on the yield strength of Fe-based dilute alloy using atomistically informed

kinetic Monte Carlo method

○Shuhei Shinzato[1], Masato Wakeda[2], Shigenobu Ogata[1] （1.Dept. of Mechanical Science and Bioengineering, Osaka Univ., Japan, 2.National Institute for Materials Science, Japan）

[P1-24] **Molecular Dynamics Simulations of Low-cycle Fatigue Behavior in Single Layer Molybdenum Disulfide**

Yu-Chieh Lo[1], ○Yu-Cheng Su[1], Ming-Chen Chung[2], Alice Hu[3] （1.National Chiao Tung University, Taiwan, 2.National Cheng Kung University, Taiwan, 3.City University of Hong Kong, Hong Kong）

[P1-25] Fracture behavior of multi-walled carbon nanotube under biaxial loading condition

○Masaomi Nishimura[1], Naoki Kazami[2], Daiki Kato[2] （1.Dept. of Mechanical Systems Engineering, Shinshu Univ., Japan, 2.Graduate School of Science and Technology, Shinshu Univ., Japan）

[P1-26] **On the role of amorphous shells on mechanical properties of fcc Ni nanoparticles under compression**

○Alexandra Goryaeva[1,2], Claudio Fusco[2], Matthieu Bugnet[2], Jonathan Amodeo[2] （1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France, 2.INSA-Lyon, Université de Lyon, MATEIS, 69621 Villeurbanne, France）

[P1-27] Molecular dynamics analysis of hydrogen diffusion behavior in alpha-Fe bi-crystal under stress gradient

○Ken-ichi Saitoh[1], Haruka Koga[2], Tomohiro Sato[1], Masanori Takuma[1], Yoshimasa Takahashi[1] （1.Kansai Univ., Japan, 2.Kobe Steel, Ltd., Japan）

[P1-28] Understanding Interactions of Dislocations with Interfaces in Nickle-based Superalloys: Insights from Molecular Dynamics Simulations

○Jian Huang[1], Yunjiang Wang[2] （1.Shanghai Institute of Ceramics Chinese Academy of Sciences, China, 2.Institute of Mechanics, Chinese Academy of Sciences, China）

[P1-29] The influence of nano-sized Ti_3Al particles on the mechanical properties of α-titanium alloys

○Yan He[1,2,3], Wang Hao[1], Dongsheng Xu[1], Yang Rui[1] （1.IMR, CAS, China, 2.Coll. of Physics Science and Technology, SYNU, China, 3.Univ. of chinese Academy of Sciences, China）

[P1-30] **The atomic study of tensile property for nickel nanowires with helium bubble**
○Hengfeng Gong, Rui Li, Tong Liu （CGN, China）

[P1-31] **Componets of fracture response of alkali-activated slag mortars with steel fibers**
○Hana Simonova, Petr Frantik, Zbynek Kersner, Pavel Schmid, Pavel Rovnanik （Brno University of Technology, Faculty of Civil Engineering, Czech Republic）

[P1-32] Molecular Dynamics Simulation of Crack Growth Behavior of Single Crystal γ-TiAl Alloy Under Different Nb Substitution Mode
○Yuxi Feng[1,2], Zhiyuan Rui[1,2], Hui Cao[1,2], Ruicheng Feng[1,2], Xiaocui Fan[1,2], Xing Yang[1,2] （1.Mechanical and Electronical Engineering College, Lanzhou University of Technology, China, 2.Key Laboratory of Digital Manufacturing Technology and Application, the Ministry of Education, Lanzhou University of Technology, China）

Poster Session | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[PO-F1] Poster Session 1
5:45 PM - 8:00 PM Poster Hall

[P1-33] UNDERSTANDING OF DELAYED HYDRIDE CRACKING FAILURE MECHANISM IN E110 ZIRCONIUM BASED FUEL CLADDINGS BY EBSD AND IN-SITU MECHANICAL TESTING
○Hygreeva Kiran NAMBURI[1], Zbynek Spirit[1], Patricie Halodova[1], Ondrej Libera[1], Jakub krejci[2] （1.Research Centre REZ, Czech Republic, 2.UJP Praha, Czech Republic）

[P1-34] Transition-metal alloying of γ '-Ni$_3$Al: Effects on the ideal uniaxial compressive strength from first-principles calculations
○Minru Wen[2,1], Chongyu Wang[2] （1.Guangdong University of Technology, China, 2.Tsinghua University , China）

[P1-35] **The Influence of Deposition Pattern on Stress and Mechanical Properties in Wire Arc Additive Manufacturing**
○Changmeng Liu, Qianru Wu, Jiping Lu, Shuyuan Ma （Beijing Institute of Technology, China）

[P1-36] On the Significance of the Higher-Order Neighbors for Abnormal Grain Growth and Recrystallization Nucleation
○Markus Kuehbach （Max-Planck-Institut fur Eisenforschung GmbH, Germany）

[P1-37] **Hydrogen trapping in carbon supersaturated a-iron and its decohesion effect in martensitic steel**
○Wen-Tong Geng[1,2], Vei Wang[1,3], Jin-Xu Li[2], Nobuyuki Ishikawa[4], Hajime Kimizuka[1], Kaneaki Tsuzaki[5,6], Shigenobu Ogata[1,6] （1.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 2.University of Science and Technology Beijing, China, 3.Department of Applied Physics, Xi'an University of Technology, China, 4.Steel Research Laboratory, JFE Steel Corporation, Japan, 5.Department of Mechanical Engineering, Kyushu University, Japan）

[P1-38] **Size Scale Effect on Energy Absorption Property of Aluminum Foam**
○zengyou liang, fudi liang, dezhi deng, chunzhuang miao, mingguang wang （North University of China, China）

[P1-39] Development of charge-transfer type interatomic potential for SiC oxidation
○So Takamoto[1], Takahiro Yamasaki[2], Takahisa Ohno[2], Chioko Kaneta[3], Asuka Hatano[1], Satoshi Izumi[1] （1.The Univ. of Tokyo, Japan, 2.NIMS, Japan, 3.Fujitsu Lab., Japan）

[P1-40] Alpha-phase in engineering aluminum alloys: a multiscale modeling approach to its mechanical behavior
○Duancheng Ma （Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria）

[P1-41] Multi-phase-field lattice Boltzmann modeling and simulation of equiaxed structure
○Ryotaro Sato[1], Tomohiro Takaki[1], Shinji Sakane[1], Munekazu Ohno[2], Yasushi Shibuta[3] （1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.Tokyo University, Japan）

[P1-42] Simulation of Extrusion Process of TiAl alloy prepared by Triple VAR
○Fan Gao, Zhenxi Li （AECC BEIJING INSTITUTE OF AERONAUTICAL MATERIALS, China）

[P1-43] Experimental-Computational Analysis of Primary Static Recrystallizazion in DC04 Steel
○Martin Diehl, Markus Kühbach, Dierk Raabe （Max-Planck-Institut fuer Eisenforschung GmbH, Germany）

[P1-44] Combining 4D experiments and phase-field modeling to determine reduced grain boundary mobilities

○Jin Zhang[1,2], Peter W Voorhees[1], Henning F Poulsen[2]　(1.Northwestern University, United States of America, 2.Technical University of Denmark, Denmark)

[P1-45] Fiber-intersectant microstructure of fish scale and biomimetic research

○Bin Chen[1], Jinghong Fan[2], Miao Li[1], Wei Ye[1]　(1.College of Aerospace Engineering, Chongqing University, China, 2.Division of Mechanical Engineering, Alfred University, United States of America)

[P1-46] Microstructures of turtle shell and biomimetic fabrication

○Bin Chen[1], Jinghong Fan[2], Wei Ye[1], Miao Li[1]　(1.College of Aerospace Engineering, Chongqing University, China, 2.Division of Mechanical Engineering, Alfred University, United States of America)

[P1-47] **Phase-field Simulation of Solidification Process in Welding Pool of Fe-C Binary Alloy**

○Ian zhan, Xiangge Qin　(Jiamusi Univ., China)

[P1-48] **Phase field simulation of the phase separation in the TiC-ZrC-WC system**

○Zelin Luo[1], Hong Ma[1], Sai Tang[1], Yingbiao Peng[2], Yong Du[1], Zikui Liu[3], Qianhui Min[1], Yafei Pan[4]　(1.State Key Lab of Powder Metallurgy, Central South University, China, 2.College of Metallurgy and Materials Engineering, Hunan University of Technology, China, 3.Department of Materials Science and Engineering, Pennsylvania State University, United States of America, 4.School of materials science and engineering, Hefei University of Technology, China)

[P1-49] Switching of coordinate transformations of a repetitive bar-and-joint framework under uniaxial compression

○Hiro Tanaka[1], Kazutoshi Hamada[1], Yoji Shibutani[1,2]　(1.Dept. of Mechanical Engineering, Osaka Univ., Japan, 2.Nanotechnology Program, Vietnam Japan Univ., Viet Nam)

[P1-50] Understanding the effect of Residual Stresses in 3D Printed Metals

○Alankar Alankar, BVSS Bharadwaja, Ritam Chatterjee　(IIT Bombay, India)

Poster Session | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[PO-H1] Poster Session 1

5:45 PM - 8:00 PM　Poster Hall

[P1-51] Multi-scale modeling of DNA-dendrimers in electrolyte solutions

○Natasa Adzic[1], Clemens Jochum[2], Gerhard Kahl[2], Christos Likos[1]　(1.Faculty of Physics, University of Vienna, Austria, 2.Institute for Theoretical Physics, Vienna University of Technology, Austria)

[P1-52] Structural and dynamical properties of star block-copolymers in shear flow.

○Diego Felipe Jaramillo - Cano[1], Manuel Camargo[2], Christos N. Likos[1]　(1.Faculty of Physics, University of Vienna, Austria, 2.CICBA, Universidad Antonio Nariño - Campus Farallones, Colombia)

[P1-53] Multiscale simulation of polymeric solids for fracture processes

○Takahiro Murashima[1], Shingo Urata[2]　(1.Dept. of Physics, Tohoku Univ., Japan, 2.AGC, Japan)

[P1-54] Quantification and validation of the mechanical properties of DNA nicks

○Jae Young Lee, Jae Gyung Lee, Do-Nyun Kim　(Dept. of Mechanical and Aerospace Engineering, Seoul National Univ., Korea)

[P1-55] Investigating the mechanical properties of azobenzene-tethered DNA for controlling self-assembling DNA nanostructures

○Jae Gyung Lee, Chanseok Lee, Do-Nyun Kim　(Dept. of Mechanical and Aerospace Engineering, Seoul National Univ., Korea)

[P1-56] FTMP-based Modeling and Simulations of Glassy Polymers.

○Soushi Miyamoto, Tadashi Hasebe　(Dept. of Mechanical Engineering, Kobe Univ., Japan)

[P1-57] Shock Wave Induced Damage in Tumor Cells: Experiments and Simulations

○Martin Steinhauser　(Fraunhofer Ernst-Mach-Institute, EMI, Germany)

Poster Session | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[PO-I1] Poster Session 1

5:45 PM - 8:00 PM　Poster Hall

[P1-58] Phase-field modeling of anisotropic grain growth with incorporation of Sigma 3 CSL grain boundaries.

○Kunok Chang　(Kyung Hee Univ., Korea)

[P1-59] Direct mapping from molecular dynamics to phase-field simulations for accurate prediction of grain growth

○Eisuke Miyoshi[1], Tomohiro Takaki[1], Yasushi Shibuta[2], Munekazu Ohno[3] （1.Kyoto Institute of Technology, Japan, 2.The University of Tokyo, Japan, 3.Hokkaido University, Japan）

[P1-60] Density functional theory plus Hubbard U study of the segregation of Pt to the CeO_{2-x} grain boundary
Guoli Zhou, Pan Li, Qingmin Ma, ○Zhixue Tian, Ying Liu （Hebei Normal Univ., China）

[P1-61] **Interfacial charge transfer and enhanced photocatalytic mechanism for Bi_2WO_6/BiOCl heterostructure: A first-principles theoretical study**
○Pan Li （Hebei Normal Univ., China）

[P1-62] Investigation of abnormal grain growth conditions by phase-field method
○Nobuko Mori, Eisuke Miyoshi, Tomohiro Takaki （Kyoto Institute of Technology, Japan）

[P1-63] **Phase Field Crystal Modeling of Mechanism of Strain-Driven for Nucleation and Grain of Deformed-Grain**
○Ying-Jun Gao （Guangxi University, China）

[P1-64] **Diffusion and trapping of hydrogen at grain boundaries scale in fcc polycrystalline nickel: some implications of the atomic volume and the interstitial self-stress**
○xavier Feaugas, jiaqi Li, abdel malek Hallil, abdelali oudriss, arnaud metsue, jamaa bouhattate （university of La Rochelle, France）

Poster Session | J. Multiscale Modeling of Heterogeneous Layered Media

[PO-J1] Poster Session 1
5:45 PM - 8:00 PM Poster Hall

[P1-65] Multiscale Model for Interlayer Defects in Heterogeneous Bilayer Material
○Shuyang Dai[1], David Joseph Srolovitz[2], Yang Xiang[3] （1.Wuhan University, China, 2.University of Pennsylvania, United States of America, 3.Hong Kong University of Science and Technology, Hong Kong）

Poster Session | L. Structure, Statistics and Mechanics in Crystal Dislocation Plasticity

[PO-L1] Poster Session 1
5:45 PM - 8:00 PM Poster Hall

[P1-66] Molecular dynamics study on temperature and loading rate dependence of nano-indentation pop-in load

○Yuji Sato[1], Shuhei Shinzato[1], Takahito Ohmura[2], Shigenobu Ogata[1,3] （1.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan, 3.Center for Elements Strategy Initiative for Structural Materials (ESISM), Kyoto University, Japan）

[P1-67] Geometry of curved surface and energetics of in graphene with defects
○Ako Kihara[1], Xiao-Wen Lei[1], Akihiro Nakatani[2] （1.Dept. of Mechanical Engineering, Univ.of Fukui, Japan, 2.Dept. of Adaptive Machine Systems, Osaka Univ., Japan）

[P1-68] Collective motion of dislocation associated with local plasticity initiation and subsequent behavior in bcc metals
○Takahito Ohmura （National Institute for Materials Science, Japan）

Poster Session | M. Time- and History-Dependent Material Properties

[PO-M1] Poster Session 1
5:45 PM - 8:00 PM Poster Hall

[P1-69] FORMATION OF PHYSICAL GELS BY ARRESTED SPINODAL DECOMPOSITION IN CHARGED COLLOIDS
○Jose Manuel Olais-Govea[1], Alonso Gomez-Canales[1], Leticia Lopez-Flores[2], Martin Chavez-Paez[2], Magdaleno Medina-Noyola[2] （1.Instituto Tecnologico y de Estudios Superiores de Monterrey, Mexico, 2.Universidad Autonoma de San Luis Potosi, Mexico）

[P1-70] How to improve the ductility of CuZr BMGs based on cyclic pre-straining: MD simulations and mechanical testing
○Jonathan Amodeo[1], Oriane Baulin[1], Damien Fabregue[1], David Rodney[2] （1.MATEIS, Univ. Lyon 1, France, 2.ILM, Univ. Lyon 1, France）

[P1-71] **Modeling plastic deformation of amorphous solids from atomic scale mechanisms**
○Francesca Boioli[1], Tristan Albaret[2], David Rodney[2] （1.LEM, CNRS-ONERA, Chatillon, France, France, 2.ILM, University of Lyon 1, France, France）

[P1-72] Thermally Activated Creep and Constant Shear Rate Deformation in Amorphous Materials
○Samy MERABIA[1], Julien LAM[2], François DETCHEVERRY[1] （1.CNRS and Universite Lyon 1, France, 2.Université de Bruxelles, Belgium）

[P1-73] Numerical analysis of shrinkage process based on the experimental data

○Barbara Kucharczykova[1], Hana Simonova[2], Petr Frantik[2] （1.Brno University of Technology, Faculty of Civil Engineering, Institute of Building Testing, Czech Republic, 2.Brno University of Technology, Faculty of Civil Engineering, Institute of Structural Mechanics, Czech Republic）

Poster Session | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[PO-O1] Poster Session 1
5:45 PM - 8:00 PM Poster Hall

[P1-74] Designing Lubricant Additives for Titanium Carbide Surface: First-principles and Molecular Dynamics Investigations

○Tasuku Onodera, Jun Nunoshige, Hiroshi Kanemoto （Research &Development Group, Hitachi, Ltd., Japan）

[P1-75] Crystal Growth Molecular Dynamics Simulation of alpha-Al_2O_3 Cutting Tools for Realizing Their Best Tribological Properties

○Shandan BAI[1], Hiroya Nakata[1], Jingxiang Xu[2], Nobuki Ozawa[2], Momoji Kubo[2] （1.KYOCERA Cop., Japan, 2.Tohoku Univ., Japan）

[P1-76] Atomistic modeling of polymer friction

○Robin Sam Vacher （SINTEF-NTNU, Norway）

[P1-77] A two degree-of-freedom extension to the Prandtl Tomlinson-model for friction strengthening in layered materials

○David Andersson[1,2], Astrid de Wijn[2] （1.Department of Physics, Stockholm University, Sweden, 2.Department of Mechanical and Industrial Engineering, Norwegian University of Science and Technology, Norway）

[P1-78] Analysis of Friction Characteristics of Steel Powders using Parallelized Discrete Element Method

○Naoki Yashiro[1,2], Kouya Oohira[2], Natsuko Sugimura[1], Hitoshi Washizu[1] （1.Graduate School of Simulation Studies, University of Hyogo, Japan, 2.Advanced Technology R&D Center, NTN Corporation, Japan）

[P1-80] Dynamics of Polymer Under Shear in Confinement Geometry

○Taiki Kawate[1], Soma Usui[1], Hiroaki Yoshida[2], Hitoshi Washizu[1] （1.Univ. of Hyogo, Japan, 2.Toyota Central R&D Labs, Japan）

[P1-81] Dynamics of a Polymer in Bulk Solution under Shear Flow

○Soma Usui[1], Taiki Kawate[1], Hiroaki Yoshida[2], Hitoshi Washizu[1] （1.Univ. of Hyogo, Japan, 2.Toyota Central R&D Labs., Japan）

[P1-82] Mechanochemistry induced atomic wear in chemical mechanical polishing processes

○Jialin Wen, Tianbao Ma, Xinchun Lu （Dept. of Mechanical Engineering, Tsinghua Univ., China）

[P1-83] Adsorption property of a fatty acid on iron surface with grain boundary

○Yuki Uchiyama, Yoshinori Shiihara, Ivan Lobzenko （Toyota Technological Institute, Japan）

Tue. Oct 30, 2018

Room1

Plenary Talk | Plenary Talk

[PL3] Plenary Talk 3
Chair: William Curtin(EPFL, Switzerland)
8:30 AM - 9:20 AM Room1

[PL3] Plenary Talk 3

○David Rodney （Institut Lumière Matière, University of

Lyon, France）

Tue. Oct 30, 2018

Room1

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C3] Symposium C-3

Chair: Francois Willaime(DEN-Departement des Materiaux pour le Nucleaire, CEA, Universite Paris-Saclay, France)
9:45 AM - 11:00 AM Room1

[SY-C3] Quantifying the effect of hydrogen on dislocation dynamics in microcrystals: A three-dimensional discrete dislocation dynamics study
Yejun Gu, ○Jaafar A. El-Awady　(Johns Hopkins University, United States of America)

[SY-C3] Discrete dislocation plasticity modelling of hydrogen dislocation interactions in micro-cantilevers
○Haiyang Yu[1], Alan Cocks[2], Ed Tarleton[1]　(1.Dept. of Materials, Univ. of Oxford, UK, 2.Dept. of Engineering, Univ. of Oxford, UK)

[SY-C3] Dislocation climb models from atomistic scheme to dislocation dynamics
○Yang Xiang[1], Xiaohua Niu[2]　(1.Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong, 2.Department of Mathematics, Jimei University, China)

[SY-C3] Investigation of the Hall-Petch Effect with DD Simulation
○Maoyuan Jiang[1,2], Benoit Devincre[2], Ghiath Monnet[1]　(1.EDF - R&D, Les Renardieres, France, 2.Laboratoire d'Etude des Microstructures, CNRS/ONERA, France)

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C4] Symposium C-4

Chair: Dan Mordehai(Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel, Israel)
11:15 AM - 12:15 PM Room1

[SY-C4] **Hydrogen consequences on cyclic behaviour of <001> nickel single crystals : a multi-scale approach.**
○xavier Feaugas, Guillaume Hachet, Arnaud Metsue, abdelali Oudriss　(université de la rochelle, France)

[SY-C4] **Atomistic and continuum approaches to analyse precipitation hardening in metallic alloys**
Gustavo Esteban-Manzanares[1,2,3], Rodrigo Santos[1,2], Anxin Ma[1], Ioannis Papadimitriou[1], Enrique Martínez[3], Laurent Capolungo[3], Javier Segurado[1,2], ○Javier

LLorca[1,2]　(1.IMDEA Materials Institute, Spain, 2.Polytechnic University of Madrid, Spain, 3.Los Alamos National Laboratory, United States of America)

[SY-C4] Dislocation-precipitate interaction in Al-Mg-Si alloys
○Inga Gudem Ringdalen[1], Sigurd Wenner[1], Jaime Marian[2]　(1.Dept. of Materials and Nanotechnology, SINTEF, Norway, 2.Dept. of Material Science and Engineering, UCLA, United States of America)

Room2

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E3] Symposium E-3

Chairs: Benoit Devincre(LEM, CNRS-ONERA, France), Alejandro Strachan(Purdue University, United States of America)
9:45 AM - 11:00 AM Room2

[SY-E3] 3D mesoscopic study of the stability of three-dimensional short cracks in FCC metals using the Discrete-Continuous Model
Laurent Korzeczek[1], Riccardo Gatti[1], Arjen Roos[2], ○Benoit Devincre[1]　(1.LEM, CNRS-ONERA, France, 2.Safran Tech, France)

[SY-E3] Role of cracks, voids and interfaces in hot spot formation and initiation of energetic materials
Michael Sakano[1], Chunyu Li[1], Nicolo Grilli[2], Brenden Hamilton[1], Camilo Duarte[2], Marisol Koslowski[2], ○Alejandro Strachan[1]　(1.School of Materials Engineering, Purdue University, United States of America, 2.School of Mechanical Engineering, Purdue University, United States of America)

[SY-E3] Precipitation hardening effects on extension twinning in magnesium
○Haidong Fan[1], Jaafar El-Awady[2], Dierk Raabe[3]　(1.Sichuan University, China, 2.The Johns Hopkins University, United States of America, 3.Max-Planck-Institut für Eisenforschung GmbH, Germany)

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E4] Symposium E-4

Chairs: Haifeng Song(Institute of Applied Physics and Computational Mathematics, China), Chenghua Sun(Swinburne University of Technology, Australia)
11:15 AM - 12:30 PM Room2

[SY-E4] **High-performance first-principles calculation software development with applications to the zirconium**

○Haifeng Song[1,2], Xingyu Gao[1,2], Jun Fang[1,2], Yafan Zhao[2], Han Wang[2], Deye Lin[2]（1.Institute of Applied Physics and Computational Mathematics, China, 2.CAEP Software Center for High Performance Numerical Simulation, China）

[SY-E4] Catalyst design for ammonia synthesis of ammonia
○Chenghua Sun （Swinburne University of Technology, Australia）

[SY-E4] A solid-solution structure model for multi-component alloys
○Xingyu Gao[1,2], Fuyang Tian[3], Yafan Zhao[2], Deye Lin[2], Haifeng Song[1,2]（1.Institute of Applied Physics and Computational Mathematics, China, 2.CAEP Software Center for High Performance Numerical Simulation, China, 3.University of Science and Technology, China）

[SY-E4] First-princples prediction of plastic deformation modes in alloys
○Song Lu, Levente Vitos （KTH Royal Institute of Technology, Sweden）

[SY-E4] The local-orbital construction of strongly correlated electrons based on the PAW method
○Yu Liu[1,2], Xingyu Gao[1,2], Jianzhou Zhao[3], Haifeng Song[1,2]（1.Institute of Applied Physics and Computational Mathematics, China, 2.CAEP Software Center for High Performance Numerical Simulation, China, 3.Southwest University of Science and Technology, China）

Room3

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F3] Symposium F-3
Chair: Carl Krill(Institute of Micro and Nanomaterials, Ulm University, Germany)
9:45 AM - 11:00 AM Room3

[SY-F3] Biomineralization in molluscan shells: From ideal to hierarchical grain growth
○Dana Zoellner, Igor Zlotnikov （B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany）

[SY-F3] **Mesoscale modeling of cement: texture, mechanics and durability**
○Katerina Ioannidou[1,2,3], Emanuela Del Gado[4], Franz J. Ulm[1], Roland J.-M. Pellenq[1,2,3]（1.Dept. of Civil and Enviromental Engineering, Massachusetts Institute of Technology, United States of America, 2.MultiScale Material Science for Energy and Environment,

Massachusetts Institute of Technology-CNRS/MIT/AMU Joint Lab. at MIT, United States of America, 3.MIT Energy Initiative, United States of America, 4.Dept. of Physics and Institute for Soft Matter Synthesis and Metrology, Georgetown Univ., United States of America）

[SY-F3] **Actuation in Metal-Polymer Nanocomposites: Chemoelectromechanical Coupling on Interfaces**
○Jana Wilmers, Swantje Bargmann （Chair of Solid Mechanics, University of Wuppertal , Germany）

[SY-F3] Mechanics of Cilia Beating - A Relationship Between Metachronal Wavelength and Fluid Flow Rate
○Jon Hall, Nigel Clarke （The University of Sheffield, UK）

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F4] Symposium F-4
Chair: Dana Zoellner(B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany)
11:15 AM - 12:30 PM Room3

[SY-F4] Showdown! Pitting computer simulations against time-resolved experimental measurements of grain growth in 3D
Mingyan Wang[1], Nan Wang[2], Jules Dake[1], Søren Schmidt[3], ○Carl Krill[1]（1.Institute of Micro and Nanomaterials, Ulm University, Germany, 2.Dept. of Physics, McGill University, Canada, 3.Dept. of Physics, Technical University of Denmark, Denmark）

[SY-F4] Coarsening and grain-growth in an SOFC-anode under surface and grain boundary self-diffusion: A Multiphase-field approach
○Paul Hoffrogge[1], Daniel Schneider[1,2], Britta Nestler[1,2], Patricia Haremski[2,3], Matthias Wieler[3], Piero Lupetin[3] （1.Karlsruhe University of Applied Sciences, Germany, 2.Karlsruhe Institute of Technology, Germany, 3.Robert Bosch GmbH, Germany）

[SY-F4] Solidification Simulation in Additive Manufacturing Process of Ti-Alloy by ICME approach
○Yusuke SHIMONO, Mototeru Oba, Sukeharu Nomoto （Itochu Techno-Solutions Corp., Japan）

[SY-F4] **Phase Field Model of Microstructural Evolution in Metal Alloy for Designing Mechanical Property**
Wooju Lee, ○Dongchoul Kim （Dept. of Mechanical Engineering, Sogang Univ., Korea）

Room4

Symposium | M. Time- and History-Dependent Material Properties

[SY-M3] Symposium M-3
Chair: Thomas Franosch(University of Innsbruck, Austria)
9:45 AM - 11:00 AM Room4

[SY-M3] Heterogeneous thermal properties in a glass from molecular dynamics calculations
○Jean-Louis BARRAT （Univ. Grenoble Alpes, France)

[SY-M3] Structural-dynamical phase transition in the phase space of histories of a polydisperse hard sphere liquid
○Matteo Campo[1,2], Thomas Speck[1] （1.Johannes Gutenberg University Mainz, Germany, Germany, 2.Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany, Germany)

[SY-M3] Time- and History-dependent Structure and Morphology of van-der-Waals Liquids forming Physical Gels and Porous Glasses
○Magdaleno Medina-Noyola, Leticia Lopez-Flores, Jose Manuel Olais-Govea, Benigno Zepeda-Lopez （Instituto de Fisica (Laboratorio Nacional de Ingenieria de la Materia Fuera de Equilibrio), Universidad Autonoma de San Luis Potosi, Mexico)

Symposium | M. Time- and History-Dependent Material Properties

[SY-M4] Symposium M-4
Chair: Leticia Lopez Flores(University of San Luis Potosi, Mexiko)
11:15 AM - 12:30 PM Room4

[SY-M4] Mechanical behavior and emerging morphologies in active matter
○Ignacio Pagonabarraga （CECAM, EPFL, Switzerland)

[SY-M4] Time dependent interaction between intruders in granular media
○Hisao Hayakawa [1], Takahiro Tanabe[2] （1.Yukawa Institute for Theoretical Physics, Kyoto Univeristy, Japan, 2.Graduate School of Advanced Mathematical Sciences, Meiji University, Japan)

[SY-M4] Hystory-dependent shear jamming of granular materials under oscillatory shear
○Michio Otsuki[1], Hisao Hayakawa[2] （1.Graduate School of Engineering Science, Osaka Univ., Japan, 2.Yukawa Institute for Theoretical Physics, Kyoto Univ., Japan)

[SY-M4] Structural predictor for nonlinear sheared dynamics in simple glass-forming liquids
○Trond S. Ingebrigtsen, Hajime Tanaka （University of Tokyo, Japan)

Room5

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O3] Symposium O-3
Chairs: Momoji Kubo(Tohoku University, Japan), Michael Moseler(Fraunhofer Institute for Mechanics of Materials IWM, Germany)
9:45 AM - 11:00 AM Room5

[SY-O3] Scale Dependence of Friction: How Elasticity Destroys Superlubricity
Joseph Monti[1], Lars Pastewka[2], ○Mark Owen Robbins[1] （1.Dept. of Physics and Astronomy, Johns Hopkins University, United States of America, 2.University of Freiburg, Germany)

[SY-O3] Coarse-Grain Simulations of Polymer Solutions with Hydrodynamics and Long-range Interactions
○Hitoshi Washizu[1,2], Hiroaki Yoshida[3], Soma Usui[1], Taiki Kawate[1] （1.Univ. Hyogo, Japan, 2.Kyoto Univ., Japan, 3.Toyota Central R&D Labs., Inc., Japan)

[SY-O3] **A Multi-Scale Approach for the Design of Novel Lubricants**
○Georgios Bletsos[1], Konstantinos Gkagkas[2], Varvara Asouti[1], Evaggelos Papoutsis-Kiachagias[1], Daniele Savio[3], Kyriakos C Giannakoglou[1] （1.National Technical University of Athens, Greece, 2.Toyota Motor Europe NV/SA, Belgium, 3.Fraunhofer Institute for Mechanics of Materials IWM, Germany)

[SY-O3] Impact of ionic liquid ordering on their triborheological properties
○Konstantinos Gkagkas[1], Andras Vernes[2,3] （1.Advanced Material Research Division, Toyota Motor Europe NV/SA, Belgium, 2.AC2T research GmbH, Austria, 3.Institute of Applied Physics, TU Wien, Austria)

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O4] Symposium O-4
Chairs: Aiichiro Nakano(Univ. of Southern California, United States of America), Shandan Bai(KYOCERA Corp., Japan)
11:15 AM - 12:30 PM Room5

[SY-O4] Molecular simulation to better understand soot-detergent interactions in engine oils
○Sophie LOEHLE[1], Elias Gebremedhn[2], Michael Mazarin[1], Stephan Steinman[2], Carine Michel[2] （1.Total M&S, France, 2.ENS Lyon, France)

[SY-O4] A Molecular Dynamics Study on the Wear Mechanisms of Hydrogenated Diamond-like Carbon

○Yang Wang[1], Jingxiang Xu[1], Yusuke Ootani[1], Yuji Higuchi[1], Nobuki Ozawa[1], Koshi Adachi[2], Momoji Kubo[1] （1.Institute for Materials Research, Tohoku University, Japan, 2.Department of Mechanical System Engineering, Graduate School of Engineering, Tohoku University, Japan）

[SY-O4] Effect of Tribochemical Reactions on Diamond-like Carbon and Wear under Water Lubrication: A Molecular Dynamics Simulation Investigation

○Jing Zhang[1], Yang Wang[1], Jingxiang Xu[1], Yusuke Ootani[1], Nobuki Ozawa[1], Koshi Adachi[2], Momoji Kubo[1] （1.Inst. for Materials Research, Tohoku Univ., Japan, 2.Dept. of Mechanical Systems Engineering, Tohoku Univ., Japan）

[SY-O4] Formation Mechanism of Tribofilm of Silicon Carbide under Water Lubrication: Molecular Dynamics Simulations

○Fumiya Nakamura, Yang Wang, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Koshi Adachi, Momoji Kubo （Tohoku Univ., Japan）

Room6

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A3] Symposium A-3
Chair: Katsuyo Thornton(University of Michigan, Ann Arbor, United States of America)
9:45 AM - 11:00 AM Room6

[SY-A3] **Challenges and gaps in length and time scaling of dislocation models**

○David L McDowell （Woodruff School of Mechanical Engineering, Georgia Institute of Technology, United States of America）

[SY-A3] From discrete to continuum dislocations and back: a two dimensional study of microstructure and interaction energies.

○Hengxu Song, Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

[SY-A3] **Advances in microstructure prediction: a FFT-based Dislocation Dynamics approach**

○Francesca Boioli[1], Benoit Devincre[1], Riccardo Gatti[1], Laurant Dupuy[2], Lionel Gélébart[2] （1.LEM, CNRS-ONERA, Chatillon, France, 2.SRMA, CEA Saclay, France）

[SY-A3] **Plasticity and microstructure evolutions at the mesoscale: towards and integrated framework.**

○Laurent Capolungo, John Graham, Aaron Kohnert, Ricardo Lebensohn, Richard Lesar, Hareesh Tummala （Los Alamos National Laboratory, United States of America）

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A4] Symposium A-4
Chair: David L McDowell(Woodruff School of Mechanical Engineering, Georgia Institute of Technology, United States of America)
11:15 AM - 12:30 PM Room6

[SY-A4] Effective Transport Properties of Polycrystalline Materials

William Beck Andrews[1], Min-Ju Choe[1], Erik Hanson[1], Max Powers[1], Hui-Chia Yu[1,2], ○Katsuyo Thornton[1] （1.University of Michigan, Ann Arbor , United States of America, 2.Michigan State University , United States of America）

[SY-A4] **A new E-VPSC polycrystal formulation: fundamentals**

○Carlos Tome[1], Youngung Jeong[2] （1.Los Alamos National Laboratory, United States of America, 2.Department of Materials Science, Changwon National University, Korea）

[SY-A4] **A new E-VPSC polycrystal formulation: applications**

○Youngung Jeong[1], Carlos Tome[2] （1.Changwon National Univ., Korea, 2.Los Alamos Natinal Lab, United States of America）

[SY-A4] Modeling microstructural material variability with uncertainty quantification and machine learning techniques

○Reese Jones, Coleman Alleman, Brad Boyce, Ari Frankel, Nathan Heckman, Mohammad Khalil （Sandia National Laboratories, United States of America）

Room7

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I3] Symposium I-3
Chair: Peter Voorhees(Northwestern University, United States of America)
9:45 AM - 11:00 AM Room7

[SY-I3] Interaction of moving grain boundaries with solutes: bridging time scales between atomistics

and continuum

○Yuri Mishin （George Mason University, United States of America）

[SY-I3] Phenomenological model for prediction of interaction parameters in grain boundary segregation

○Pavel Lejcek[1], Siegfried Hofmann[2] （1.Institute of Physics, AS CR, Praha, Czech Republic, 2.Max-Planck-Institute for Intelligent Systems, Stuttgart, Germany）

[SY-I3] Influence of Solutes at Grain Boundaries on Phase Transformations and Mechanical Response

○Stephen M Foiles, Nathan Heckman, Christopher Barr, Fadi Abdeljawad, Khalid Hattar, Brad Boyce （Sandia National Laboratories, United States of America）

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I4] Symposium I-4

Chairs: Shen J Dillon(University of Illinois, USA), Daniel Pino Munoz(Mines ParisTech / PSL Research University, France)
11:15 AM - 12:30 PM　Room7

[SY-I4] Atomistic modeling of helium segregation to grain boundaries in tungsten and its effect on de-cohesion

○Enrique Martinez Saez[1], Blas Pedro Uberuaga[1], Brian D Wirth[2,3] （1.Material Science and Technology Division, MST-8,Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America, 2.Department of Nuclear Engineering, University of Tennessee, Knoxville, TN 37996, United States of America, United States of America, 3.Oak Ridge National Laboratory, PO Box 2008, MS-6003, Oak Ridge, TN 37831, United States of America, United States of America）

[SY-I4] Thermodynamic properties of bcc Fe grain boundaries with segregation of 3d-transition-metal solutes

○Zhuo Xu, Shingo Tanaka, Masanori Kohyama （AIST, Japan）

[SY-I4] A new thermodynamic model for the austenite-ferrite massive transformation in Fe-C-X alloys.

○Alexandre MATHEVON[1], Michel PEREZ[1], Damien FABREGUE[1], Veronique MASSARDIER[1], Philippe ROCABOIS[2], Patrice CHANTRENNE[1] （1.INSA Lyon, France, 2.FIVES KEODS, France）

[SY-I4] Multiscale simulation of solid phase sintering of nano copper powder

○Xinyu Zhu, Xiangge Qin （School of Materials Science

and Engineering, Jiamusi Univ., China）

Room8

Symposium | L. Structure, Statistics and Mechanics in Crystal Dislocation Plasticity

[SY-L3] Symposium L-3

Chairs: Peter M Derlet(Paul Scherrer Institut, Switzerland), Cynthia Reichhardt(Los Alamos National Laboratory, United States of America)
9:45 AM - 11:00 AM　Room8

[SY-L3] Intermittent micro-plasticity and its relation to dislocation structure - a linear stability analysis.

○Peter M Derlet[1], Gábor Péterffy[2], Péter Dusán Ispán ovity[2] （1.Paul Scherrer Institut, Switzerland, 2.Department of Materials Physics, Eötvös University, Hungary）

[SY-L3] Discrete dislocation dynamics simulations of complexity in crystal plasticity: strain burst statistics and machine learning

○Lasse Laurson （Aalto University, Finland）

[SY-L3] Nanoindentation in the ultra-nano scale: Microstructure-property relationships using statistical approaches

Hengxu Song[1,2], Ryder Bolin[1], Michael Tzimas[1], ○S tefanos Papanikolaou[1,2] （1.west virginia university, United States of America, 2.johns hopkins university, United States of America）

Symposium | L. Structure, Statistics and Mechanics in Crystal Dislocation Plasticity

[SY-L4] Symposium L-4

Chair: Lasse Laurson(Aalto University, Finland)
11:15 AM - 12:30 PM　Room8

[SY-L4] Dynamic phases, pinning, and pattern formation for driven dislocation assemblies

○Cynthia Reichhardt[1], Caizhi Zhou[2], Charles Reichhardt[1], Irene Beyerlein[3] （1.Los Alamos National Laboratory, United States of America, 2.Missouri University of Science and Technology, United States of America, 3.University of California, Santa Barbara, United States of America）

[SY-L4] Effect of solute atoms and Peierls stress on the critical behaviour of discrete dislocations

○Peter Dusan Ispanovity[1], Gabor Peterffy[1], Peter M. Derlet[2] （1.Eotvos Universty, Hungary, 2.Paul Scherrer Institut, Switzerland）

[SY-L4] Temporal and spatial plastic instability of

micrometer-scaled materials

○Yinan Cui[1], Giacomo Po[1], Nasr Ghoniem[1] （1. Mechanical and Aerospace Engineering Department, University of California, Los Angeles, United States of America）

Room9

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H1] Symposium H-1

Chair: Turab Lookman(Los Alamos National Laboratory, United States of America)
9:45 AM - 11:00 AM Room9

[SY-H1] **Multiscale modeling of electro-responsive gels**
○Masao Doi （Beihang University, China）

[SY-H1] Non-monotonic particle size effect on the glass transition in polymer-particle blends and its application to shape memory polymers
○Elias M. Zirdehi, Fathollah Varnik （Ruhr-University Bochum, Germany）

[SY-H1] **Thermomechanical behavior of shape-memory polyurethane copolymer : A coarse-grained molecular dynamics simulation**
○SUNGWOO PARK, JUNGHWAN MOON, BYUNGJO KIM, MAENGHYO CHO （Seoul National University, South Korea, Korea）

[SY-H1] **Investigation of photo-mechanical behavior of azobenzene-based polymer: A coarse-grained molecular dynamics study**
○Junghwan Moon[1], Byungjo Kim[1], Joonmyung Choi[2], Maenghyo Cho[1,3] （1.Divison of Multiscale Mechanical Design, School of Mechanical and Aerospace Engineering, Seoul National University, Korea, 2.Mechatronics R&D center, SAMSUNG ELECTRONICS CO., LTD, Korea, 3.Institute of Advanced Machines and Design, Seoul National University, Korea）

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H2] Symposium H-2

Chair: Hansohl Cho(Los Alamos National Laboratory, United States of America)
11:15 AM - 12:30 PM Room9

[SY-H2] **Hydrogels with Dynamic Sacrificial Bonds - From Toughness to Adhesion to Composites -**
○Jian Ping Gong[1,2] （1.Faculty of Advanced Life Science, Hokkaido University, Japan, 2.Soft Matter GI-CoRE, Hokkaido University, Japan）

[SY-H2] Elastic properties and effective interactions of *in silico* realistic microgels
○Lorenzo Rovigatti[1,2], Nicoletta Gnan[1,2], Emanuela Zaccarelli[1,2] （1.Institute for Complex Systems, Uos Sapienza - CNR, Italy, 2.Dipartimento di Fisica, Sapienza Università di Roma, Italy）

[SY-H2] Controlling the mechanics of a synthetic hydrogel with motor-like internal contractility
Marcos Fernandez-Castano Romera[1], Rint P Sijbesma[1], ○Cornelis Storm[1] （1.Theory of Polymers and Soft Matter, Technische Universiteit Eindhoven, The Netherlands）

[SY-H2] **Study on viscoelastic behavior of natural rubber with multiscale approach**
○Byungjo Kim, Junghwan Moon, Maenghyo Cho （Seoul National University, Korea）

Room10

Symposium | J. Multiscale Modeling of Heterogeneous Layered Media

[SY-J3] Symposium J-3

Chairs: Ramesh Talreja(Texas A&M University, United States of America), Tong-Earn Tay(National University of Singapore, Singapore)
9:45 AM - 11:00 AM Room10

[SY-J3] Fundamentals of Generalized Particle (GP) Multiscale Methods with Applications to Analyses of Alternatively-Arranged Soft and Hard Layers
○Jinghong Fan （Kazuo Inamori School of Engineering, Alfred University, United States of America）

[SY-J3] **The effect of layer thickness ratio on the plastic deformation mechanisms of nonoindented Ti/TiN nanolayered composite: A molecular dynamics study**
○Georges Y Ayoub[1], Wei yang[2], Iman Salehinia[3], Bilal Mansoor[2], Hussein Zbib[4] （1.Dept. of Industrial and manufacturing system Engineering, Univ. of Michigan, United States of America, 2.Dept. of Mechanical Engineering, Texas A&M Univ., United States of America, 3.Dept. of Mechanical Engineering, Northern Illinois Univ., United States of America, 4.School of Mechanical and Materials Engineering, Washington State Univ., United States of America）

[SY-J3] The attenuation of stress wave propagation in multilayer structure
○Fengyuan Yang, Zhanli Liu （Tsinghua University,

China）

[SY-J3] Multiscale molecular-dynamics simulations of structure and mechanics of polymer nanocomposites

○Alexey Lyulin[1,2] （1.Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands, 2.Center for Computational Energy Research, Department of Applied Physics, Eindhoven University of Technology, Netherlands）

Symposium | J. Multiscale Modeling of Heterogeneous Layered Media

[SY-J4] Symposium J-4

Chairs: Brian Cox(Arachne Consulting Inc., United States of America), Tomonaga Okabe(Tohoku University, Japan)
11:15 AM - 12:30 PM Room10

[SY-J4] Validation of analytical models for ply cracking of general symmetric composite laminates

○TOMONAGA OKABE （Department of Aeroscpace Engineering, Tohoku University, Japan）

[SY-J4] Two-way coupled modeling of lithium diffusion and diffusion induced finite elastoplastic bending of bilayer electrodes in lithium-ion batteries

Jun Yin, ○Junqian Zhang （Shanghai University, China）

[SY-J4] Micro-Scale Model of Thermomechanics in Solidifying Saturated Porous Media

○Michal Benes, Alexandr Zak （Czech Technical University in Prague, Czech Republic）

Wed. Oct 31, 2018

Room1

Plenary Talk | Plenary Talk

[PL4] Plenary Talk 4
Chair: Erik Bitzek(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)
8:30 AM - 9:20 AM Room1

[PL4] Plenary Talk 4
○Yuichi Ikuhara （The University of Tokyo/Japan Fine Ceramics Center, Japan）

Wed. Oct 31, 2018

Room1

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C5] Symposium C-5

Chair: Christopher Woodward(Air Force Research Laboratory, United States of America)
9:45 AM - 11:00 AM Room1

[SY-C5] **Plasticity and Fracture in Transition Metal Carbides**

○Giacomo Po[1], Suneel Kodambaka[2], Jeffrey M Wheeler[3], Davide Sangiovanni[4]　(1.University of California Los Angeles, Mechanical Engineering Department, United States of America, 2.University of California Los Angeles, Materials Science and Engineering Department, United States of America, 3.Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Mechanics of Materials and Nanostructures, Swaziland, 4.Department of Physics, Chemistry and Biology, Linköping University, Sweden)

[SY-C5] Atomic Scale Investigation of Plasticity in Laves phases

○Julien Guenole[1], Fatim-Zahra Mouhib[1], Christoffer Zehnder[1], James Gibson[1], Blazej Grabowski[2], Sandra Korte-Kerzel[1]　(1.Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Germany, 2.Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany)

[SY-C5] Nucleation of dislocation in ultra-hard ceramic nanoparticles modelled by molecular dynamics and nudged elastic band simulations

○Jonathan Amodeo[1], Emile Maras[2]　(1.MATEIS, Univ. Lyon 1, France, 2.SRMP, DEN, CEA, Gif-sur-Yvette, France)

[SY-C5] Multiscale discrete dislocation dynamics modeling of nano-indentation near the grain boundary

○Xu Zhang, Songjiang Lu　(School of Mechanics and Engineering, Southwest Jiaotong University, China)

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C6] Symposium C-6

Chair: Jaime Marian(Dept. of Materials Science and Engineering, University of California Los Angeles, United States of America)
11:15 AM - 12:30 PM Room1

[SY-C6] Effect of interstitial solutes on the structure and mobility of screw dislocations in bcc metals

○Berengere Lüthi[1], Lisa Ventelon[1], David Rodney[2], Emmanuel Clouet[1], Bernard Legrand[1], Fabienne Berthier[3], ○Francois Willaime[4]　(1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, France, 2.Institut Lumière Matière, CNRS-Université Claude Bernard Lyon 1, France, 3.Synthèse, Propriétés et Modélisation des Matériaux /Institut de Chimie Moléculaire et des Matériaux d'Orsay, Université Paris-Saclay, France, 4.DEN-Département des Matériaux pour le Nucléaire, CEA, Université Paris-Saclay, France)

[SY-C6] Effect of solutes on dislocation motion in dilute hcp and bcc alloys

○Tomohito Tsuru[1,2], Mitsuhiro Itakura[1], Masatake Yamaguchi[1,2], Tomoaki Suzudo[1], Masato Wakeda[3], Shigenobu Ogata[2,4], Daryl C Chrzan[5]　(1.Japan Atomic Energy Agency, Japan, 2.ESISM, Kyoto University, Japan, 3.National Institute for Materials Science, Japan, 4.Osaka University, Japan, 5.University of California, Berkeley, United States of America)

[SY-C6] Investigation of the energy pathway for generation of dislocations in silicon at $\Sigma 3$ grain boundaries with the kinetic Activation-Relaxation Technique

○Simen Nut Hansen Eliassen[1], Normand Mousseau[3], Mickaël Trochet[3], Yanjun Li[1], Jesper Friis[2], Inga Gudem Ringdalen[2]　(1.Dept. of Materials Science and Engineering, Norwegian Univ. of Science and Technology, Norway, 2.SINTEF Materials and Chemistry, Norway, 3.Dept. of Physics, Univ. de Montréal, Canada)

[SY-C6] Prediction of mechanical twinning in post-perovskite structure

○Philippe Carrez, Alexandra Goryaeva, Patrick Cordier　(Lille University, Lab. UMET UMR-CNRS 8207, France)

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C7] Symposium C-7

Chair: David Rodney(Institut Lumiere Matiere, Universite Lyon 1, France)
2:00 PM - 3:30 PM Room1

[SY-C7] **Predictive simulations of crystal plasticity: multiscale or cross-scale?**

○Vasily V Bulatov[1], Alexander Stukowski[2], Luis A Zepeda-Ruiz[1], Tomas Oppelstrup[1]　(1.Lawrence

Livermore National Laboratory, United States of America, 2.Darmstadt University, Germany）

[SY-C7] **Molecular dynamics simulations of dislocation avalanche emissions in FCC and BCC crystals**

○Javier Varillas[1,2], Jan Očenášek[2], Jorge Alcalá[1] （1.New Technologies Research Centre, University of West Bohemia in Pilsen, Czech Republic, 2.Department of Materials Science and Metallurgical Engineering, InSup, ETSEIB. Universitat Politècnica de Catalunya, Spain）

[SY-C7] Scrutinizing screw dislocation glide initiation at finite temperatures in BCC metals

○Tomoaki Suzudo[1], Takashi Onitsuka[2], Ken-ichi Fukumoto[2] （1.Japan Atomic Energy Agency, Japan, 2.Fukui Univ., Japan）

[SY-C7] Uranium plastic deformation: A multiscale approach

○Pavel A. Pokatashkin, Denis K. Ilnitsky, Alexei V. Yanilkin （Dukhov Research Institute of Automatics (VNIIA), Russia）

[SY-C7] Understanding the grain refinement mechanism in surface mechanical attrition treatment of Fe14Ni18Cr by molecular dynamics simulations

○Ali Rida[1], Matthieu Micoulaut[2], Emmanuelle Rouhaud[1], Ali Makke[1,3] （1.University of Technology of Troyes , France, 2.Sorbonne Université, France, 3.EPF, Engineering school, France）

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C8] Symposium C-8

Chair: Yinan Cui(Mechanical and Aerospace Engineering Department, University of California, Los Angeles, United States of America)
4:00 PM - 5:30 PM Room1

[SY-C8] Thermal fluctuations of dislocations reveal the interplay between their core energy and long-range elasticity.

○Pierre-Antoine Geslin[1,2,3], David Rodney[4] （1.Mateis lab, INSA Lyon/CNRS, France, 2.Institute for Materials Research, Tohoku University, Japan, 3.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan, 4.Institut Lumière Matière, Université Lyon 1, France）

[SY-C8] Tension of fluctuating dislocation lines

○Max Boleininger[1], Thomas D Swinburne[2], Laurent Dupuy[3], Sergei L Dudarev[1] （1.Culham Centre for Fusion Energy, UK, 2.Theoretical Division T-1, Los

Alamos National Laboratory, United States of America, 3.DEN-Service de Recherches Métallurgiques Appliquées s, CEA, France）

[SY-C8] Stress-Dependent Activation Parameters for Cross-Slip in FCC Metals

○Alon Malka-Markovitz, Dan Mordehai （Technion—Israel Institute of Technology, Israel）

[SY-C8] The influence of precipitate size and shape on the strengthening and hardening rate as observed within metallic alloys.

○Benjamin A Szajewski, Joshua Crone, Jaroslaw Knap （Army Research Laboratory, United States of America）

[SY-C8] Molecular dynamics simulations of dislocation dynamics

Eyal Oren, ○Guy Makov （Ben-Gurion University of the Negev, Israel）

Room2

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E5] Symposium E-5

Chairs: Anthony D Rollett(Carnegie Mellon University, United States of America), Evgeniya Kabliman(Austrian Institute of Technology, Austria)
9:45 AM - 11:00 AM Room2

[SY-E5] Use of FFT-based micromechanical modeling for analysis of synchrotron-based diffraction experiments

Vahid Tari[1], Ricardo A Lebensohn[2], Reeju Pokharel[2], Rachel E Lim[1], Darren C Pagan[3], Yufeng Shen[1], Joel V Bernier[4], Robert M Suter[1], ○Anthony D Rollett[1] （1.Carnegie Mellon University, United States of America, 2.Los Alamos National Laboratory, United States of America, 3.Cornell High Energy Synchrotron Source, United States of America, 4.Lawrence Livermore National Laboratory, United States of America）

[SY-E5] Computational Design of Hysteresis-Free and Linear Super-Elastic, and Ultralow Modulus Ferroelastic Materials

○Jiaming Zhu[1], Yipeng Gao[2], Dong Wang[3], Tong-Yi Zhang[4], Yunzhi Wang[2] （1.City University of Hong Kong, Hong Kong, 2.Ohio State University, United States of America, 3.Xi'an Jiaotong University, China, 4.Shanghai University, China）

[SY-E5] A biphasic continuum model for large deformation visco-elastic mechanics of uncured carbon fibre prepregs

○Amir Hosein Sakhaei, Timothy James Dodwell
（College of Engineering, Mathematics and Physical Sciences, University of Exeter, UK）

[SY-E5] Strong coupling of deformation and microstructure/microchemistry evolution in hot compression tests

○Evgeniya Kabliman[1], Johannes Kronsteiner[1], Ernst Kozeschnik[2] （1.Light Metals Technologies Ranshofen, Center for Low-Emission Transport, Austrian Institute of Technology, Austria, 2.Institute of Materials Science and Technology, TU Wien, Austria）

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E6] Symposium E-6

Chairs: Ying-Jun Gao(Guangxi University, China), Masaki Tanaka(Kyushu Univ., Japan)
11:15 AM - 12:30 PM Room2

[SY-E6] **Phase Field Crystal Simulation of Crack Extension and Brittle-Ductile Transition Behavior on Nano-Scale**

○Ying-Jun Gao （Guangxi University, China）

[SY-E6] Continuum elasticity and correlations of plastic strain fluctuations in sheared glasses: The effect of hard boundaries

○Muhammad Hassani, Fathollah Varnik （Ruhr-University Bochum, Germany）

[SY-E6] Modeling approaches to tetragonal-to-monoclinic transformations in MgO partially stabilized zirconia

○Michael Budnitzki （TU Bergakademie Freiberg, Germany）

[SY-E6] Delamination cracks in wire-drawn fully pearlitic steels.

○Masaki Tanaka[1], Yelm Okuyama[1], Tatsuya Morikawa[1], Toshiyuki Manabe[2] （1.Kyushu Univ., Japan, 2.Nippon Steel &Sumitomo Corporation, Japan）

[SY-E6] FTMP-based Modeling and Simulations of Inhomogeneous Recovery-Triggered Accelerated Creep Rupture in Lath Martensite Structures

○yasutaka matsubara, tadashi hasebe, yuta amano （Kobe Univ., Japan）

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E7] Symposium E-7

Chairs: Daisuke Matsunaka(Shinshu Univ., Japan), Shiyu Du(Chinese Academy of Sciences, China)
2:00 PM - 3:30 PM Room2

[SY-E7] The Activation Parameters for Dislocation Nucleation in Molybdenum Nanoparticles under Compression

Doron Chachamovitz, ○Dan Mordehai （Mechanical Engineering, Technion, 32000 Haifa, Israel）

[SY-E7] Dislocation density-based crystal plasticity analysis for the evolution of atomic vacancies during plastic slip deformation

○Tetsuya Ohashi （Kitami institute of technology, Japan）

[SY-E7] Structural Stability of Long-period Stacking Ordered Magnesium Alloys

○Daisuke Matsunaka[1], Yoji Shibutani[2] （1.Dept. of Mechanical Systems Engineering, Shinshu Univ., Japan, 2.Dept. of Mechanical Engineering, Osaka Univ., Japan）

[SY-E7] **First-principles-based prediction of yield strength in the RhIrNiPdPtCu high entropy alloy**

○Binglun Yin, William A. Curtin （LAMMM, EPFL, Switzerland）

[SY-E7] Metal-coated carbon nanotube reinforced aluminum composites

○Samaneh Nasiri[1,2], Michael Zaiser[1,2] （1.Institute for Materials Simulation WW8, Deptartment of Materials Science, Friedrich-Alexander University Erlangen-Nuernberg, Germany, 2.Cluster of Excellence EAM/FUMIN, Germany）

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E8] Symposium E-8

Chairs: Hao Wang(Institute of Metal Research, CAS, China), Jun-Ping Du(Kyoto University, Japan)
4:00 PM - 5:30 PM Room2

[SY-E8] **Effect of hydrogen on the vacancy diffusion in metals**

○Jun-Ping Du[1,2], W.T. Geng[3], Kazuto Arakawa[4], Shigenobu Ogata[2,1] （1.Elements Strategy Initiative for Structural Materials, Kyoto University, Japan, 2.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 3.University of Science and Technology Beijing, China, 4.Department of Materials Science, Faculty of Science and Engineering, Shimane University, Japan）

[SY-E8] Promotional effects of anisotropic strain on vacancy mobility in tungsten: the independence on the sign of strain

○Zhong Zhu Li, Yu Hao Li, Hong Bo Zhou, Guang Hong

Lu （Department of Physics, Beihang University, China)

[SY-E8] **Ab initio investigation on the stacking fault energy and the *c/a* ratio in hexagonal metals and alloys**

○Gang Zhou, Hao Wang, Dong sheng Xu, Rui Yang （Institute of Metal Research, Chinese Academy of Sciences, China)

[SY-E8] Role of vacancies and grain boundaries of 2D materials for the catalytic ammonia synthesis

○Qinye Li[1], Lizhong He[1], Chenghua Sun[2,3], Xiwang Zhang[1] （1.Monash University, Australia, 2.Swinburne University of Technology, Australia, 3.Dongguan University of Technology, China)

[SY-E8] First-principles Investigation on the Stability and Oxygen Adsorption Behavior of a $Ti_2AlNb/TiAl$ Interface

○Yue Li, Jianhong Dai, Yan Song （School of Materials Science and Engineering, Harbin Institute of Technology at Weihai, China)

[SY-E8] **DFT predictions of hydrogen storage properties of Mg_7TiX_2 (X= F, O, S, P and Cl)**

○Yuying Chen, Jianhong Dai, Yan Song （School of Materials Science and Engineering, Harbin Institute of Technology at Weihai, China)

Room3

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F5] Symposium F-5
Chair: Ingo Steinbach(Ruhr-University Bochum, Germany)
9:45 AM - 11:00 AM Room3

[SY-F5] Solidification microstructure formation by phase-field simulation with multi-GPU acceleration

○Tomohiro Takaki[1], Shinji Sakane[1], Munekazu Ohno[2], Yasushi Shibuta[3], Takayuki Aoki[4] （1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.The University of Tokyo, Japan, 4.Tokyo Institute of Technology, Japan)

[SY-F5] **Phase-field study of eutectic colony formation in NiAl-34Cr**

○Michael Kellner[1,2], Johannes Hötzer[1,2], Markus Linnenberg[1], Marco Seiz[1], Britta Nestler[1,2] （1.Institute of Applied Materials - Computational Materials Science (IAM-CMS), Karlsruhe Institute of Technology, Germany, 2.Institute of Digital Materials Science (IDM), Karlsruhe University of Applied Science, Germany)

[SY-F5] Solidification analysis by non-equilibrium phase

field model using thermodynamics data estimated by machine learning

○Sukeharu Nomoto[1], Hiroshi Wakameda[1], Masahito Segawa[1], Toshiyuki Koyama[2], Akinori Yamanaka[3] （1.ITOCHU techno-Solutions Coorporation, Japan, 2.Materials Design Innovation Engineering, Nagoya Univ., Japan, 3.Department of Mechnical Systems Engneering, Tokyo University of Agriculture and Technology, Japan)

[SY-F5] Phase field modeling of deformation twinning in β -metastable titanium alloys

○Juba Hamma[1], Benoît Appolaire[2], Yann Le Bouar[1], Alphonse Finel[1] （1.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay F-92322 Châtillon, France, 2.IJL, UMR 7198 CNRS-Université de Lorraine, 54000 Nancy, France)

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F6] Symposium F-6
Chair: Benoit Appolaire(Institut Jean Lamour, Univ. de Lorraine, France)
11:15 AM - 12:30 PM Room3

[SY-F6] Atomistically informed full-field simulation of tempered martensite:Quenching, tempering and mechanical characterization

○Ingo Steinbach （Ruhr-University Bochum, Germany)

[SY-F6] **Characterisation and modelling of drawn martensite**

○Marius Gintalas[1], Miguel A. Santajuana[2], Carlos Garcia-Mateo[2], David San-Martin[2], Jose A. Jiménez[2], Wim Van Haver[3], Pedro E. J. Rivera-Diaz-del-Castillo[4] （1.The University of Cambridge, Department of Materials Science &Metallurgy, 27 Charles Babbage Road, Cambridge CB3 0FS, UK, 2.Materalia research group, Department of Physical Metallurgy, Spanish National Centre for Metallurgical Research (CENIM-CSIC), Avda. Gregorio del Amo 8, Madrid E-28040, Spain, 3.NV Bekaert SA, Bekaertstraat 2, Zwevegem B-8550, Belgium, 4.The University of Lancaster, Department of Engineering, Engineering Building, Lancaster University, Gillow Ave, Bailrigg, Lancaster LA1 4YW, UK)

[SY-F6] 3D modeling of microstructure evolution in Ni-based superalloys under creep loading

○Maeva Cottura[1], Benoît Appolaire[1], Alphonse Finel[2], Yann Le Bouar[2] （1.Institut Jean Lamour , France, 2.LEM - CNRS/Onera, France)

[SY-F6] Phase field study of the effect of coherency strains and applied load in material couples
○Sourav Chatterjee, Nele Moelans （Department of Materials Engineering, KU Leuven, Belgium）

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F7] Symposium F-7

Chair: Tomohiro Takaki(Kyoto Institute of Technology, Japan)
2:00 PM - 3:30 PM Room3

[SY-F7] A Cosserat crystal plasticity and phase field theory for grain boundary migration
○Benoit Appolaire[1,2], Anna Ask[3], Samuel Forest[3], Kais Ammar[3] （1.Institut Jean Lamour, Univ. de Lorraine, France, 2.LEM, CNRS-Onera, France, 3.Centre des Materiaux, Mines ParisTech, France）

[SY-F7] Phase-field modeling of precipitation growth and ripening during heat-treatment conditions in Ni-base superalloys
○Michael Fleck, Felix Schleifer, Markus Holzinger, Yueh-Yu Lin, Uwe Glatzel （Metals and Alloys, University Bayreuth, Germany）

[SY-F7] Two-dimensional Simulation of Cyclic Phase Transformation in Fe-C-Mn-Si Alloy using Non-equilibrium Multi-Phase-Field Model
○Masahito Segawa[1], Nomoto Sukeharu[1], Akinori Yamanaka[2] （1.ITOCHU Techno-Solutions Corporation, Japan, 2.Division of Advanced Mechanical Systems Engineering, Institute of Engineering, Tokyo University of Agriculture and Technology, Japan）

[SY-F7] Prediction of the microstructure evolution in Electron Beam Melting Alloy 718 through phase field modelling
○Chamara Kumara[1], Dunyong Deng[2], Johan Moverare[2], Per Nylén[1] （1.Department of Engineering Science, University West, Sweden, 2.Department of Management and Engineering, Linköping University, Sweden）

[SY-F7] Phase-field simulation of solidification morphology in laser powder deposition of Fe-B alloys
○Xiaoxia Li, Xiangge Qin （School of Materials Science and Engineering, Jiamusi Univ., China）

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F8] Symposium F-8

Chair: Martin Diehl(Max-Planck-Institut fuer Eisenforschung GmbH, Germany)

4:00 PM - 5:30 PM Room3

[SY-F8] From state parameter-based microstructure modeling to temperature and strain rate-dependent yield stress
○Ernst Kozeschnik （Institute of Materials Science and Technology, TU Wien, Austria）

[SY-F8] **Modelling of grain boundary segregation and precipitation in multi-component Al alloys subjected to heat treatment**
○Dongdong Zhao[1], Sylvain Gouttebroze[2], Jesper Friis[3], Yanjun Li[1] （1.Norwegian University of Science and Technology (NTNU), 7491, Trondheim , Norway, 2.SINTEF Materials and Chemistry, 0314 Oslo, Norway, 3.SINTEF Materials and Chemistry, 7491 Trondheim, Norway）

[SY-F8] Modeling the microstructure and electrical conductivity evolution during aging of Al-Mg-Si alloys
○Yijiang Xu, Yanjun Li （Norwegian University of Science and Technology , Norway）

[SY-F8] Thermo-kinetic modeling of long-term precipitate evolution in heat-resistant alloys
○Jae-Hyeok Shim[1], Magdalena Speicher[2], Mahesh Chandran[3], Woo-Sang Jung[1] （1.Korea Institute of Science and Technology, Korea, 2.Materials Testing Institute, Germany, 3.Indo-Korea Science and Technology Centre, India）

[SY-F8] **Simultaneous Transformation Kinetics Model for Additive Manufacturing**
○Narendran Raghavan, Srdjan Simunovic, John Turner （Oak Ridge National Laboratory , United States of America）

Room4

Symposium | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[SY-N1] Symposium N-1

Chair: Danny Perez(Los Alamos National Laboratory, United States of America)
9:45 AM - 10:45 AM Room4

[SY-N1] Increasing the power of accelerated molecular dynamics methods and plans to exploit the coming exascale
○Arthur F Voter （Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, United

States of America)

[SY-N1] Atomistic processes at interfaces on extended timescales

○Jutta Rogal[1] （1. Ruhr University Bochum, Germany）

Symposium | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[SY-N2] Symposium N-2
Chair: Erik Bitzek(FAU Erlangen-Nuernberg, Germany)
11:15 AM - 12:15 PM Room4

[SY-N2] *Modeling Microstructure Evolution in Rapid Solidification Phenomena Using Structural Phase Field Crystal Models*

○Nikolas Provatas （McGill University, Canada）

[SY-N2] The Phase Field Method: Crystal Structures and Facets

○Peter Voorhees[1], Eli Alster[1], Nana Ofuri-Opoku[1,3], David Montiel[2], Katsuyo Thornton[2], James Warren[3] （1.Northwestern University, United States of America, 2.University of Michigan, United States of America, 3.National Institute for Standards and Technology, United States of America）

[SY-N2] Using free energy calculations and statistical mechanics to probe the brittle to ductile transition of bcc metals

○Thomas Swinburne[1] （1.CINaM, CNRS/Aix-Marseille Univ., France）

Symposium | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[SY-N3] Symposium N-3
Chair: Arthur F. Voter(Los Alamos National Lab, United States of America)
2:00 PM - 3:30 PM Room4

[SY-N3] Kinetics of Fivefold-Twinned Nanowire Growth

○Kristen Fichthorn （Penn State University, United States of America）

[SY-N3] Accelerated quantum molecular dynamics simulations of chemistry under extreme conditions

○Romain Perriot, Marc Cawkwell, Enrique Martinez （Los Alamos National Laboratory, United States of America）

[SY-N3] Hydrogen diffusion in TiH_x: insights from PRD accelerated QMD

○Ivan Novoselov[1,2], Alexey Yanilkin[1] （1.Dukhov

Research Institute of Automatics, Russia, 2.Moscow Institute of Physics and Technology, Russia）

[SY-N3] Shape fluctuation of metallic nanoclusters: observations from long-timescale simulations

○Rao Huang[1], Li-Ta Lo[2], Arthur F. Voter[2], Danny Perez[2] （1.Xiamen University, China, 2.Los Alamos National Lab, United States of America）

Symposium | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[SY-N4] Symposium N-4
Chair: Laurent Karim Beland(Queen's University, Canada)
4:00 PM - 5:30 PM Room4

[SY-N4] Multiscale diffusion method for simulations of long-time defect evolution with application to dislocation climb

○Kristopher Baker[1], William Curtin[2] （1.Knolls Atomic Power Laboratory, United States of America, 2.Swiss Federal Institute of Technology, Switzerland）

[SY-N4] Accelerated Quantum Molecular Dynamics

○Enrique Martinez Saez[1], Christian Negre[2], Romain Perriot[2], Danny Perez[2], Eduard Kober[2], Marc Cawkwell[2], Arthur F. Voter[2], Anders Niklasson[2] （1.Material Science and Technology Division, MST-8,Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America, 2.Theoretical Division, T-1, Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America）

[SY-N4] On the effect of hydrogen on vacancy diffusion

○Sebastian Echeverri Restrepo[1], Anthony T Paxton[2] （1.Department of Metallic Materials &Ceramics, SKF, Netherlands, 2.Department of Physics, King's College London, UK）

Room5

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O5] Symposium O-5
Chairs: Hitoshi Washizu(University of Hyogo, Japan), Sophie Loehle(TOTAL Marketing &Services, Solaize, France)
9:45 AM - 11:00 AM Room5

[SY-O5] On the formation of superlubricious layers during boundary lubrication of diamond and diamond-like carbon

○Michael Moseler[1,2] （1.Fraunhofer Institute for Mechanics of Materials IWM, Germany, 2.University of

Freiburg, Germany）

[SY-O5] Unveiling the chemical reactions involved in moisture-induced weakening of adhesion between aluminum and epoxy resin: a hybrid quantum-classical simulation study

○Shuji Ogata, Masayuki Uranagase （Dept. of Physical Science and Engineering, Nagoya Institute of Technology, Japan）

[SY-O5] Efficient evaluation of adhesion free energy between a liquid and polymer-grafted substrate

○Masayuki Uranagase, Shuji Ogata （Nagoya Institute of Technology, Japan）

[SY-O5] **Ultimate response of confined fluids under extreme conditions: a Molecular Dynamics analysis**

○Alejandro Porras-Vazquez, Laetitia Martinie, Philippe Vergne, Nicolas Fillot （INSA Lyon, France）

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O6] Symposium O-6

Chairs: Yoshitaka Umeno(The University of Tokyo, Japan), Yoshinori Shiihara(Toyota Technological Institute,Japan)
11:15 AM - 12:30 PM Room5

[SY-O6] Modeling the plastic deformation of a metal crystal induced by contact with a rough rigid surface

○Lucia Nicola[1,2] （1.Delft University of Technology, Netherlands, 2.University of Padova, Italy）

[SY-O6] On the potential use of liquid crystals as 'smart' lubricants - an MD simulation study

○Kerstin Falk[1], Konstantinos Gkagkas[2], Gianpietro Moras[1], Michael Moseler[1,3] （1.Dept. of Tribology, Fraunhofer IWM, Freiburg, Germany, 2.Toyota Motor Europe, Technical Center, Zaventem, Belgium, 3.Dept. of Physics, University of Freiburg, Germany）

[SY-O6] **Sliding on physisorbed cetyltrimethylammonium bromide (CTAB)**

○Johannes Laurin Hoermann, Lars Pastewka （University of Freiburg, Germany）

[SY-O6] Atomistic simulations of amines as organic friction modifiers

Rafael Pereira de Matos[1], Sophie Loehlé[2], Clotilde Minfray[1], ○Manuel Cobian[1] （1.LTDS ECL, Universite de Lyon, France, 2.TOTAL Marketing &Services, Solaize, France）

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O7] Symposium O-7

Chairs: Lucia Nicola(Delft University of Technology, Netherlands), Shuji Ogata(Nagoya Institute of Technology, Japan)
2:00 PM - 3:30 PM Room5

[SY-O7] Toward Exascale Atomistic Simulations of Interfaces

○Aiichiro Nakano （Univ. of Southern California, United States of America）

[SY-O7] Molecular Dynamics Simulation Study on the Structure, Role, and Formation Mechanism of Tribofilms of Silicon-Based Materials in Water

○Yusuke Ootani[1], Jingxiang Xu[1], Naoki Takahashi[1], Koshi Adachi[2], Momoji Kubo[1] （1.Institute for Materials Research, Tohoku University, Japan, 2.Department of Mechanical Systems Engineering, Graduate School of Engineering, Tohoku University, Japan）

[SY-O7] Influence of Tribo-Film Structure Generated from MoDTC at DLC/DLC Interface on Friction Behavior : A Molecular Dynamics Simulation

○Masahiro Saito[1], Jingxiang Xu[1], Yusuke Ootani[1], Nobuki Ozawa[1], Koshi Adachi[2], Momoji Kubo[1] （1.Institute for Materials Research, Tohoku Univ., Japan, 2.Graduate School of Engineering, Tohoku Univ., Japan）

[SY-O7] **Shear-induced amorphization of silicon and diamond yields liquid-like amorphous solids**

○Gianpietro Moras[1], Andreas Klemenz[1], Thomas Reichenbach[1], Adrien Gola[2], Hiroshi Uetsuka[3], Michael Moseler[1,4], Lars Pastewka[1,5] （1.Fraunhofer Institute for Mechanics of Materials IWM, Germany, 2.Institute for Applied Materials, Karlsruhe Institute of Technology, Germany, 3.Asahi Diamond Industrial Co. Ltd., Japan, 4.Institute of Physics, University of Freiburg, Japan, 5.Department of Microsystems Engineering, University of Freiburg, Germany）

[SY-O7] A new damage implementation for Smooth Particle Hydrodynamics and its application to simulating the wear response of metals.

○Alban de Vaucorbeil, Christopher Hutchinson （Monash University, Australia）

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O8] Symposium O-8

Chairs: Tianbao Ma(Tsinghua University, China), Yang Wang(Institute for Materials Research, Tohoku University, Japan)

4:00 PM - 5:00 PM Room5

[SY-O8] Friction mechanism of nanostructured steel in lubricant: A coarse-grained molecular dynamics study
○Yoshitaka Umeno Umeno, Atsushi Kubo, Yuta Sudo （The University of Tokyo, Japan）

[SY-O8] Coarse-Grained Molecular Dynamic Simulation on the Wear Mechanism of Polymer Brush with Different Chain Topologies
○Zhongmin Liu, Shuichi Uehara, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Material Research,Tohoku Univ., Japan）

[SY-O8] Molecular Dynamics Simulation Study on Friction of Bottlebrush Polymer with a Cationic Anchor Block Adsorbed on Substrate
○Shuichi Uehara, Zhongmin Liu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Materials Research, Tohoku Univ., Japan）

[SY-O8] Temperature dependent dynamics simulation of traction fluid by molecular dynamics method
○Eiji Tomiyama[1,2], Takeshi Iwasaki[3], Hitoshi Washizu[2] （1.Research Organization for Information Science and Technology, Japan, 2.Graduate School of Simulation Studies, Univ. of Hyogo, Japan, 3.Lubricants Research Laboratory, Idemitsu Kosan Co., Ltd., Japan）

Room6

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A5] Symposium A-5
Chair: Sinisa Dj Mesarovic(Washington State University, United States of America)
9:45 AM - 11:00 AM Room6

[SY-A5] Parameters to consider in the modelling of dislocation boundary evolution
○Grethe Winther Winther （Technical University of Denmark, Denmark）

[SY-A5] Data Mining of Indentation Induced Dislocation Microstructures
○Dominik Steinberger[1], Shyamal Roy[1], Dan Mordehai[2], Stefan Sandfeld[1] （1.Chair of Micromechanical Materials Modelling, TU Bergakademie Freiberg, Germany, 2.Department of Mechanical Engineering, Technion - Israel Institute of Technology, Israel）

[SY-A5] Lattice continua for polycrystal grains: Climb and glide of dislocations, diffusion and grain boundary

kinematics.
○sinisa Dj Mesarovic （Washington State University, United States of America）

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A6] Symposium A-6
Chair: Emma Griffiths(University of Cape Town, South Africa)
11:15 AM - 12:30 PM Room6

[SY-A6] Design of patchy nanoparticles via the self-assembly of triblock terpolymers in selective solvents
○Eliot Fried, Nicolás Moreno （Okinawa Institute of Science and Technology, Japan）

[SY-A6] Nanoporous Composites: Giving Polymers Strength and Helping Metals Move
○Emma Griffiths[1], Jana Wilmers[2], Swantje Bargmann[2], BD Reddy[1] （1.University of Cape Town, South Africa, 2.University of Wuppertal, Germany）

[SY-A6] Multiscale modeling of advanced materials for hybrid organic-inorganic solar cells
○Alexander E. Kobryn （Nanotechnology Research Center, National Research Council Canada, Canada）

[SY-A6] **From cellulose and lignin to kerogen: molecular simulations of a geological process**
○Roland PELLENQ[1], Pierre-Louis Valdenaire[1], Christophe Bichara[3], Franz Ulm[1], Jean-Marc Leyssale[2] （1.<MSE>2, MIT- CNRS - AMU, United States of America, 2.ISM, CNRS - Bordeaux U., France, 3.CINaM, CNRS - Aix-Marseille U., France）

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A7] Symposium A-7
Chair: Michael Zaiser(FAU University of Erlangen-Nuremberg, Germany)
2:00 PM - 3:30 PM Room6

[SY-A7] Mathematical challenges for a mesoscale theory of dislocations
○Thomas Hochrainer （TU Graz, Austria）

[SY-A7] **Dislocation multiplication in the discrete-continuum transition regime**
○Katrin Schulz[1], Markus Sudmanns[1], Kolja Zoller[1], Peter Gumbsch[1,2] （1.Karlsruhe Institute of Technology, Germany, 2.Fraunhofer Institute for Mechanics of Materials, Germany）

[SY-A7] The fundamental instability of dislocation transport equations
○Michael Zaiser, Ronghai Wu （FAU University of

Erlangen-Nuremberg, Germany）

[SY-A7] 2D continuum theory of dislocations

○Istvan Groma （Eotvos Lorand University, Hungary）

[SY-A7] Continuum dislocation dynamics for finite deformation mesoscale plasticity

○Anter El-Azab （Purdue University, United States of America）

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A8] Symposium A-8

Chair: Thomas Hochrainer(TU Graz, Austria)
4:00 PM - 5:30 PM Room6

[SY-A8] Pattern formation in doubly curved thin shells

○Eleni Katifori[1], Desislava Todorova[1], Octavio Albarran[2], Lucas Goehring[2] （1.University of Pennsylvania, United States of America, 2.Max Planck Institute, Germany）

[SY-A8] Phase-field model for microstructure change in $L1_0$ type ordering with lattice distortion

○Ryuichiro Oguma[1], Long-Qing Chen[2], Syo Matsumura[3] （1.Fukuoka Univ., Japan, 2.The Pennsylvania State Univ., United States of America, 3.Kyushu Univ., Japan）

[SY-A8] Coupling multi-component phase field models for oxide systems to thermodynamic databases - breaking the curse of dimensionality

○Inge Bellemans[1], Nico Vervliet[2], Lieven De Lathauwer[2,3], Nele Moelans[4], Kim Verbeken[1] （1.Department of Materials, Textiles and Chemical Engineering, Ghent University , Belgium, 2.Department of Electrical Engineering, KU Leuven, Belgium, 3.Group Science, Engineering and Technology, KU Leuven - Kulak, Belgium, 4.Department of Materials Engineering, KU Leuven, Belgium）

[SY-A8] A Sharp Phase Field Method

○Alphonse FINEL[1], Yasunori YAMADA[2], Yann LE BOUAR[1], Benoît DABAS[1], Benoît APPOLAIRE[1], Tetsuo MOHRI[2] （1.Laboratoire d'Etude des Microstructures, CNRS, ONERA, France, 2.Institute for Materials Research, Tohoku University, Japan）

Room7

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I5] Symposium I-5

Chairs: Stephen M Foiles(Sandia National Laboratories, United States of America), Mitra L Taheri(Drexel University, United States of America)
9:45 AM - 11:00 AM Room7

[SY-I5] **Heterogeneous disconnections nucleation mechanisms during grain boundary migration**

○Nicolas Combe[1,2], Frederic Mompiou[1], Marc Legros[1] （1.CEMES Toulouse, France, 2.Univ. Toulouse, UPS, France）

[SY-I5] Motion of Grain Boundaries Based on Disconnections

○Chaozhen Wei[1,2], Luchan Zhang[5], Yang Xiang[2], Jian Han[4], Spencer Thomas[4], kongtao Chen[4], David J. Srolovitz[3,1] （1.HKUST Jockey Club Institute for Advanced Study, Hong Kong University of Science and Technology, Hong Kong, 2.Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong, 3.Materials Science and Engineering, Mechanical Engineering and Applied Mechanics, Computer and Information Science, University of Pennsylvania, United States of America, 4.Materials Science and Engineering, University of Pennsylvania, United States of America, 5.Department of Mathematics, National University of Singapore, Singapore）

[SY-I5] Dislocation-mediated boundary motion, dislocation-boundary interaction, and their effect on the mechanical behavior in fcc materials

○Bob Svendsen[1,2], Jaber Rezaei Mianroodi[2], Juan Li[3], Christoph Kirchlechner[3], Gerhard Dehm[3] （1.Material Mechanics, RWTH Aachen University, Germany, 2.Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Germany, 3.Structure and Nano-/Micromechanics of Materials, Max-Planck-Institut für Eisenforschung GmbH , Germany）

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I6] Symposium I-6

Chairs: Garritt Tucker(Colorado School of Mines, United States of America), Chuang Deng(University of Manitoba, Canada)
11:15 AM - 12:30 PM Room7

[SY-I6] Migration mechanisms of faceted vicinal grain boundaries

○Sherri Hadian[1], Blazej Grabowski[1], Mike W Finnis[2], Jörg Neugebauer[1] （1.Max-Planck-Institut fuer Eisenforschung, Germany, 2.Imperial College London, UK）

[SY-I6] Multiscale model for the structure and energy of low-angle general grain boundaries in Al, Cu and Ni

○Shuyang Dai[1], Yang Xiang[2], David Joseph Srolovitz[3]

(1.Wuhan University, China, 2.Hong Kong University of Science and Technology, Hong Kong, 3.University of Pennsylvania, United States of America)

[SY-I6] The influence of normal stress on the structural transformation and migration of grain boundaries
○Chuang Deng, Mohammad Aramfard (University of Manitoba, Canada)

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity
[SY-I7] Symposium I-7
Chairs: Nicolas Combe(CEMES Toulouse, France), Brandon Runnels(University of Colorado Colorado Springs, United States of America)
2:00 PM - 3:30 PM Room7

[SY-I7] Insights into recrystallisation: atomistic simulations of the properties of grain boundaries in heavily deformed material
○Chris P Race (University of Manchester, UK)

[SY-I7] Continuum Dislocation Dynamic Based Grain Fragmentation Modeling for Severe Plastic Deformation in FCC Metals
○Ali Al-Hadi I. Kobaissy[1], Georges Ayoub[2], Mu'Tasem Shehadeh[1] (1.Department of Mechanical Engineering, American University of Beirut, Lebanon, 2.Department of Industrial and Manufacturing Systems Engineering, University of Michigan-Dearborn, United States of America)

[SY-I7] Atomistic Investigation on Interaction of Stress-Assisted Grain Boundary Motion with Crack
○Mohammad Aramfard, Chuang Deng (Univ. Manitoba, Canada)

[SY-I7] **Effect of grain boundary structure on its Dynamic Response using Molecular Dynamics**
○Saryu Fensin[1], Timothy Frolov[2] (1.Los Alamos National Lab, United States of America, 2.Lawrence Livermore National Laboratory, United States of America)

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity
[SY-I8] Symposium I-8
Chair: Srikanth Patala(North Carolina State University, United States of America)
4:00 PM - 5:00 PM Room7

[SY-I8] New Approaches for Understanding Nanocrystalline Mechanics: Physical Microstructures, Grain Boundary Descriptors and Deformation Mechanisms

○Garritt Tucker, Jacob Tavenner, Ankit Gupta (Colorado School of Mines, United States of America)

[SY-I8] **Grain Boundary Sliding: the best supporting role in ductile localization**
○Alexandre Dimanov[1], Jean Raphanel[1], Michel Bornert[2], Eva Héripré[3], Mathieu Bourcier[1], Ababacar Gaye[2], Alexandre El Sabbagh[1], Wolfgang Ludwig[4], Andrew King[5] (1.LMS, CNRS-UMR7649, Ecole Polytechnique, France, 2.Laboratoire Navier, CNRS-UMR8205, Ecole des Ponts, France, 3.MSSMAT, CNRS-UMR8579, Centrale-Supélec, France, 4.MATEIS, UMR5510, INSA-Lyon, France, 5.SOLEIL Synchrotron, Beam line Psiché, France)

[SY-I8] Polycrystal plasticity with anisotropic grain boundary energy described on the five-dimensional grain boundary space
○Nikhil Chandra Admal[1], Javier Segurado[2,1], Jaime Marian[1] (1.University of California Los Angeles, United States of America, 2.IMDEA, Spain)

Room8

Symposium | G. Modeling Mechanical Behavior of Materials under Harsh Environments
[SY-G1] Symposium G-1
Chairs: Byeongchan Lee(KyungHee Univ., Korea), Keonwook Kang(Yonsei University, Korea)
9:45 AM - 11:00 AM Room8

[SY-G1] A systematic method to develop a potential model for harsh environments
○Takuji Oda, Sehyeok Park, Woonghee Cho (Dept. of Nuclear Engineering, Seoul National Univ., Korea)

[SY-G1] Molecular dynamics study of the bulk cascades in W-Re alloy
○Hyunggyu Lee[1], Byeongchan Lee[2], Keonwook Kang[1] (1.yonsei university, Korea, 2.kyung hee university, Korea)

[SY-G1] Defect Energetics in W-Based Transition-Metal Ternary Systems
○Younggak Shin, Byeongchan Lee (KyungHee Univ., Korea)

[SY-G1] A numerical study of channel deformation and fracture in irradiated stainless steel single crystals
○Jean-Michel Scherer[1,2], Samuel Forest[2], Jacques Besson[2], Benoit Tanguy[1], Jérémy Hure[1] (1.DEN-Service d'Etudes des Matériaux Irradiés, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette cedex, France, France, 2.MINES ParisTech, PSL-Research University, Centre des

matériaux, CNRS UMR 7633, 63-65 rue Henri Auguste DesbruèresBP 87 91003 Evry Cedex, France, France)

Symposium | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[SY-G2] Symposium G-2

Chairs: Seunghwa Ryu(Korea Advanced Institute of Science and Technology, Korea), Keonwook Kang(Yonsei University, Korea)
11:15 AM - 12:30 PM Room8

[SY-G2] **Multiscale modeling of strength enhancement of aluminium honeycombs under combined shear-compression at high strain rate**

○Han Henri ZHAO[1], Bing Hou[2] （1.Ecole Normale Paris-Saclay, France, 2.School of aeronautics, NWPU, , China）

[SY-G2] Multiscale mechanical analysis of silicon and silicon dioxide as high capacity anode materials for lithium ion batteries.

○Janghyuk Moon[1], Kyeongjae Cho[2], Maenghyo Cho[3] （1.School of Energy System Engineering, Chung-Ang Univ., Korea, 2.Department of Materials Science and Engineering, University of Texas at Dallas, United States of America, 3.School of Mechanical &Aerospace Engineering, Seoul National University, Korea）

[SY-G2] **Finite element analysis of the effect of interfacial bubbles on performance of epoxy coatings under the alternating hydrostatic pressure**

○Li Liu （Institute of Metal Research, Chinese Academy of Sciences, China）

[SY-G2] **Multiscale Modeling and Design of High-Strength and Low-Density 3D-Archecticured Metamaterial Systems**

○Hussein M Zbib[1], Mehdi Hamid[1], Rahul Panat[2], Sadeq Saleh[2] （1.Washington State university, United States of America, 2.Carnegie Mellon University, United States of America）

[SY-G2] Multiscale-multiphysics simulations of metal nanotips under high electric field

○Mihkel Veske[1], Andreas Kyritsakis[1], Kyrre Ness Sjobak[2], Vahur Zadin[3], Flyura Djurabekova[1] （1.Helsinki Institute of Physics, University of Helsinki, Finland, 2.Department of Physics, University of Oslo, Norway, 3.Institute of Technology, University of Tartu, Estonia）

Symposium | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[SY-G3] Symposium G-3

Chairs: Seunghwa Ryu(Korea Advanced Institute of Science and

Technology, Korea), Keonwook Kang(Yonsei University, Korea)
2:00 PM - 3:30 PM Room8

[SY-G3] Simulations on severely transient FSI problems associated with shock compression of matters in extreme conditions

○Jai-ick Yoh （Seoul National University, Korea）

[SY-G3] **Modeling and simulation of shock waves in solids using branched Hugoniots**

Jae-Wan Lee[1], Jimin Choi[1], Keonwook Kang[1], Soonho Song[1], ○Won-Suk Ohm[1], Jung Su Park[2] （1.Yonsei University, Korea, 2.Agency for Defense Development, Korea）

[SY-G3] Branched Hugoniot curve of aluminum in strong shock using molecular dynamics

○Jimin Choi[1], Sanghyuk Yoo[1], Soonho Song[1], Jung Su Park[2], Keonwook Kang[1] （1.Yonsei Univ., Korea, 2.Agency for Defense Development, Korea）

[SY-G3] **Shear relaxation behind the shock front in <1 1 0> molybdenum**

○Roman Kositski[1], Dominik Steinberger[2], Stefan Sandfeld[2], Dan Mordehai[1] （1.Department of Mechanical Engineering, Technion - Israel Institute of Technology, 32000 Haifa, Israel, 2.Chair of Micromechanical Materials Modelling (MiMM), Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, 09599 Freiberg, Germany）

[SY-G3] **Hypervelocity shock behavior of graphene-metal nanocomposites via molecular dynamics simulations**

○Stefano Signetti, Seunghwa Ryu （Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea）

Symposium | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[SY-G4] Symposium G-4

Chairs: Keonwook Kang(Yonsei University, Korea), Byeongchan Lee(KyungHee Univ., Korea)
4:00 PM - 4:45 PM Room8

[SY-G4] Effect of surface and internal defects on the mechanical properties of metallic glasses

Sunghwan Kim, ○Seunghwa Ryu （Dept. of Mechanical Engineering, Korea Advanced Institute of Science and Technology, Korea）

[SY-G4] Weighted Voronoi Tessellation for metallic glasses by molecular dynamics and powder packing by discrete element method

○Junyoung Park[1], Jaehee Lyu[1], Shibutani Yoji[2] （1.Dept. of Mechanical Design Engineering, Kumoh National Institute of Technology, Korea, 2.Dept. of Mechanical Engineering, Osaka University, Japan）

[SY-G4] Potential of lineal-path function as a characterization parameter related to material properties

○Tong-Seok Han, JI-SU KIM （Yonsei University, Korea）

Room9

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H3] Symposium H-3
Chair: Hansohl Cho(Los Alamos National Laboratory, United States of America)
9:45 AM - 11:00 AM Room9

[SY-H3] Polydomain liquid crystal elastomers1

○Kaushik Bhattacharya （California Institute of Technology, United States of America）

[SY-H3] **Mechanical behavior of hydrated polymers at nanoscale: from elasticity to rupture.**

○William Goncalves[1], Takuya Mabuchi[2], Takashi Tokumasu[1] （1.Institute of Fluid Science, Tohoku University, Sendai, Miyagi 980-8577, Japan, 2.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Sendai, Miyagi 980-8577, Japan）

[SY-H3] Structural properties of mixtures of stars polymers and long chains

○Emanuele Locatelli[1], Daniele Parisi[2,3], Maria Merola[2], Domenico Truzzolillo[4], Mario Gauthier[5], Christos N. Likos[1], Dimitris Vlassopoulos[2,3] （1.Faculty of Physics, University of Vienna, Austria, 2.Institute of Electronic Structure and Laser, FORTH, Greece, 3.Department of Materials Science and Technology, University of Crete, Greece, 4.Laboratoire Charles Coulomb, UMR 5221 CNRS - Universitè de Montpellier, France, 5.Faculty of Science, University of Waterloo, Canada）

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H4] Symposium H-4
Chair: Meredith Silberstein(Cornell University, United States of America)
11:15 AM - 12:30 PM Room9

[SY-H4] **Enhanced Dissipation Behavior of Main-Chain LCE Networks**

○Thao D Nguyen （Johns Hopkins University, United States of America）

[SY-H4] Thermo-mechanically coupled model for large strain of ultra-high molecular weight semi-crystalline polymers

○Chrystelle A. Bernard[1], Tiana Deplancke[4], Olivier Lame[4], Kazuhiro Ogawa[3], Jean-Yves Cavaillé[2] （1.Frontier Research Institute for Interdisciplinary Sciences (FRIS), Tohoku Univ., Japan, 2.Engineering Science Lyon Tohoku joint lab for Materials under Extreme Conditions (ELyTMaX) UMI3757, Tohoku Univ., Japan, 3.Fracture and Reliability Research Institute (FRI), Tohoku Univ., Japan, 4.Materials Engineering and Science (MATEIS), CNRS, INSA-Lyon, UMR5510 Univ. de Lyon, France）

[SY-H4] Design principles for high modulus and toughness of assembled hairy nanoparticles

Nitin Krishnamurthy Hansoge, Tianyu Huang, Robert Sinko, Wenjie Xia, Wei Chen, ○Sinan Keten （Northwestern University, United States of America）

[SY-H4] Effect of Chain Alignment on Entanglements, Diffusion and Polymer Weld Strength

Marco Galvani, Thomas C O'Connor, ○Mark Owen Robbins （Dept. Physics and Astronomy, Johns Hopkins Univ., United States of America）

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H5] Symposium H-5
Chair: Alexey Lyulin(Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands)
2:00 PM - 3:30 PM Room9

[SY-H5] Microstructural Effects in the Dynamic Response of Random 3D Structural Polymeric Foams

○Axinte Ionita, Brittany Branch, Brian M. Patterson, Brad E. Clements, Dana M. Dattelbaum, Alexander H. Mueller （Los Alamos National Laboratory, United States of America）

[SY-H5] Monte Carlo simulation predicting generation and growth of spherulites in thermoplastic polymer

○Ryota Osawa[1], Yoshiteru Aoyagi[2] （1.Dept. of Mechanical Engineering, Tohoku Univ., Japan, 2.Tohoku Univ., Japan）

[SY-H5] Determination of mechanical properties of polymers from coarse grained molecular dynamics simulations: a few case studies

○Sumit Basu （Indian Institute of Technology Kanpur,

India)

[SY-H5] Modulating Elastomer Strength and Toughness with Metal Ligand Cross-linking

○Meredith Silberstein Silberstein, Yuval Vidavsky, Suwon Bae （Cornell University, United States of America）

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H6] Symposium H-6

Chair: Alexey Lyulin(Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands)
4:00 PM - 5:15 PM Room9

[SY-H6] Coarse-Grained Molecular Dynamics Simulation of Filled Rubber under Cyclic Tensile Deformation

○Takashi Kojima, Masataka Koishi （The Yokohama Rubber Co.,Ltd., Japan）

[SY-H6] Modelling of Influence of Fatigue Damage on Oxygen Diffusion in Rubbers

○Jan Heczko, Radek Kottner （NTIS - New Technologies for the Information Society, Faculty of Applied Sciences, University of West Bohemia, Czech Republic）

[SY-H6] On the modeling and calculation of tensile properties of real rubber using molecular dynamics simulation

○Osamu HIno （TOYO TIRE&RUBBER CO.,LTD., Japan）

[SY-H6] A molecular dynamics study of dissolution of covalent adaptable networks in organic solvent

○Yaguang Sun[1], Hua Yang[2], Yafang Guo[1] （1.Dept. of Mechanics, Beijing Jiaotong Univ., China, 2.State Key Lab. for Geomechanics and Deep Underground Engineering, China Univ. of Mining and Tech., China）

[SY-H6] A minimal micromechanical model for the viscoelasticity in biophysical filamentous networks

Arjan E. Boerma[1], Patrick R. Onck[1], ○Erik Van der Giessen[1], Stefanos Papanikolaou[2] （1.Univ. of Groningen, Netherlands, 2.West Virginia Univ., United States of America）

Room10

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B1] Symposium B-1

Chair: Lorenzo Malerba(CIEMAT, Energy, Environment and Technology Research Centre, Spain)
9:45 AM - 11:00 AM Room10

[SY-B1] Thermal stability of carbon-vacancy complexes in iron alloys and steels

○Milan J Konstantinovic, Lorenzo Malerba （Belgian nuclear institute, SCK.CEN, Belgium）

[SY-B1] Computational study of phosphorous migration to grain-boundary in alpha-iron

○Ken-ichi Ebihara, Tomoaki Suzudo （Center for Computational Science &e-Systems, Japan Atomic Energy Agency, Japan）

[SY-B1] **Properties of interstitials in concentrated Fe-Cr alloys from first principles**

○Marcin Roland Zemla[1], Jan Stanislaw Wrobel[1], Marek Muzyk[1], Tomasz Wejrzanowski[1], Duc Nguyen-Manh[2], Sergei L. Dudarev[2], Luca Messina[3], Par Olsson[3], Christophe Domain[4] （1.Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland, 2.CCFE, Culham Centre for Fusion Energy, Abingdon, Oxon OX14 3DB, UK, 3.KTH Royal Institute of Technology, Nuclear Engineering, 106 91 Stockholm, Sweden, 4.Dép artement Matériaux et Mécanique des Composants, EDF-R&D, Les Renardières, F-77250 Moret sur Loing, France）

[SY-B1] **Defect production in cascade overlap with defect clusters in iron and tungsten**

○Jesper Byggmastar[1], Fredric Granberg[1], Andrea E Sand[1], Kai Nordlund[1] （1. Department of Physics, University of Helsinki, Finland）

[SY-B1] Multiscale modelling of radiation damage evolution in Fe and Fe-based alloys

○Fredric Granberg[1], Haixuan Xu[2], Kai Nordlund[1] （1.Department of Physics, University of Helsinki, Finland, 2.Department of Materials Science and Engineering, University of Tennessee, United States of America）

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B2] Symposium B-2

Chair: Davide Pizzocri(Politecnico di Milano, Italy)
11:15 AM - 12:30 PM Room10

[SY-B2] Atomic scale calculations of nuclear fuel properties to sustain multiscale modeling of fuel behavior

○Emeric Bourasseau, Marjorie Bertolus, Michel Freyss, Gérald Jomard, Ibrahim Cheik Njifon, Martin-Stéphane Talla Noutack, Cyrille Takoukam Takoundjou

（CEA/DEN/DEC, Centre CEA de Cadarache, France）

[SY-B2] Influence of vibrational entropy on the concentrations of uranium vacancies in UO$_2$

○Jean-Paul Crocombette[1], Fabien Bruneval[1], Aurélien Soulié[1], Mihai-Cosmin Marinica[1], Samuel Murphy[2]

（1.CEA Saclay, France, 2.Lancaster University, UK）

[SY-B2] **Modelling of defect and rare gas transport properties in UO$_2$ from the atomic to the grain scale**

○Marjorie Bertolus, Michel Freyss, Emerson Vathonne, Emeric Bourasseau, Serge Maillard, Gérald Jomard

（CEA, DEN, Département d'Etude des Combustibles, Centre de Cadarache, 13108 Saint-Paul-lez-Durance, France）

[SY-B2] **Intragranular bubble impact on nuclear fuel thermomechanical properties**

Fabienne Ribeiro[1], Mehdi Colbert[1], ○Jack Arayro[1], Guy Tréglia[2]（1.Institut de Radioprotection et de Sûreté Nucléaire/PSN-RES/SEMIA/LPTM, France, France, 2.Centre Interdisciplinaire de Nanoscience de Marseille, CNRS, France, France）

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B3] Symposium B-3

Chair: Kazuto Arakawa(Shimane University, Japan)
2:00 PM - 3:15 PM Room10

[SY-B3] **Formation of radiation-induced Re and Os precipitation in W and its effects on mechanical properties**

○Guang-Hong Lu, Yu-Hao Li, Hong-Bo Zhou（Beihang University, China）

[SY-B3] **Elastic fields and interaction between self-interstitial atom defects in bcc metals.**

○Sergei L Dudarev, Pui-Wai Ma（UK Atomic Energy Authority, UK）

[SY-B3] Molecular dynamics simulation study of the interaction of Re with interstitial defects in tungsten bulk

Yangchun Chen[1], Jingzhong Fang[1], Ning Gao[2], Hong-Bo Zhou[3], Wangyu Hu[4], Fei Gao[4,5], ○Huiqiu Deng[1,4]

（1.School of Physics and Electronics, Hunan University, China, 2.Institute of Modern Physics, Chinese Academy of Sciences, China, 3.Department of Physics, Beihang University, China, 4.College of Materials Science and Engineering, Hunan University, China, 5.Department of Nuclear Engineering and Radiological Science,

University of Michigan, United States of America）

[SY-B3] **Hydrogen super-saturated layers in plasma loaded tungsten: a global model combining Density Functional Theory data, Thermodynamic and Kinetic models**

○Yves Ferro, Etienne Hodille（Aix-Marseille University, France）

[SY-B3] Mobility of small vacancy and interstitial prismatic dislocation loops in BCC tungsten

○Jan Fikar[1], Roman Gröger[1], Robin Schäublin[2]

（1.Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic, Switzerland, 2.Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, Switzerland）

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B4] Symposium B-4

Chair: Gary S Was(University of Michigan, United States of America)
4:00 PM - 5:15 PM Room10

[SY-B4] **Kinetics of Precipitation in Fe-Cr and Fe-Cr-C alloys under Irradiation**

○Frederic Soisson（CEA Saclay, France）

[SY-B4] **The complex problem of the experimental validation of atomistic and microstructural evolution models**

○Lorenzo Malerba（CIEMAT, Energy, Environment and Technology Research Centre, Spain）

[SY-B4] Physically based prediction of radiation hardening: application to steels and model alloys

○Ghiath Monnet（EDF - R&D, MMC, France）

[SY-B4] **Oxygen diffusion in bcc Fe under the influence of foreign atoms and vacancies**

○Xiaoshuang Wang, Matthias Posselt, Jürgen Faßbender（Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany）

Wed. Oct 31, 2018

Poster Hall

Poster Session | A. Advances in Materials Theory for Multiscale Modeling

[PO-A2] Poster Session 2
5:45 PM - 8:00 PM Poster Hall

[P2-01] Multiscale model of solid state amorphization during processing of pharmaceutical materials

○Chunyu Li[1], Yifei Zeng[1], Lorena Alzate-Vargas[1], Pilsun Yoo[1], Rachel Frocino[2], Jeff Brum[2], Peilin Liao[1], Marisol Koslowski[1], ○Alejandro Strachan[1] （1.Purdue University, United States of America, 2.GlaxoSmithKline, Analytical Sciences and Development, United States of America）

[P2-02] FTMP-based Modeling and Simulations of HCP Mg Single Crystal

○Takahiro Kitano, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P2-03] Nonlinear elasticity on Riemannian manifold and its application to general surface development

○Yuto Horikawa[1], Ryuichi Tarumi[2], Yoji Shibutani[1] （1.Dept. of Mechanical Engineering, Osaka Univ., Japan, 2.Grad. Sch. of Engineering Science, Osaka Univ., Japan）

[P2-04] The challenge of achieving quantitative phase field models for microstructure evolution in irradiated solids - the case of voids

○Anter El-Azab （Purdue University, United States of America）

[P2-05] A Molecular-Dynamics Study of Surface Tension: From Alloy Droplets to Bubbles in Molten Alloy

○Xiangming Ma, Hongtao Liang, Yang Yang （East China Normal Univercity, China）

Poster Session | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[PO-B2] Poster Session 2
5:45 PM - 8:00 PM Poster Hall

[P2-06] Effects of rhenium on the mechanical behavior of irradiated tungsten: a molecular dynamics study using neural-network potential

○Ryo KOBAYASHI （Nagoya Institute of Technology (NITech), Japan）

[P2-07] Diffusion behavior and temperature dependence of hydrogen in tungsten and molybdenum under isotropic strain state

○QuanFu Han[1], Yue-Lin Liu[2], Ying Zhang[1], Guang-Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

[P2-08] **Diffusion of Point Defects on Tungsten Surface**

Jiannan Hao[1], ○Shuo Jin[1], Haixuan Xu[2], Xiaolin Shu[1], Guanghong Lu[1] （1.School of Physics and Nuclear Energy Engineering, Beihang University, China, 2.Department of Material Science and Engineering, The University of Tennessee, Knoxville, United States of America）

[P2-09] Influence of anisotropic strain and temperature on hydrogen dissolution in tungsten

○Ying zhang[1], Quan Fu Han[1], Yue lin Liu[2], Guang Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

[P2-10] Screw dislocation-interstitial solute coevolution in W-O alloys using atomistically-informed kinetic Monte Carlo simulations

○Yue Zhao[1], Lucile Dezerald[3], Jaime Marian[1,2] （1.Dept. of Materials Science and Engineering, University of California, Los Angeles, United States of America, 2.Dept. of Mechanical Engineering, University of California, Los Angeles, United States of America, 3.Institut Jean Lamour, University of Lorraine, France）

[P2-11] Kinetic Monte-Carlo Simulations of Radiation Damage in W(Re,Os) Alloys

○Matthew James Lloyd[1,2], David Armstrong[1], Enrique Martinez Saez[3], Duc Nguyen-Manh[2] （1.Department of Materials, University of Oxford, UK, 2.Culham Centre for Fusion Energy, UK, 3.Los Alamos National Laboratory, United States of America）

[P2-13] **Dynamics of Magnetism in Neutron Irradiated Iron-Chromium Steels**

○Jacob B. J. Chapman, Pui-Wai Ma, Sergei L. Dudarev （Culham Centre for Fusion Energy (CCFE), UK）

[P2-14] **Atomistic insights into the grain boundaries interaction with radiation-induced point defects in bcc Fe-Cr alloys**

○Marcin Roland Zemla, Jan Stanislaw Wrobel, Tomasz Wejrzanowski （Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland）

[P2-15] Production and Process of Cascade Development in Irradiated Pure α-Zr from Molecular Dynamics Simulations

○Rongjian Pan[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Bang Wen[1], Wen He[1], Y.R. Ovcharenko[3], D.O.

Kharchenko[3] （1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine）

[P2-16] Microstructure evolution of cascade annealing in irradiated pure α-Zr from molecular dynamics simulations

○Bang Wen[1], Rongjian Pan[1], Wei Zhang[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3] （1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine）

Poster Session | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[PO-C2] Poster Session 2
5:45 PM - 8:00 PM Poster Hall

[P2-18] **Prediction of Biaxial Tensile Deformation Behavior of Aluminum Alloy Sheets using Crystal Plasticity Finite Element Method and Machine Learning**

○Kota Koenuma[1], Akinori Yamanaka[1], Ikumu Watanabe[2], Toshihiko Kuwabara[1] （1.Tokyo University of Agriculture and Technology, Japan, 2.National Institute of Materials Science, Japan）

[P2-19] MobiDiC: A 3-D Dislocation Dynamics Simulation

○Ronan MADEC[1], Laurent COLOMBET[1], Ladislas KUBIN[2] （1.CEA, DAM, DIF, France, 2.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay, France）

[P2-20] Temperature dependence of fatigue crack growth in Ti-6Al-4V

○Bhargavi Rani Anne, Masaki Tanka, Tatsuya Morikawa （Dept. of Materials Science and Engineering, Kyushu University, Japan）

[P2-21] Parametric model of discrete dislocation dynamics based on mathematical theory of moving curves

○Miroslav Kolar, Jan Kratochvíl, Petr Pauš, Michal Beneš （Czech Technical University in Prague, Czech Republic）

[P2-22] On Visualization of Multiscale Information Transfer/Exchange Processes via FTMP-based Duality Diagram Representation Scheme

○Takuya Takagi, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P2-23] **Rotational Field Evolutions based on Field Theory of Multiscale Plasticity (FTMP)**

○Tadashi Hasebe[1], Yasutaka Matsubara[2] （1.Kobe Univ., Japan, 2.Graduate School of Kobe Univ., Japan）

[P2-24] **A 2D MESOSCALE STUDY OF DISLOCATIONS, CRACKS AND MARTENSITIC PHASE TRANSFORMATIONS**

○Rachel Derby, Michael Budnitzki, Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

[P2-25] Effects of Stress Distribution on the Plastic Deformation of Metallic Glasses under Different Geometries

○Chih-Jen Yeh[1], Hsuan-Teh Hu[1], Chang-Wei Huang[2], Yu-Chieh Lo[3] （1.National Cheng Kung University, Taiwan, 2.Chung Yuan Christian University, Taiwan, 3.National Chiao Tung University, Taiwan）

Poster Session | D. Data-Driven and Physics-Informed Materials Discovery and Design

[PO-D2] Poster Session 2
5:45 PM - 8:00 PM Poster Hall

[P2-26] Generalized nano-thermodynamic model for predicting size-dependent surface segregation in multi-metal alloy nanoparticles from smaller particles

○Abhijit Chatterjee （Dept. of Chemical Engg., Indian Institute of Technology Bombay, India）

[P2-27] Development of thermodynamic database of Nd-Fe-B-based permanent magnet alloys

○Jiang Wang, Lei Xu, Kaicheng Yang, Qingrong Yao, Guanghui Rao, Huaiying Zhou （School of Material Science and Engineering, Guilin University of Electronic Technology, China）

[P2-28] Design of proteins and biopolymers: role of directional interactions and of water.

○Valentino Bianco[1], Ivan Coluzza[2] （1.University of Vienna, Austria, 2.CIC biomaGUNE, center for cooperative research in biomaterials, Spain）

[P2-29] Aquatic pollutant removal by adsorption in zeolite structures: An experimental and molecular simulation study

○Mate Erdos[1], Nan Jiang[2], Sebastian G. J. Heijman[2], Othonas A. Moultos[1] （1.Process &Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology,

Netherlands, 2.Department of Water Management, Faculty of Civil Engineering and Geosciences, Delft University of Technology, Netherlands）

[P2-30] Optimizing elastic moduli of the silicate glasses through high-throughput atomistic modeling and machine learning techniques

Yong-Jie Hu[1], Ge Zhao[2], Tyler Del Rose[1], ○Liang Qi[1] （1.Dept. of Materials Science and Engineering, University of Michigan, United States of America, 2.Department of Statistics, Pennsylvania State University, United States of America）

[P2-31] High pressure phase transition and structural stability of transition metal compounds

○Fanyan Meng[1], Wandong Xing[1,2], Rong Yu[2] （1.Dept. of Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-32] Development of artificial neural network model for prediction of electronic density of states in atomistic systems

○Atsushi Kubo, Yoshitaka Umeno （Institute of Industrial Science, the University of Tokyo, Japan）

[P2-33] Development of First-principles Platform Technology for Energy Research

○Kanghoon Yim[1], Chan-Woo Lee[1], Jehyun Lee[1], Incheol Jeong[2], Yong Youn[3], Seungwu Han[3] （1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Dept. of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science &Technology, Korea, 3.Seoul National University, Korea）

Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E2] Poster Session 2
5:45 PM - 8:00 PM Poster Hall

[P2-34] Dynamics of a solidification front made by invasion of fluid with a different temperature

○So Kitsunezaki, Chika Yamanaka （Nara Women's Univ., Japan）

[P2-35] Strengthening through solid solution in $W_{1-x}Ta_xB$ system

○lijuan liu[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-36] Desiccation crack patterns based on phase-field modeling and their statistical properties

○Shin-ichi Ito[1], Satoshi Yukawa[2] （1.The Univ. of Tokyo, Japan, 2.Osaka Univ., Japan）

[P2-37] Ce-terminated (111) surface of CeO_2

○YaNan Zhao[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-39] **Numerical analysis of elasto-plastic behavior of metallic architectured materials**

○Filip Siska[1], Ivo Dlouhy[1], Jan Cizek[2], Hanus Seiner[3] （1.Institute of Physics of Materials, Czech Academy of Sciences, Czech Republic, 2.Institute of Materials Science and Engineering, Brno University of Technology, Czech Republic, 3.Institute of Thermomechanics, Czech Academy of Sciences, Czech Republic）

[P2-40] Automatic analysis and numerical prediction of flow stress curves for aluminium alloys

○Evgeniya Kabliman, Johannes Kronsteiner, Ana-Helena Kolody （Light Metals Technologies Ranshofen, Center fo Low-Emission Transport, Austrian Institute of Technology, Austria）

[P2-41] Comparison of different alkali activated mortars with hemp fibres response during fracture test by acoustic emission method

Libor Topolar[1], ○Hana Simonova[1], Barbara Kucharczykova[1], Zbynek Kersner[1], Jelena Dragas[2], Ivan Ignjatovic[2], Miroslav Komljenovic[3], Violeta Nikolic[3] （1.Brno University of Technology, Faculty of Civil Engineering, Czech Republic, 2.University of Belgrade, Faculty of Civil Engineering, Serbia, 3.University of Belgrade, Institute for Multidisciplinary Research, Serbia）

Poster Session | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[PO-F2] Poster Session 2
5:45 PM - 8:00 PM Poster Hall

[P2-43] Design of spontaneous formation-based 3D plasmonic optical structure, using multyphysics modeling

○Jihwan Song[1], Inhee Choi[2], Yonghee Shin[3], SoonGweon Hong[5], Younggeun Park[5], Dongchoul Kim[4], Taewook Kang[3], Luke Lee[5] （1.Dept. of Mechanical Engineering, Hanbat National University, Korea, 2.Dept. of Life Science, University of Seoul, Korea, 3.Dept. of Chemical and Biomolecular Engineering, Sogang

University, Korea, 4.Dept. of Mechanical Engineering, Sogang University, Korea, 5.Dept. of Bioengineering and Berkeley Sensor and Actuator Center, University of California, Berkeley, United States of America）

[P2-44] **Characterization of $K_xNa_{1-x}NbO_3$ powders and ceramics prepared by hydrothermal synthesis**

○Jing Yang, Aifen Tian, Xuan Xi, Huiling Du （Dept. of Materials Science and Engineering, Xi An Univ. of Science and Technology, China）

[P2-45] Numerical and experimental investigation of liquid metal dealloying of Cu-Ni alloy in liquid silver.

○Pierre-Antoine Geslin[1,2,3], Takumi Suga[2], Takeshi Wada[2], Hidemi Kato[2] （1.INSA Lyon/CNRS, France, 2.Institute for Materials Research, Tohoku University, Japan, 3.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan）

[P2-46] **Application of DLVO theory to predict dispersion stability of ZrO_2 submicron particles in electrolyte solutions**

○Ming-Hong Chiueh, Tien-Jung Huang （Industrial Technology Research Institute, Taiwan）

[P2-47] Multi-GPU large-scale phase-field lattice Boltzmann simulation of dendrite growth with thermal-solutal convection

○Shinji Sakane[1], Tomohiro Takaki[1], Munekazu Ohno[2], Yasushi Shibuta[3], Takayuki Aoki[4] （1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.The University of Tokyo, Japan, 4.Tokyo Institute of Technology, Japan）

[P2-48] Stress analysis of 4H-SiC power devices via FEM and Raman spectroscopy

○Hiroki Sakakima[1], Asuka Hatano[1], Akihiro Goryu[2], Kenji Hirohata[2], Satoshi Izumi[1] （1.The Univ. of Tokyo, Japan, 2.Toshiba, Japan）

[P2-49] A Functionally Graded Multi-Phase Micromechanical Model for Carbon Nanotube - Polymer Composites

○Vahidullah Tac[1,2], Ercan Gurses[1] （1.Middle East Technical University, Turkey, 2.Turkish Aerospace Industries, Turkey）

[P2-50] **Atomic surface treatment of copper nanowires by electron beam irradiation simulated by first principle calculation**

○Shih Kuang Lee （National Chiao Tung University, Taiwan）

[P2-51] Molecular-Dynamic Simulation of Rapid Solidification of Dipolar Molecular Crystal from Its Melt

○Xianqi Xu, Yang Yang （East China Normal University, China）

[P2-52] Intrinsic Analysis of Structural Order Parameter at Equilibrium Crystal-Melt Interfaces

○Wenliang Lu, Hongtao Liang, Yang Yang （EAST CHINA NORMAL UNIVERSITY, China）

[P2-53] Multiscale Modelling of Indirect-to-Direct Band Gap Transition in Silicon Nanosheets

○Byung-Hyun Kim[1], Chan-Woo Lee[1], Mina Park[2], Gyubong Kim[2], Kersti Hermansson[3], Peter Broqvist[3], Heon-Jin Choi[4], Kwang-Ryeol Lee[2] （1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Computational Science Research Center, Korea Institute of Science and Technology, Korea, 3.Dept. of Chemistry-Ångström Laboratory, Uppsala University, Sweden, 4.Dept. of Materials Science and Engineering, Yonsei University, Korea）

Poster Session | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[PO-G2] Poster Session 2
5:45 PM - 8:00 PM Poster Hall

[P2-54] **Component-wise Effect of Incompatibility Tensor on Misorientation Development in Lath Block Structure Model based on FTMP**

○Yuta Amano, Tadashi Hasebe, Yasutaka Matsubara （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P2-55] Construction of virtual ITZ specimens using extended stochastic optimization and evaluation of their permeability

○Se-Yun Kim, Tong-Seok Han （Dept. of Civil and Environmental Engineering, Yonsei Univ., Korea）

[P2-56] Estimation for probabilistic distribution of material response according to microstructural characteristics

○JI-SU KIM, Tong-Seok Han （Yonsei Univ., Korea）

[P2-57] **Hypervelocity impact and shock behavior of pillared graphene foams**

○Stefano Signetti, Seunghwa Ryu （Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea）

Poster Session | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[PO-H2] Poster Session 2
5:45 PM - 8:00 PM Poster Hall

[P2-58] Studying the kinetics of a self-propelled cruiser in 2D granular media under gravity
○Guo-jie Jason Gao （Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan）

[P2-59] A Discrete Tetris model showing two flow regimes for hard particles exiting a hopper with an adjustable obstacle
○Tomoya Yasuno[1,2], Guo-jie Jason Gao[1] （1.Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan, 2.Dept. of Complex Systems Science, Nagoya Univ., Japan）

[P2-60] Effect of water molecules on polymer chain motion in dense chain ensembles of nafion membrane
○Isamu Riku, Ryoma Oka, Koji Mimura （Osaka Prefecture Univ., Japan）

[P2-61] A Coarse-Grained Model for Competitive Adsorption on the Surface of Inorganic Nanomaterials
○Stefano Poggio[1], Hender Lopez[2], David Power[1], Vladimir Lobaskin[1] （1.School of Physics, University College Dublin, Ireland, 2.Institute Laue-Langevin, Grenoble, France）

[P2-62] Molecular Dynamics of Inorganic and Organic Interfaces with Force-Field Parameters Based on DFT Simulations
○Kosuke Ohata, Hiroya Nitta, Kenta Chaki, Taku Ozawa （JSOL Corporation, Japan）

[P2-63] **Molecular dynamics screening for developing compounds of electrolytes with high performance in lithium ion batteries**
○Yoshihiro Takai[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] （1.Graduate school of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan）

[P2-64] Molecular dynamics study on transmission mechanism of torsional deformation in cellulose nanofibers with hierarchical structure
○Kentaro Takada[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] （1.Graduate School of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan）

[P2-65] Bubble dynamics of foam flow around an obstacle
○Antti Puisto, Juha Koivisto, Leevi Viitanen, Mikko J Alava （Aalto University, Department of Applied Physics, Finland）

[P2-66] Shape Deformation and Mechanical Relationship of Ionic Droplet Under An Electric Field
Bo-Yu Shih[1], ○Wei-Chun Lin[1], Alice Hu[2], Hsuan-Teh Hu[1], Yu-Chieh Lo[3] （1.Department of Civil Engineering,National Cheng Kung University, Taiwan, 2.Department of Mechanical and Biomedical Engineering, City University of Hong Kong, Hong Kong, 3.Department of Materials Science and Engineering, National Chiao Tung University, Taiwan）

[P2-67] Multiscale modeling of surface functionalized graphene/polymer nanocomposites: insight into the effect of covalent grafting
○Jeong-ha Lee[1], Seunghwa Yang[2] （1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea）

[P2-68] Durability analysis on the environmental aging of epoxybased nanocomposite
○Sunyong Kwon[1], Man Young Lee[2], Seunghwa Yang[3] （1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Agency for Defense Development, Korea, 3.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea）

Poster Session | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[PO-I2] Poster Session 2
5:45 PM - 8:00 PM Poster Hall

[P2-69] **Topological evolution of the microstructures of thin films during grain growth**
○Ahu Oencue[1], Thorsten Halle[2], Dana Zoellner[3] （1.Institute of Experimental Physics, Otto-von-Guericke University Magdeburg, Germany, 2.Institute of Materials and Joining Technology, Otto-von-Guericke University Magdeburg, Germany, 3.B CUBE Center for Molecular Bioengineering, TU Dresden, Germany）

[P2-70] Molecular dynamics simulations of phase transformations in nanocrystalline NiTi shape-memory alloys
○Won-Seok Ko （University of Ulsan, 93 Daehak-ro, Nam-gu, Ulsan, 44610, Korea）

[P2-71] An attempt to connect migration of grain boundaries to their atomic structures with help of Molecular Dynamics
Zakaria El Omari, ○Sylvain Queyreau, Charlie Kahloun,

Brigitte Bacroix（Universite Paris XIII, Sorbonne Paris Cite, Laboratoire des Sciences des Procedes et des Materiaux, LSPM UPR 3407, France）

[P2-72] Disconnection interaction in Cu grain boundaries

○Christian Brandl（Karlsruhe Institute of Technology, Germany）

[P2-73] Phase-field Approach to Thermo-mechanical Behavior of Through-silicon Vias

Wooju Lee, ○jaekeun yoon, Dongchoul Kim（Sogang Univ., Korea）

[P2-74] **Grain-Growth in Nanocrystalline Metals under Ion Irradiation: A Thermal Spike Model**

○Djamel Kaoumi[1], Robert Birtcher[2], Arthur Motta[3] （1.North Carolina State University, United States of America, 2.Argonne National Laboratory, United States of America, 3.Penn State University, United States of America）

Poster Session | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[PO-N2] Poster Session 2
5:45 PM - 8:00 PM Poster Hall

[P2-75] **Why the structure-property relationship in metallic glasses should be established beyond short-range order: Insight from potential energy landscape**

○Dan Wei[1,2], Yunjiang Wang[1,2], Lanhong Dai[1,2] （1.University of Chinese Academy of Sciences, China, 2.Institute of Mechanics, Chinese Academy of Sciences, China）

[P2-76] Vacancy segregation analysis near grain boundaries in metallic systems by long-time atomistic simulations

○Shotaro Hara（Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan）

[P2-77] **EXPERIMENTAL AND DENSITY FUNCTIONAL THEORY STUDIES OF PRECIPITATE INTERFACES IN ALUMINIUM ALLOYS, WITH FOCUS ON β'' & β**

○Haris Rudianto, Deni Hariadi, Andriansyah Andriansyah （Gunadarma University, Indonesia）

Poster Session | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[PO-O2] Poster Session 2
5:45 PM - 8:00 PM Poster Hall

[P2-78] Adsorption of Volatile Organic Compounds (VOCs) on Silicene by Density Functional Theory Calculations

○Thi Viet Bac Phung[1], Trong Lam Pham[1], Van An Dinh[1,2] （1.Nanotechnology Program, Vietnam Japan University - Vietnam National University, Viet Nam, 2.Center for Atomic and Molecular Technologies, Graduate School of Engineering, Osaka University, Japan）

[P2-79] Atomistic insights into defect formation mechanism in single crystal SiC based on molecular dynamics simulation

○Kenji Nishimura[1], Koji Miyake[1], Ken-ichi Saitoh[2] （1.AIST, Japan, 2.Kansai Univ., Japan）

[P2-80] **Potential cathode material Na_xVOPO_4 for rechargeable Sodium - ion batteries: DFT investigation**

○Duc Huu Luong[1], An Van Dinh[1,2], Yoshitada Morikawa[3], Yoji Shibutani[2,1]（1.Nano Technology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan, 3.Department of Precision Science and Technology, Graduate School of Engineering, Osaka University, Japan）

[P2-81] **Two-dimensional Na_xSiS as a promising anode material for rechargeable Sodium-based batteries: Ab initio material design.**

Thi Dung Pham[1], ○Van An Dinh[1,2], Kazunori Sato[3], Yoji Shibutani[1,2]（1.Nanotechnology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan, 3.Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, Japan）

[P2-82] Modelling and analysis of SiO2 interfaces of non-firing solids

○Tomohiro Sato[1], Ken-ichi Saitoh[1], Masayoshi Fuji[2], Chika Yamashita Takai[2], Hadi Razavi[2], Masanori Takuma[1], Yoshimasa Takahashi[1]（1.Dept. of Mechanical Engineering, Kansai Univ., Japan, 2.Advanced Ceramics Reserch Center, Nagoya Institute of Technology, Japan）

Thu. Nov 1, 2018

Room1

Plenary Talk | Plenary Talk

[PL5] Plenary Talk 5
Chair: Dongsheng Xu(IMR-CAS, China)
8:30 AM - 9:20 AM Room1

[PL5] Plenary Talk 5
○Rui Yang （Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China）

Thu. Nov 1, 2018

Room1

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C9] Symposium C-9

Chair: Vasily Bulatov(Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, United States of America)
9:45 AM - 11:00 AM Room1

[SY-C9] Interstitial Shuffling Mechanism for Solute-Induced Embrittlement of Titanium
○Daryl C. Chrzan （Department of Materials Science and Engineering, University of California, Berkeley, United States of America）

[SY-C9] Screw dislocation mediated solution strengthening of substitutional α-Ti alloys - First principles investigation
○Piotr Kwasniak （Warsaw University of Technology, Poland）

[SY-C9] Microstructural effects on strain rate sensitivity in dual-phase titanium alloys
○Sana Waheed[1], Zebang Zheng[2], Daniel S. Balint[1], Fionn P. E. Dunne[2] （1.Dept. of Mechanical Engineering, Imperial College London , UK, 2.Dept. of Materials, Imperial College London , UK）

[SY-C9] **Understanding thermal alleviation in cold dwell fatigue in titanium alloys using crystal plasticity model**
○Zebang Zheng[1], Adam Stapleton[2], Kate Fox[2], Fionn P.E. Dunne[1] （1.Dept. of Materials, Imperial College London, UK, 2.Rolls-Royce plc, UK）

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C10] Symposium C-10

Chair: Tomohito Tsuru(Japan Atomic Energy Agency, Japan)
11:15 AM - 12:15 PM Room1

[SY-C10] First Principles Calculations of Dislocations in Model Engineering Alloys (Ni, Ni3Al, hcp-Ti, and a Refractory Metal BCC-HEA)
○Christopher Woodward （Air Force Research Laboratory, United States of America）

[SY-C10] **Hybrid QM/MM study of dislocation glide in tungsten in the presence of plasma components**
○Petr Grigorev[1], Tom Swinburne[2], James Kermode[1] （1.Warwick Centre for Predictive Modelling, UK, 2.Los Alamos National Laboratory, United States of America）

[SY-C10] First-principles Calculations of Deformation Twins in Hexagonal Titanium Alloys
○Daisuke Matsunaka, Ryosuke Amano （Dept. of Mechanical Engineering, Shinshu Univ., Japan）

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C11] Symposium C-11

Chair: Nikhil Chandra Admal(University of California Los Angeles, United States of America)
2:00 PM - 3:30 PM Room1

[SY-C11] A Multi-Scale Dislocation Language - Data Mining, Statistical Analysis, and Steps Towards a Community-Driven Data Base
○Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

[SY-C11] **The effect of dislocation character on dislocation line tension in bcc tungsten and its impact on kink-pair enthalpy**
○David Cereceda[1], Vasily Bulatov[3], Jaime Marian[2] （1.Dept. of Mechanical Engineering, Villanova University, United States of America, 2.Department of Materials Science and Engineering, University of California Los Angeles, United States of America, 3.Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, United States of America）

[SY-C11] Atomistic modeling of thermally activated plasticity in UO_2
Aurélien Soulié[1], ○Jean-Paul Crocombette[1], Antoine Kraych[1], Frédérico Garrido[2], Gaël Sattonnay[2], Emmanuel Clouet[1] （1.CEA Saclay, SRMP, France, 2.CSNSM, CNRS-IN2P3-Université Paris-Sud, France）

[SY-C11] **FTMP-based Simulations and Evaluation of Geometrically-Necessary Boundaries (GNBs) of Dislocation**
○Shiro Ihara, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[SY-C11] Improved phase field model of dislocation intersections
○Songlin Zheng[1], Yong Ni[2] （1.China Academy of Engineering Physics, China, 2.University of Science and Technology of China, China）

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C12] Symposium C-12

Chair: Irene Beyerlein(University of California at Santa Barbara, United States of America)
4:00 PM - 5:15 PM Room1

[SY-C12] Modeling the interaction between martensitic phase transformations and dislocation dynamics
○Rachel Derby, Michael Budnitzki, Stefan Sandfeld (TU Bergakademie Freiberg, Germany)

[SY-C12] The effect of microscopic slip deformation on the yield stress in dispersion hardened alloys analyzed by using crystal plasticity FEM
○Yelm Okuyama[1], Masaki Tanaka[1], Tatsuya Morikawa[1], Tetsuya Ohashi[2] (1.Dept. of Materials Science and Engineering, Kyushu University, Japan, 2.Dept. of Engineering, Kitami Institute of Technology, Japan)

[SY-C12] Deformation Behaviour for Two-Phase Composites under Large Deformations using Micromechanical Analysis
○Srihari Dodla (Madanapalle Institute of Technology (MITS) Madanapalle, India)

[SY-C12] Dislocation dynamics simulation of FCC single crystals in high strain rate deformation
○Ronan MADEC (CEA, DAM, DIF, France)

[SY-C12] Comparison of two methods to cross-slip modeling by means of mathematical theory of moving curves
○Miroslav Kolar, Jan Kratochvíl, Petr Pauš, Michal Beneš (Czech Technical University in Prague, Czech Republic)

Room2

Symposium | E. Deformation and Fracture Mechanism of Materials
[SY-E9] Symposium E-9
Chairs: Andrej Ostapovec(Institute of Physics of Materials ASCR, Czech Republic), Yujie Wei(Chinese Academy of Sciences, China)
9:45 AM - 11:00 AM Room2

[SY-E9] **The motion of a single dislocation from molecular dynamics simulations and its physical interpretation**
○Yujie Wei[1,2], Shenyou Peng[1,2] (1.Chinese Academy of Sciences, China, 2.School of Engineering Sciences, University of Chinese Academy of Sciences, China)

[SY-E9] **Atomistic study on the super-elasticity of single crystal bulk NiTi shape memory alloy under adiabatic condition**
○Bing Wang[1], Guozheng Kang[1], Qianhua Kan[1], Wenping Wu[2], Kun Zhou[3], Chao Yu[1] (1.School of Mechanics and

Engineering, Southwest Jiaotong University, China, 2.School of Civil Engineering, Wuhan University, China, 3.School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapore)

[SY-E9] Atomistic Modelling of Fracture with Non-Linear Elastic Boundary Conditions
○Punit Patel, James Kermode (University of Warwick, UK)

[SY-E9] **Atomistic simulation of the deformation and crack nucleation mechanisms in titanium alloys**
○Dongsheng Xu (Institute of Metal Research, Chinese Academy of Sciences, China)

Symposium | E. Deformation and Fracture Mechanism of Materials
[SY-E10] Symposium E-10
Chairs: Irene Beyerlein(University of California at Santa Barbara, USA), Dongsheng Xu(Institute of Metal Research, CAS, China)
11:15 AM - 12:30 PM Room2

[SY-E10] Study of atomic trajectories during twinning transformation in magnesium
○Andrej Ostapovec[1], Tomáš Káňa[1], Václav Paidar[2] (1.Institute of Physics of Materials ASCR, Czech Republic, 2.Institute of Physics ASCR, Czech Republic)

[SY-E10] **Understanding nanocontact plasticity through massive MD simulations**
○Jorge Alcala[1], Javier Varillas[2,1], Jordi Torner[2], Jan Očenášek[1] (1.Universidad Politecnica de Catalunya, Spain, 2.New Technologies Research Centre, Czech Republic)

[SY-E10] Atomistically informed mesoscale modeling of fracture
○Hamad ul Hassan[1], Johannes Möller[2,3], Erik Bitzek[2], Alexander Hartmaier1[1], Rebecca Janisch[1] (1.ICAMS, Ruhr-Universität Bochum, Germany, 2.Friedrich-Alexander Universität Erlangen-Nürnberg , Germany, 3.Fraunhofer Institut für Werkstoffmechanik, Freiburg, Germany)

[SY-E10] **Lattice Distortion Effect on Cross-Slip in High Entropy Alloys and Lennard-Jones Systems for Face-Centered Cubic**
○Chao-Chun Yen[1], Junping Du[2,3], Jia-An Lin[4], Yu-Chieh Lo[4] (1.National Tsing Hua University, Taiwan, 2.Kyoto University, Japan, 3.Osaka University, Japan, 4.National Chiao Tung University, Taiwan)

[SY-E10] **Atomic structure of gamma/alpha2 interface and**

its influence on plastic deformation of lamellar TiAl alloys

○Hao Wang[1], Aidong Tu[1], Yanxia Liu[2], Dongsheng Xu[1], Rui Yang[1]　(1.Institute of Metal Research, CAS, China, 2.Dept. of Physics, Liaoning University, China)

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E11] Symposium E-11
Chairs: Xiaoyu Yang(Computer network information center, CAS, China), Denise Reimann(ICAMS, Ruhr-Universität Bochum, Germany)
2:00 PM - 3:30 PM　Room2

[SY-E11] Thermodynamically consistent directional distortional hardening of wrought Mg alloys: experimental investigation and constitutive modeling

○Baodong Shi[1], Yan Peng[1], Chong Yang[1], Jianliang Sun[1], Fusheng Pan[2]　(1.NECSR, School of Mechanical Engineering, Yanshan Univ., China, 2.NERC-MA, Chongqing Univ., China)

[SY-E11] **A computational infrastructure for multiscale materials simulation**

○Xiaoyu Yang　(Computer network information center of the Chinese Academy of Sciences, China)

[SY-E11] Using machine learning methods to homogenize damage from micro- to macroscale

Denise Reimann[1], Hamad ul Hassan[1], Tobias Glasmachers[2], ○Alexander Hartmaier[1]　(1.ICAMS, Ruhr-Universität Bochum, Germany, 2.Institut für Neuroinformatik, Ruhr-Universität Bochum, Germany)

[SY-E11] Graph theory analysis of rich fiber-scale data yields very fast simulations of damage evolution in composites

jerry quek[2], ○brian n cox[1]　(1.arachne consulting, United States of America, 2.IHPC, Singapore)

[SY-E11] A deep learning-based constitutive model for finite element analysis

Fariborz Ghavamian[1], ○Angelo Simone[2,1]　(1.Delft University of Technology, Netherlands, 2.University of Padova, Italy)

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E12] Symposium E-12
Chairs: Baodong Shi(NECSR, School of Mechanical Engineering, Yanshan Univ., China), Ligang Zhang(Central South University, China)
4:00 PM - 5:00 PM　Room2

[SY-E12] **Diffusivities and atomic mobilities in bcc Ti-Mo-**

Nb-Ta-Zr alloys

○Weimin Bai[1], Guanglong Xu[2], Libin Liu[1], Ligang Zhang[1]　(1.School of Materials Science and Engineering, Central South Univ., China, 2.Tech Inst. for Advanced Materials &School of Materials Science and Engineering, Nanjing Tech Univ., China)

[SY-E12] Design of Ti-alloy by Integrating High Throughput Experiments and Calculations

○Ligang Zhang, Libin Liu, Di Wu　(Central South University, China)

[SY-E12] Simulation of Plasticity in Amorphous Solids

○Shingo Urata[1], Takahiro Murashima[2], Shaofan Li[3]　(1.Innovative Technology Research Center, Asahi Glass Co., Ltd (AGC)., Japan, 2.Dept. of Physics, Tohoku University, Japan, 3.Dept. of Civil and Environmetal Engineering, Univ. of California Berkeley, United States of America)

[SY-E12] Computational generation of the yield surfaces using stress based loading

○mayank chouksey, Sumit Basu　(Indian Institute of Technology, Kanpur, India)

Room3

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F9] Symposium F-9
Chair: Ernst Kozeschnik(Institute of Materials Science and Technology, TU Wien, Austria)
9:45 AM - 11:00 AM　Room3

[SY-F9] Programmable Materials - tuning effective materials response

○Peter Gumbsch[1,2], Chris Eberl[1,3], Claudio Findeisen[1,2], Alexander Butz[1], Jan Pagenkopf[1,2]　(1.Fraunhofer IWM, Germany, 2.Karlsruhe Institute of Technology (KIT), Germany, 3.Albert-Ludwigs-Universität Freiburg, Germany)

[SY-F9] **Equilibrium crystal shape of GaAs by ab-initio thermodynamics**

In Won Yeu[1,2], Gyuseung Han[1,2], Cheol Seong Hwang[2], ○Jung-hae Choi[1]　(1.Center for Electronic Materials, Korea Institute of Science and Technology, Korea, 2.Department of Materials Science and Engineering, and Inter-university Semiconductor Research Center, Seoul National University, Korea)

[SY-F9] Elastic field of lattice defects in low-dimensional nano-carbon materials

○Xiao-Wen LEI[1], Akihiro NAKATANI[2], Tomoya TANIGUCHI[1] （1.Dept. of Mechanical Engineering, Univ. of Fukui, Japan, 2.Dept. of Adaptive Machine Systems, Osaka Univ. , Japan）

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F10] Symposium F-10

Chair: Ricardo Lebensohn(Los Alamos National Laboratory, United States of America)
11:15 AM - 12:30 PM Room3

[SY-F10] **Data Analytics for Mining Process-Structure-Property Linkages for Hierarchical Materials**
○Surya Raju Kalidindi （Georgia Tech, United States of America）

[SY-F10] Maximization of strengthening effect of microscopic morphology in duplex elastoplastic solids
○Ikumu Watanabe[1], Gaku Nakamura[2], Kohei Yuge[2] （1.National Institute for Materials Science, Japan, 2.Seikei University, Japan）

[SY-F10] Assessment of formability limit diagram prediction by crystal plasticity finite element method
○Duancheng Ma （Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria）

[SY-F10] Analysis of gradient microstructures using crystal plasticity
○Balaji Selvarajou, Jerry Quek Siu Sin （IHPC, Singapore, Singapore）

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F11] Symposium F-11

Chair: Peter Gumbsch(Fraunhofer IWM, Germany)
2:00 PM - 3:30 PM Room3

[SY-F11] **Mesoscale plasticity models of polycrystalline materials for efficient computation of microstructure/property relationships**
○Ricardo Lebensohn （Los Alamos National Laboratory, United States of America）

[SY-F11] Development of a new consistent discrete Green operator for FFT-based methods to solve heterogeneous problems with eigenstrains
○Komlavi Senyo ELOH[1,2,3], Alain JACQUES[2,1], Stéphane BERBENNI[1,3] （1.University of Lorraine, France, 2.Institut Jean Lamour, France, 3.Laboratoire d'etudes de microstructures et de mécanique des matériaux, France）

[SY-F11] Efficient FFT-based Homogenisation without Linear Reference Medium
○Till Junge （EPFL, Mech. Engineering, Multiscale Mechanics Modeling, Switzerland）

[SY-F11] Multiscale modelling of the effective viscoplastic behavior of constituents of the mantle transition zone (Mg_2SiO_4 wadsleyite and ringwoodite): bridging atomic and polycrystal scales
Olivier Castelnau[1], Katell Derrien[1], Sebastian Ritterbex[2], Philippe Carrez[2], ○Patrick Cordier[2] （1.Process and Engineering in Mechanics and Materials, CNRS/ENSAM/CNAM, Paris, France, 2.Unité Matériaux et Transformations, CNRS / Univ. Lille, Lille, France）

[SY-F11] Scalable and Directionally-Sensitive Three-Dimensional Quantifying of Orientation and Dislocation Density Gradients in Crystal Plasticity Computer Simulations
○Markus Kuehbach, Franz Roters （Max-Planck-Institut fur Eisenforschung GmbH, Germany）

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F12] Symposium F-12

Chair: Yasushi Shibuta(The University of Tokyo, Japan)
4:00 PM - 5:30 PM Room3

[SY-F12] Microstructure formation in large-scale molecular dynamics simulation
○Yasushi Shibuta[1], Shin Okita[1], Eisuke Miyoshi[2], Shinji Sakane[2], Tomohiro Takaki[2], Munekazu Ohno[3] （1.The University of Tokyo, Japan, 2.Kyoto Institute of Technology, Japan, 3.Hokkaido University, Japan）

[SY-F12] Directed assembly of structured nanoparticles through rapid micromixing
○Arash Nikoubashman[1], Nannan Li[2], Athanassios Z. Panagiotopoulos[2] （1.Johannes Gutenberg University of Mainz, Germany, 2.Princeton University, United States of America）

[SY-F12] Various interfaces related to twinning in hexagonal metals
○Vaclav Paidar[1], Andriy Ostapovets[2] （1.Institute of Physics AS CR Prague, Czech Republic, 2.Institute of Physics of Materials AS CR Brno, Czech Republic）

[SY-F12] Multiscale mean-field modelling of mechanochemical processes in heterogeneous

materials for energy storage

○Mikhail Poluektov[1], Łukasz Figiel[1,2] （1.International Institute for Nanocomposites Manufacturing, WMG, University of Warwick, UK, 2.Warwick Centre for Predictive Modelling, University of Warwick, UK）

[SY-F12] Impact of local symmetry breaking on the physical properties of tetrahedral liquids

○Rui Shi, Hajime Tanaka （University of Tokyo, Japan）

Room4

Symposium | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[SY-G5] Symposium G-5

Chairs: Keonwook Kang(Yonsei University, Korea), Akiyuki Takahashi(Tokyo University of Science, Japan)
9:45 AM - 11:00 AM Room4

[SY-G5] Metallic materials under extreme pressure: Interplay of plasticity and phase transitions

○Nina Gunkelmann[1], Hoang-Thien Luu[1], Diego R. Tramontina[3], Carlos J. Ruestes[3], Yudi Rosandi[4], Herbert M. Urbassek[2] （1.Clausthal University of Technology, Germany, 2.University of Kaiserslautern, Germany, 3.National University of Cuyo, Argentine, 4.University of Padjadjaran, Indonesia）

[SY-G5] Dislocation dynamics modeling of fracture behavior with considering dislocation shielding effect

○Akiyuki Takahashi, Hayato Sugasawa, Masanori Nagura （Tokyo University of Science, Japan）

[SY-G5] Dynamic behaviors of dislocations and grain boundaries induced by phonon scattering in nanoscale

○Soon Kim, Sung Youb Kim （Dept. of Mechanical Engineering, UNIST, Korea）

[SY-G5] Investigation on 1/2<11-1>{112} and 1/2<11-1>{123} mixed dislocations in BCC iron by classical molecular dynamics

○Tomohisa Kumagai[1], Akiyoshi Nomoto[1], Akiyuki Takahashi[2] （1.Central Research Institute of Electric Power Industory, Japan, 2.Tokyo University of Science, Japan）

Symposium | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[SY-G6] Symposium G-6

Chairs: Akiyuki Takahashi(Tokyo University of Science, Japan), Keonwook Kang(Yonsei University, Korea)

11:15 AM - 12:15 PM Room4

[SY-G6] Repulsive Correction in Tersoff Potential for Irradiated Si

○Youhwan Jo, Taeyeon Kim, Byeongchan Lee （Kyung Hee University, Korea）

[SY-G6] Phase-field modeling of microstructural evolution of Fe-Cr-Al system

○Kunok Chang （Kyung Hee Univ., Korea）

[SY-G6] Dissolution kinetics of ejecta in hydrogen at megabar pressure

○Arslan B. Mazitov[1,2], Artem R. Oganov[3,1,4], Alexey V. Yanilkin[1,2] （1.Dukhov Research Institute of Automatics (VNIIA), Moscow, Russian Federation, Russia, 2.Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation, Russia, 3.Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russian Federation, Russia, 4.International Center for Materials Discovery, Northwestern Polytechnical University, Xi'an, China）

[SY-G6] MD simulation study of displacement damage in bulk wurtzite GaN by proton irradiation

○SangHyuk Yoo, Yongwoo Kim, Keonwook Kang （Dept. of Mechanical Engineering, Yonsei Univ., Korea）

Symposium | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[SY-N5] Symposium N-5

Chair: Jutta Rogal(ICAMS Ruhr University Bochum, Germany)
2:00 PM - 3:30 PM Room4

[SY-N5] Understanding the impact of extended defects on the behaviour of C atoms: a multi technique approach

○Christophe Domain[1], charlotte S becquart[2] （1.EDF, France, 2. Univ.Lille, CNRS, INRA, ENSCL, UMR 8207, UMET, Unité Matériaux et Transformations, France）

[SY-N5] Localised on-the-fly Kinetic Monte Carlo

○Johannes Bulin （Fraunhofer-Institut SCAI, Germany）

[SY-N5] A Preconditioning scheme for Minimum Energy Path finding methods

○Stela Makri, James Kermode, Christoph Ortner （University of Warwick, UK）

[SY-N5] Temperature Programmed Molecular Dynamics - Accessing rare events using a combination of finite time sampling and bias potentials

○Abhijit Chatterjee （Dept. of Chemical Engineering, Indian Institute of Technology Bombay, India）

Symposium | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[SY-N6] Symposium N-6

Chair: Chad W Sinclair(Dept. of Materials Engineering, University of British Columbia, Canada)
4:00 PM - 5:30 PM Room4

[SY-N6] **Modelling metals, alloys and cement paste across length and time scales**
○Laurent Karim Beland[1], Roger E Stoller[3], Yuri N Osetsky[3], Tingtao Zhou[2], Katerina Katerina Ioannidou[2], Franz-Josef Ulm[2], Roland Pellenq[2] (1.Queen's University, Canada, 2.Massachusetts Institute of Technology, United States of America, 3.Oak Ridge National Laboratory, United States of America)

[SY-N6] BCA-MD-KMC hybrid simulation for long time helium plasma irradiation inducing fuzzy nanostructure on tungsten
○Atsushi M Ito[1,2], Arimichi Takayama[1], Hiroaki Nakamura[1,3] (1.National Institute for Fusion Science, National Institutes of Natural Sciences, Japan, 2.The Graduate University for Advanced Studies, Japan, 3.Department of Electrical Engineering, Graduate School of Engineering, Nagoya University, Japan)

[SY-N6] Atomistic Modelling of Pipe Diffusion: a Direct Comparison of MD, KMC, aKMC and DMD
Frederic Houlle[1], Jutta Rogal[2], ○Erik Bitzek[1] (1.FAU Erlangen-Nuernberg, Germany, 2.ICAMS Ruhr University Bochum, Germany)

[SY-N6] Strategies for optimal construction of Markov chain representations of atomistic dynamics
○Danny Perez, Thomas Swinburne (Los Alamos National Laboratory, United States of America)

[SY-N6] Simulating the collective diffusion mechanism of amorphous solids at experimentally relevant time scales
○Yunjiang Wang[1,2], Shigenobu Ogata[3] (1.Institute of Mechanics, Chinese Academy of Sciences, China, 2.School of Engineering Science, University of Chinese Academy of Sciences, China, 3.Graduate School of Engineering Science, Osaka University, Japan)

Room5

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K1] Symposium K-1

Chairs: Momoji Kubo(Institute for Materials Research, Tohoku University, Japan), Tomoaki Niiyama(Kanazawa Univ., Japan)
11:15 AM - 12:30 PM Room5

[SY-K1] Supercomputer Post-K Project "Challenge of Basic Science - Exploring Extremes through Multi-Physics and Multi-Scale Simulations"
○Momoji Kubo (Tohoku Univ., Japan)

[SY-K1] Universal avalanche statistics across 16 decades in length: From nanocrystals (and neurons) to earthquakes and stars?
○Karin Dahmen (University of Illinois at Urbana Champaign, United States of America)

[SY-K1] Predicting avalanches and failure: wood and paper
○Mikko Alava, Juha Koivisto, Tero Mäkinen, Leevi Viitanen (Aalto University, Finland)

[SY-K1] System-spanning shear avalanches induced by thermal structural relaxation in metallic glasses
○Tomoaki Niiyama[1], Masato Wakeda[2], Tomotsugu Shimokawa[4], Shigenobu Ogata[3] (1.College of Science and Engineering, Kanazawa Univ., Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan, 3.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 4.Faculty of Mechanical Engineering, Kanazawa University, Japan)

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K2] Symposium K-2

Chairs: Ferenc Kun(University of Debrecen, Hungary), Ian Main(University of Edinburgh, UK)
2:00 PM - 3:30 PM Room5

[SY-K2] Predictability of catastrophic failure in porous media
○Ian Main[1], Ferenc Kun[2], Jeremie Vasseur[3], Andrew Bell[1] (1.University of Edinburgh, UK, 2.University of Debrecen, Hungary, 3.Ludwig Maximilian University, Munich, Germany)

[SY-K2] Deciphering the dynamics of precursors to failure in quasi-brittle solids: an inspiration for understanding the statistics of earthquakes ?
○Laurent Ponson[1], Estelle Berthier[1], Vincent Démery[2] (1.Institut Jean le Rond d'Alembert, CNRS - Sorbonne University, Paris, France, 2.Gulliver, CNRS - ESPCI, Paris, France)

[SY-K2] Avalanche precursors and fracture strength in the

limit of high disorder

○Ferenc Kun[1,2], Viktória Kádár[1] （1.Department of Theoretical Physics, University of Debrecen, Hungary, 2.Institute for Nuclear Research (Atomki), Debrecen, Hungary）

[SY-K2] Jump statistics of epicenters in thermally induced cracking of fiber bundles

○Naoki Yoshioka[1], Ferenc Kun[2], Nobuyasu Ito[1,3] （1.RIKEN Center for Computational Science, Japan, 2.Department of Theoretical Physics, University of Debrecen, Hungary, 3.Department of Applied Physics, Graduate Schoold of Engineering, The University of Tokyo, Japan）

[SY-K2] Time dependent fracture under unloading in a fiber bundle model

○Reka Korei, Ferenc Kun （Department of Theoretical Physics, University of Debrecen, Hungary）

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K3] Symposium K-3

Chairs: Takahiro Hatano(University of Tokyo, Japan), Akio Nakahara(Nihon Univ., Japan)

4:00 PM - 5:30 PM Room5

[SY-K3] Creep of strongly disordered materials: Plasticity, damage and approach to failure

○Michael Zaiser, David Fernandez Castellanos （Inst,. of Materials Simulation, Dept of Materials Science, FAU University of Erlangen-Nuremberg, Germany）

[SY-K3] **Creep rupture and Omori-Utsu law: Fiber bundle model approach**

○Takahiro Hatano[1], Subhadeep Roy[2] （1.University of Tokyo, Japan, 2.Norwegian University of Science and Technology, Norway）

[SY-K3] **Temperature dependent shear friction in metallic glass**

○Akio Ishii[1], Tomoaki Niiyama[2], Takahiro Hatano[3], Tomotsugu Shimokawa[2], Shigenobu Ogata[1] （1.Osaka Univ., Japan, 2.Kanazawa Univ., Japan, 3.Tokyo Univ., Japan）

[SY-K3] Mechanism of controlled crack formation induced by memory effect of clay paste

○Akio Nakahara[1], Rokuya Hayashi[1], Tomoki Hiraoka[1], Yousuke Matsuo[1], So Kitsunezaki[2] （1.Nihon Univ., Japan, 2.Nara Women's University, Japan）

[SY-K3] Effects of Shockwave-Induced Nanobubble Collapse on Precision Polishing : Molecular

Dynamics Study

○yoshimasa aoyama[1], Jingxiang Xu[2], Yuske Ootani[1], Nobuki Ozawa[1], Momoji Kubo[1] （1.Dept. of Materials Science, Tohoku Univ., Japan, 2.Dept. of Mechanical Engineering, Shanghai Ocean Univ., China）

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O9] Symposium O-9

Chairs: Yusuke Ootani(Tohoku University, Japan), Shuichi Uehara(Tohoku University, Japan)

9:45 AM - 11:00 AM Room5

[SY-O9] **Combined experimental and computational study on the superlubricity mechanism of 2D Materials at the microscale**

○Tianbao Ma （Tsinghua University, China）

[SY-O9] Quantum chemistry vs. rheology of some EMIM-based ionic liquids

Szerena Kisztina Ujvari[1,2], Konstantinos Gkagkas[1], ○Andras Vernes[2,3] （1.Advanced Material Research Division, Toyota Motor Europe NV/SA, Technical Center, Hoge Wei 33B, 1930 Zaventem, Belgium, 2.AC2T research GmbH, Viktor-Kaplan-Str. 2/C, 2700 Wiener Neustadt, Austria, 3.Institute of Applied Physics, TU Wien, Wiedner Hauptstr. 8-10/134, 1040 Vienna, Austria）

[SY-O9] Lubrication with a refrigerant : a challenge made possible thanks to fluid/surface chemistry

Stéphane TROMP[1], Laurent JOLY[2], Manuel COBIAN[3], ○Nicolas FILLOT[1] （1.Univ Lyon, INSA-Lyon, , CNRS UMR5259, LaMCoS, F-69621 Villeurbanne, France, 2.Univ Lyon, Universite Claude Bernard Lyon 1, CNRS, Institut Lumiere Matiere, F-69622 Villeurbanne, France, 3.Univ Lyon, Ecole Centrale de Lyon, ENISE, ENTPE, CNRS UMR5513, Laboratory of Tribology and System Dynamics, F-69134 Ecully, France）

[SY-O9] Meso-scale SPH simulation for friction and wear between elastic-plastic solids with various asperities

○Natsuko Nakagawa Sugimura[1,2], Le Van Sang[2], Yuji Mihara[1], Hitoshi Washizu[2] （1.Dept. of Mechanical Engineering, Tokyo City Univ., Japan, 2.Grad. Sch. of Simulation Studies, Univ. of Hyogo,, Japan）

Room6

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A9] Symposium A-9

Chair: Eliot Fried(Okinawa Institute of Science and Technology, Japan)
9:45 AM - 11:00 AM Room6

[SY-A9] Group-theoretical construction for constitutive
equation of the first strain gradient elasticity
○Ryuichi Tarumi[1], Shunsuke Kobayashi[2], Yoji Shibutani[2]
（1.Graduate School of Engineering Science, Osaka
Univ., Japan, 2.Dept. of Mechanical Engineering, Osaka
Univ., Japan）

[SY-A9] Physically based strain gradient plasticity model
for length scale dependent yield strength
○Peter Gudmundson （Department of Solid Mechanics,
KTH Royal Institute of Technology, Sweden）

[SY-A9] **FTMP-based Seamless Description of
Deformation-Fracture Transitions**
○Tadashi Hasebe （Kobe Univ., Japan）

[SY-A9] On the crucial role played by instantaneous and
hidden multifield features
of lattice dynamics in their nonlocal
pseudocontinuum modeling
○Miguel Charlotte （University of Toulouse, Institute
Clement Ader, CNRS -- UMR 5312 INSA/UPS/ISAE-
SupAero/Mines Albi, France）

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A10] Symposium A-10

Chair: Steve Fitzgerald(University of Leeds, UK)
11:15 AM - 12:30 PM Room6

[SY-A10] Interdiffusion and atomic mobilities in fcc Ag-
Mg, Ag-Mn and Ag-Mg-Mn alloy
○Qianhui Min[1], Yuling Liu[1], Yong Du[1], Huixin Liu[1], Li
Chen[1], Biao Hu[3], Changfa Du[2], Zhoushun Zheng[2]
（1.Powder Metallurgy Research Institute,Central
South University, China, 2.School of mathematics and
statistics,Central South University, China, 3.School of
Material Science and Engineering, Anhui University Of
Science And Technology, China）

[SY-A10] **Stacking and Multilayered Nature of Martensite
in Copper Based Shape Memory Alloys**
○Osman ADIGUZEL （Firat University , Turkey）

[SY-A10] Mesoscale understanding of ionic conduction in
yttria stabilized zirconia
○Abhijit Chatterjee （Dept. of Chemical Engineering,
Indian Institute of Technology Bombay, India）

[SY-A10] cancellation

[SY-A10] Accelerating stochastic simulations with path
integrals
○Steve Fitzgerald （University of Leeds, UK）

Room7

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I9] Symposium I-9

Chairs: Yuri Mishin(George Mason University, United States of
America), Yang Xiang(Hong Kong University of Science and
Technology, Hong Kong)
9:45 AM - 11:00 AM Room7

[SY-I9] Grain Boundary Microstates Under Irradiation: A
Moment in Time?
○Mitra L Taheri （Drexel University, Department of
Materials Science &Engineering, United States of
America）

[SY-I9] The Role of Grain Boundaries under Long-Time
Radiation
○Jing Luo[1], Yichao Zhu[1], Xu Guo[1], Yang Xiang[3], Stephen
Jonathan Chapman[2] （1.Dalian University of Technology,
China, 2.Mathematical Institute, University of Oxford, UK,
3.Department of Mathematics, The Hong Kong University
of Science and Technology, Hong Kong）

[SY-I9] Quantifying point defect fluxes to interfaces and
the role of interface structure
○Shen J Dillon （University of Illinois , United States of
America）

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I10] Symposium I-10

Chair: Saryu Fensin(Los Alamos National Lab, United States of
America)
11:15 AM - 12:15 PM Room7

[SY-I10] Structure and Mobility of Dissociated Cacancies
at Twist Grain Boundaries and Screw Dislocations
in Ionic Compounds
○Blas Pedro Uberuaga, Enrique Martinez, Kedarnath
Kolluri, Xiang-Yang Liu （Los Alamos National
Laboratory, United States of America）

[SY-I10] Reverse engineering the kinetics of grain growth
Mingyan Wang[1], Jules Dake[1], Søren Schmidt[2], ○Carl
Krill[1] （1.Institute of Micro and Nanomaterials, Ulm
University, Germany, 2.Dept. of Physics, Technical
University of Denmark, Denmark）

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I11] Symposium I-11
Chairs: Bob Svendsen(RWTH Aachen University, Germany), Jeremy K Mason(University of California, Davis, United States of America)
2:00 PM - 3:30 PM Room7

[SY-I11] Recent advances in the Full-Field modeling of microstructural evolutions using a finite-element level set integrated framework.

$^{\bigcirc}$Daniel Pino Munoz, Thomas Toulorge, Charbel Moussa, Nathalie Bozzolo, Marc Bernacki （Mines ParisTech / PSL Research University, France）

[SY-I11] The effect of strong anisotropic grain boundary energy and mobility on microstructure formation and evolution: mesoscale modeling and simulation

$^{\bigcirc}$Brandon Runnels[1], Josep Maria Gras Ribot[1], Ian Chesser[2] （1.University of Colorado Colorado Springs, United States of America, 2.Carnegie Mellon University, United States of America）

[SY-I11] A Machine Learning Exploration of Grain Boundary Mobility Mechanisms

Leila Khalili[1], Eric R Homer[2], $^{\bigcirc}$Srikanth Patala[1] （1.North Carolina State University, United States of America, 2.Brigham Young University, United States of America）

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I12] Symposium I-12
Chairs: Blas Pedro Uberuaga(Los Alamos National Laboratory, United States of America), Chris P Race(University of Manchester, UK)
4:00 PM - 5:15 PM Room7

[SY-I12] Formation and shrinkage of grain boundary loops in two-dimensional colloidal crystals

Francois Lavergne, Arran Curran, Dirk Aarts, $^{\bigcirc}$Roel Dullens （University of Oxford, UK）

[SY-I12] Growth and characterization of two-dimensional poly(quasi)crystals

$^{\bigcirc}$Petri Hirvonen[1], Gabriel Martine La Boissonière[2], Zheyong Fan[1], Cristian Achim[3], Nikolas Provatas[4], Ken R. Elder[5], Tapio Ala-Nissila[1,6] （1.Dept. of Applied Physics, Aalto Univ., Finland, 2.Dept. of Mathematics and Statistics, McGill Univ., Canada, 3.Dept. of Chemical Engineering, Univ. of Concepción, Chile, 4.Dept. of Physics, McGill Univ., Canada, 5.Dept. of

Physics, Oakland Univ., United States of America）

[SY-I12] A Parallel Algorithm for High Resolution 3D Phase Field Simulations of Polycrystalline Solidification

$^{\bigcirc}$Pavel Strachota, Aleš Wodecki （Czech Technical University in Prague, Czech Republic）

[SY-I12] Properties of β / ω phase interfaces in Ti and their implications on mechanical properties and ω morphology

$^{\bigcirc}$Shuo Cao[1], Qing-Miao Hu[1], Rui Yang[1], Yong Jiang[2] （1.Institute of Metal Research, Chinese Academy of Science , China, 2.Central South University, China）

Room8

Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D1] Symposium D-1
Chair: Daniel Urban(Fraunhofer IWM, Germany)
9:45 AM - 11:00 AM Room8

[SY-D1] **Data-Driven Discovery of new materials**

$^{\bigcirc}$Isao Tanaka （Dept. Materials Science and Engineering, Kyoto Univ. , Japan）

[SY-D1] Machine Learning and Materials Discovery*

$^{\bigcirc}$Gus Hart （Brigham Young University, United States of America）

[SY-D1] Data-Driven Materials Design in an Industrial Environment

$^{\bigcirc}$Thomas Eckl, Lothar Kunz, Benedikt Ziebarth （Robert Bosch GmbH, Germany）

Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D2] Symposium D-2
Chair: Tilmann Hickel(MPIE, Germany)
11:15 AM - 12:30 PM Room8

[SY-D2] Using Machine-Learning to Create Predictive Material Property Models

$^{\bigcirc}$Chris Wolverton （Northwestern University, United States of America）

[SY-D2] Designing mesoscale structures of Li-ion battery electrode using FIB-SEM image via machine learning

$^{\bigcirc}$Yoichi Takagishi, Tatsuya Yamaue （Kobelco Research Institute Inc., Japan）

[SY-D2] **Stability Engineering of Halide Perovskite via Machine Learning**

$^{\bigcirc}$Wan-Jian YIN, Wanjian YIN （Soochow University,

China）

[SY-D2] Systematic evaluation of ionization potentials of divalent cation binary oxides

○Yoyo Hinuma[1,2,3], Hiroyuki Hayashi[2,3], Yu Kumagai[4], Isao Tanaka[2,3], Fumiyasu Oba[2,5] （1.Center for Frontier Science, Chiba Univ., Japan, 2.Center for Materials Research by Information Integration, National Institute for Materials Science, Japan, 3.Department of Materials Science and Engineering, Kyoto Univ., Japan, 4.Materials Research Center for Element Strategy, Tokyo Institute of Technology, Japan, 5.Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology, Japan）

Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D3] Symposium D-3
Chair: Daryl Chrzan(UC Berkeley, USA)
2:00 PM - 3:30 PM Room8

[SY-D3] Finding the needle in the haystack: Materials discovery through high-throughput ab initio computing and data mining

○Geoffroy Hautier （Universite catholique de Louvain, Belgium）

[SY-D3] High-entropy alloys investigation using machine-learned potentials

○Tatiana Kostiuchenko, Alexander Shapeev （Dept. of Material Science and Engeneering , Skolkovo Institute of Science and Technology, Moscow, Russia）

[SY-D3] Stability evaluation of high-entropy alloys via accurate on-lattice model

○Evgenii Meshkov[1], Ivan Novoselov[1], Alexander Shapeev[2], Alexey Yanilkin[1] （1.All-Russian Research Institute of Automatics (VNIIA), Russia, 2.Skolkovo Institute of Science and Technology, Russia）

[SY-D3] Atomistically informed atomic mobility databases for continuum diffusion simulations

○Katrin Abrahams[1], Daniel Gaertner[2], Maximilian Grabowski[3], Irina Roslyakova[1], Oleg Shchyglo[1], Sergiy V. Divinski[2], Ingo Steinbach[1] （1.Scalebridging Thermodynamic and Kinetic Simulation (ICAMS), Ruhr-University Bochum, Germany, 2.Institute of Materials Physics, University of Münster, Germany, 3.Atomistic Modelling and Simulation (ICAMS), Ruhr-University Bochum, Germany）

[SY-D3] The European Materials Modelling Council: standardization, interoperability and data

management tools for materials modelling

○Luca Bergamasco[1], Emanuele Ghedini[2], Gerhard Goldbeck[3], Eliodoro Chiavazzo[1], Pietro Asinari[1] （1.Politecnico di Torino, Italy, 2.Università di Bologna, Italy, 3.Goldbeck Consulting Ltd, UK）

Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D4] Symposium D-4
Chair: Minoru Otani(AIST, Japan)
4:00 PM - 5:30 PM Room8

[SY-D4] Exploration of large ab initio data spaces to design structural materials with superior mechanical properties

○Joerg Neugebauer, Jan Janssen, Tilmann Hickel, Blazej Gabowski （Max-Planck-Institut fuer Eisenforschung, Germany）

[SY-D4] Toward a machine learning aided interatomic potential for multi-element alloys: Application to binary compounds

○Doyl Dickel, David Francis, Christopher Barrett （Mississippi State University, United States of America）

[SY-D4] **Machine Learning potentials for modeling iradiation defects in iron and tungsten**

○Alexandra Goryaeva[1], Jean-Bernard Maillet[2], Mihai-Cosmin Marinica[1] （1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France, 2.CEA-DAM DIF, 91297 Arpajon Cedex, France）

[SY-D4] Effect of friction and ductility on relaxation dynamics and mechanical memory of crumpled materials

○Mehdi Habibi, Eric van Bruggen （Wageningen University, Netherlands）

[SY-D4] Big-data insights into solute-GB segregation

○Liam Huber, Blazej Grabowski, Joerg Neugebauer （MPIE, Germany）

Room9

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H7] Symposium H-7
Chair: Patrick R. Onck(Univ. of Groningen, Netherlands)
9:45 AM - 11:00 AM Room9

[SY-H7] Computational modeling approach for the

rational design of DNA nanostructures

○Do-Nyun Kim, Jae Young Lee, Jae Gyung Lee, Young-Joo Kim, Kyung Soo Kim, Chanseok Lee （Department of Mechanical and Aerospace Engineering, Seoul National University, Korea）

[SY-H7] Quantitative Multiscale Modelling of Bionano Interface

○Vladimir Lobaskin[1], Stefano Poggio[1], David Power[1], Hender Lopez[2] （1.School of Physics, University College Dublin, Ireland, 2.Institute Laue-Langevin, Grenoble, France）

[SY-H7] Multiscale modelling of intrinsically-disordered proteins

Ankur Mishra, Henry De Vries, Hamid Jafarinia, Erik Van der Giessen, ○Patrick R. Onck （University of Groningen, Netherlands）

[SY-H7] Tracing the interplay of polymer topology and hydrodynamics

○Lisa B. Weiss[1], Arash Nikoubashman[2], Christos N. Likos[1] （1.University of Vienna, Austria, 2.Johannes Gutenberg University Mainz, Germany）

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H8] Symposium H-8

Chair: Patrick R. Onck(Univ. of Groningen, Netherlands)
11:15 AM - 12:30 PM Room9

[SY-H8] Modeling and Simulation of DNA Foldback Intercoil Structure

○Moon Ki Kim, Byung Ho Lee, Soojin Jo （School of Mechanical Engineering, Sungkyunkwan University, Korea）

[SY-H8] DNA-particle vitrimer systems

○francesco sciortino （Sapienza Universita' di Roma, Italy）

[SY-H8] Relation between Macroscopic Flows in a Contraction-Expansion Channel and Dynamics of Well-Entangled Polymer Chains

○Takeshi Sato, Takashi Taniguchi （Dept. of Chemical Engineering, Kyoto Univ., Japan）

[SY-H8] Origin of large scale spatial organization of DNA-polymer in bacterial chromosomes.

○Apratim Chatterji[1], Tejal Agarwal[2], Manjunath G.P.[3], Farhat Habib[4] （1.IISER-Pune, India 411008, India, 2.IISER-Pune, India, 411008, India, 3.NYU, USA, United States of America, 4.Inmobi, Bangalore, India 560103., India）

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H9] Symposium H-9

Chair: Kees Storm(Eindhoven University of Technology, Netherlands)
2:00 PM - 3:30 PM Room9

[SY-H9] **Micromechanics and instabilities in soft composite materials**

○Stephan Rudykh （University of Wisconsin - Madison, United States of America）

[SY-H9] Deformation analysis of UV curing 3d printed materials by combined molecular dynamics-finite element method

Jiwon Jung, Chanwook Park, ○Gunjin Yun （Seoul National University, Korea）

[SY-H9] Modelling and 3D Printing Kelvin Cell Acoustic Metamaterial

○Huina MAO[1], Peter Göransson[1], John Kennedy[2], Henry Rice[2], Umberto Iemma[3] （1.Dept. of Aeronautical and Vehicle Engineering, KTH Royal Institute of Technology, Sweden, 2.Dept. of Mechanical and Manufacturing Engineering, Trinity College Dublin, Ireland, 3.Engineering Department, Roma Tre University, Italy）

[SY-H9] Theoretical approach for EUV resist fabrication: DFT-MD-FDM study

○Muyoung Kim[1], Junghwan Moon[1], Joonmyung Choi[3], Sungwoo Park[1], Byunghoon Lee[3], Changyoung Jeong[3], Maenghyo Cho[2,1] （1.Divison of Multiscale Mechanical Design, School of Mechanical and Aerospace Engineering, Seoul National University, Korea, 2.Institute of Advanced Machines and Design, Seoul National University, Korea, 3.SAMSUNG ELECTRONICS CO., LTD, Korea）

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H10] Symposium H-10

Chair: Kees Storm(Eindhoven University of Technology, Netherlands)
4:00 PM - 5:30 PM Room9

[SY-H10] In silico design of self-assembly nanostructured polymer systems by multiscale molecular modelling

○Maurizio Fermeglia （University of Trieste , Italy）

[SY-H10] Dynamical properties of suspensions of star block-copolymers in shear flow.

○Diego Felipe Jaramillo - Cano[1], Manuel Camargo[2],

Christos N. Likos[1]　(1.Faculty of Physics, University of Vienna, Austria, 2.CICBA, Universidad Antonio Nariño - Campus Farallones, Colombia)

[SY-H10] Heterogeneous flow and internal friction in amorphous carbon

○Richard Jana[1], Lars Pastewka[1], Daniele Savio[2], Volker L Dehringer[3], Gábor Csányi[3], Julian von Lautz[2], Michael Moseler[2], Peter Gumbsch[2,4]　(1.Albert Ludwigs Universitaet Freiburg, Germany, 2.Fraunhofer-Institut für Werkstoffmechanik IWM, Germany, 3.University of Cambridge, UK, 4.Institue for Applied Materials, Karlsruhe Institute of Technology, Germany)

[SY-H10] **Increasing the thermal conductivity of polymer nanocomposites filled with carbon nanotubes via molecular dynamics simulation**

○Yangyang Gao[1], Liqun Zhang[1], Florian Müller-Plathe[2]　(1.Beijing University of Chemical Technology, China, 2.Technische Universität Darmstadt, Germany)

[SY-H10] **Thermal transport in polymer-based nanocomposite materials across multiple scales**

Rajat Srivastava, ○Matteo Fasano, Shahin Mohammadnejad, Hernan Chavez Thielemann, Eliodoro Chiavazzo, Pietro Asinari　(Energy Department, Politecnico di Torino, Italy)

Room10

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B5] Symposium B-5
Chair: Jean-Paul Crocombette(CEA, Univ. Paris-Saclay, France)
9:45 AM - 11:00 AM Room10

[SY-B5] He impurities in boron carbide : structure, kinetics, and Raman signatures

○Guido Roma, Kevin Gillet, Anton Schneider, Jean-Paul Crocombette　(CEA, Univ. Paris-Saclay, France)

[SY-B5] Irradiation damage in nuclear graphite at the atomic scale

○Alain Chartier[1], Laurent Van Brutzel[1], Justin Pageot[2]　(1.DEN, Service de la Corrosion et du Comportement des Materiaux dans leur Environment, CEA Saclay, France, 2.DEN, Service d'Etudes des Materiaux Irradies, CEA Saclay, France)

[SY-B5] Using computational modeling to understand radiation damage tolerance in complex oxides both from the bottom-up and the top-down

○Blas Pedro Uberuaga　(Los Alamos National Laboratory, United States of America)

[SY-B5] **Development of defect mechanics-based multi-scale simulation techniques for reliability study of high performance electronic devices in radiation environments**

○Yukeun Eugene Pak[1], Youjung Seo[2], Dhaneshwar Mishra[1], Keonwook Kang[3], Jihyun Kim[4]　(1.Advanced Institutes Convergence Technology, Korea, 2.Seoul National University, Korea, 3.Yonsei University, Korea, 4.Korea University , Korea)

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B6] Symposium B-6
Chair: Jaime Marian(University of California Los Angeles, United States of America)
11:15 AM - 12:30 PM Room10

[SY-B6] Ion Irradiation as a Surrogate for Reactor Irradiation: The Expected and the Surprises

○Gary S Was[1], Zhijie Jiao[1], David Woodley[1], Stephen Taller[1], Gerrit Vancoevering[1], Anthony Monterrosa[1], Elizabeth Getto[4], Brian Wirth[2], Arthur Motta[3]　(1.University of Michigan, United States of America, 2.University of Tennessee, United States of America, 3.Pennsylvania State University, United States of America, 4.United Stated Naval Academy, United States of America)

[SY-B6] **Dose Effect on the Irradiation Induced Loop Density and Burgers Vector in Ion-Irradiated Ferritic/Martensitic Steel HT9 Through In-Situ TEM**

Ce Zheng[1], Stuart Maloy[2], ○Djamel Kaoumi[1]　(1.North Carolina State University, United States of America, 2.Los Alamos National Laboratory, United States of America)

[SY-B6] **Novel Deformation Mechanism of Helium Irradiated Copper**

○WEIZHONG HAN　(Xi'an Jiaotong University, China)

[SY-B6] Isotope effect on quantum diffusion of interstitial hydrogen in face-centered cubic metals

○Hajime Kimizuka[1], Shigenobu Ogata[1,2], Motoyuki Shiga[3]　(1.Osaka University, Japan, 2.Kyoto University, Japan, 3.Japan Atomic Energy Agency, Japan)

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B7] Symposium B-7

Chair: Marjorie Bertolus(CEA/DEN/DEC, Centre CEA de Cadarache, France)
2:00 PM - 3:30 PM Room10

[SY-B7] Thermal properties of fluorite-type metal dioxides: CeO_2, ThO_2, UO_2, NpO_2, PuO_2 and AmO_2
 ○Masato Kato (Japan Atomic Energy Agency, Japan)

[SY-B7] **SCIANTIX: A new inert gas behaviour module ready for use**
 ○Davide Pizzocri, Tommaso Barani, Lelio Luzzi
  (Politecnico di Milano, Italy)

[SY-B7] Modeling swelling in U_3Si_2 nuclear fuel using a multi-scale computational approach
 ○Larry Aagesen[1], Karim Ahmed[2], Benjamin Beeler[1], Daniel Schwen[1], Yongfeng Zhang[1] (1.Idaho National Laboratory, United States of America, 2.Texas A&M University, United States of America)

[SY-B7] Why Multiscale Modeling of Nuclear Fuel is Absolutely Essential and Why it is so Challenging
 ○Michael R Tonks[1], Yongfeng Zhang[2], David Andersson[3], Simon Phillpot[1], Christopher Stanek[3]
  (1.University of Florida, United States of America, 2.Idaho National Laboratory, United States of America, 3.Los Alamos National Laboratory, United States of America)

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B8] Symposium B-8
Chair: Guang-Hong Lu(Beihang University, China)
4:00 PM - 5:30 PM Room10

[SY-B8] Kinetic Monte Carlo study of tungsten fuzz formation under low energy helium irradiation
 ○Zhangcan Yang, Yingzhao He, Quansong Peng
  (School of Energy and Power Engineering, Huazhong University of Science and Technology, China)

[SY-B8] Constrained thermodynamic model for multi-component alloys under irradiation: A matrix formulation from first-principles Hamiltonian
 ○Duc Nguyen-Manh[1], J.S Wrobel[2], A. Fernandez_Caballero[3], S.L. Dudarev[1] (1.Materials Science and Scientific Computing Department, Culham Centre for Fusion Energy, UKAEA, UK, 2.Faculty of Materials Science and Engineering, Warsaw University of Technology, Poland, 3.School of Mechanical Aerospace and Civil Engineering, University of Manchester , UK)

[SY-B8] Kinetic Monte-Carlo Simulations of Radiation Damage in W(Re,Os) Alloys

 ○Matthew James Lloyd[1,2], David Armstrong[1], Enrique Martinez Saez[3], Duc Nguyen-Manh[2] (1.Department of Materials, University of Oxford, UK, 2.Culham Centre for Fusion Energy, UK, 3.Los Alamos National Laboratory, United States of America)

[SY-B8] Modeling Re-precipitate hardening in neutron irradiated W and W-Re alloys: from point defects to macroscopic hardening
 Chen-Hsi Huang[1], Leili Gharaee[2], Paul Erhart[2], ○Jaime Marian[1] (1.University of California Los Angeles, United States of America, 2.Chalmers University, Sweden)

[SY-B8] In-situ TEM of Formation Processes of Defects in Tungsten under Irradiation: Comparison between Electron and Self-ion Irradiations
 ○Kazuto Arakawa (Shimane University, Japan)

Fri. Nov 2, 2018

Room1

Plenary Talk | Plenary Talk

[PL6] Plenary Talk 6
Chair: Karin Dahmen(University of Illinois at Urbana Champaign, USA)
8:30 AM - 9:20 AM Room1

[PL6] Plenary Talk 6
○Muneo Hori （Earthquake Research Institute, The University of Tokyo, Japan）

Fri. Nov 2, 2018

Room1

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C13] Symposium C-13

Chair: Jaafar A. El-Awady(Johns Hopkins University, United States of America)
9:45 AM - 11:00 AM Room1

[SY-C13] Mesoscopic studies of slip and twinning processes in hcp polycrystalline materials
○Irene Beyerlein[1], Marat Latypov[1], Jason Mayeur, Wyatt Witzen[1], Mitra Taheri[2], Tresa Pollock[1]
（1.University of California at Santa Barbara, United States of America, 2.Drexel University, United States of America）

[SY-C13] **Crystal plasticity formulation involving volume fraction-based deformation twinning model**
○Yuichi Tadano （Department of Mechanical Engineering, Saga University, Japan）

[SY-C13] **An Elastic-Viscoplastic Crystal Plasticity Modeling for Plane Strain Deformation of Pure Magnesium**
○Weidong Song, Liansong Dai （Beijing Institute of Technology, China）

[SY-C13] The Minimum Energy Pathways Identifications of Twinning Dislocation Loop Nucleation of Extension Twinning in Magnesium
○Xiao-Zhi Tang[1], Qun Zu[2], Lixin Sun[4], Yue Fan[3], Ya-Fang Guo[1] （1.Inst. of Mechanics, Beijing Jiaotong Univ., China, 2.Schl. of Mechanical Engineering, Hebei Univ. of Tech., China, 3.Dept. of Mechanical Engineering, Univ. of Michigan, United States of America, 4.Dept. of Nuclear Science and Engineering, MIT, United States of America）

Room2

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E13] Symposium E-13

Chairs: Erik Bitzek(FAU Erlangen-Nuernberg, Germany), Kisaragi Yashiro(Gifu University, Japan)
9:45 AM - 11:00 AM Room2

[SY-E13] 3D Aspects of Fracture in Crack - Obstacle Interactions and Effects of Crack Front Curvature
○Erik Bitzek[1], Polina Baranova[1], Johannes J. Möller[2]
（1.FAU Erlangen-Nuernberg, Germany, 2.Fraunhofer IWM, Germany）

[SY-E13] Vortex instabilities in the deformation of Cu|Au nanolaminates
Adrien Gola[1,2], Peter Gumbsch[2,3], ○Lars Pastewka[1,3,2]
（1.University of Freiburg, Germany, 2.Karlsruhe Institute of Technology, Germany, 3.Fraunhofer IWM, Germany）

[SY-E13] **Molecular dynamics simulation of the interaction between grain boundary and point defects**
○Liang Zhang[1], Yasushi Shibuta[1], Cheng Lu[2] （1.The University of Tokyo, Japan, 2.University of Wollongong, Australia）

[SY-E13] Deformation mode analysis by the eigenvectors of the atomic elastic stiffness
○Kisaragi Yashiro （Gifu University, Japan）

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E14] Symposium E-14

Chairs: Thierry Auger(CNRS, France), Jamila Rahmoun(LAMIH-ENSIAME, Valenciennes University, France)
11:15 AM - 12:30 PM Room2

[SY-E14] Stability Controlled Crack Evolution in Staggered Laminate Bio-material
○Yi Yan, Akihiro Nakatani （Dept. of Adaptive Machine Systems, Osaka University, Japan）

[SY-E14] A brittle to ductile transition modeling for liquid metal embrittlement
○Thierry Auger （CNRS, France）

[SY-E14] Buckling delamination of ductile thin films on rigid substrates
○Nadia Ben Dahmane, Guillaume Parry, Rafael Estevez
（Univ. Grenoble Alpes, SIMAP, F-38000 Grenoble, France）

[SY-E14] An analytical model of the peeling forces at edges of multilayers subjected to temperature variations
○Chengyin Zhang[2], Neng-Hui Zhang[1,2]
（1.Department of Mechanics, College of Sciences, Shanghai University, China, 2.Shanghai Key Laboratory of Mechanics in Energy Engineering, Shanghai Institute of Applied Mathematics and Mechanics, Shanghai University, China）

[SY-E14] **Characterization and multi-scale modeling of the mechanical response of the human humerus under dynamic loading**
○Jamila Rahmoun[1], Hakim Naceur[1], Pascal Drazetic[2],

Christian Fontaine[3] （1.LAMIH-ENSIAME, Valenciennes University, France, 2.LAMIH-IUT, Valenciennes University, France, 3.Lab. d'anatomie, Lille University, France）

Room3

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F13] Symposium F-13
Chair: Takayuki Aoki(Tokyo Institute of Technology, Japan)
9:45 AM - 11:00 AM Room3

[SY-F13] Advanced analysis tools for atomistic microstructure modeling
○Alexander Stukowski （Dept. of Materials Science, Darmstadt University of Technology, Germany）

[SY-F13] Studing thermo-oxidative degradation of polyimide in oxygen enviorment using MD simulations
○Ashwani Kumar Sengar, Sumit Basu （IIT Kanpur, India）

[SY-F13] In-plane characterization of structural and thermodynamic properties for steps at faceted chemically heterogeneous solid/liquid interfaces
○Hongtao Liang[1], Brian B. Laird[2], Mark Asta[3], Yang Yang[1] （1.Physics Department and State Key Laboratory of Precision Spectroscopy, School of Physical and Material Science, East China Normal Universit, China, 2.Department of Chemistry, University of Kansas, United States of America, 3.Department of Materials Science and Engineering, UC Berkeley, United States of America）

[SY-F13] Design of neural network for thermodynamics data of non-equilibrium multiphase field model
○Hiroshi Wakameda[1], Sukeharu Nomoto[1], Akinori Yamanaka[3], Toshiyuki Koyama[2] （1.ITOCHU Techno-Solutions Corporation, Japan, 2.Materials Design Innovation Engineering, Nagoya Univ., Japan, 3.Department of Mechanical Systems Engineering, Tokyo University of Agriculture and Technology, Japan）

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F14] Symposium F-14
Chair: Markus Kuehbach(Max-Planck-Institut fur Eisenforschung GmbH, Germany)
11:15 AM - 12:30 PM Room3

[SY-F14] Large-scale multiphase flow simulations on a GPU supercomputer
○Takayuki Aoki （Tokyo Institute of Technology, Japan）

[SY-F14] **Transport Properties Of Fluid Mixtures In Micro- And Mesoporous Kerogen Membranes**
○Patrick Alain Bonnaud[1], Romain Vermorel[1], Julien Collell[2], Guillaume Galliéro[1] （1.University of Pau and Adour Countries, France, 2.Total E&P, France）

[SY-F14] Numerical simulation of ionic transport through deformable porous media: application to cortical bone tissue modeling
○Jana Turjanicova[1,2], Eduard Rohan[1,2], Vladimír Lukeš[2] （1.Dept. of Mechanis, Univ. of West Bohemia in Pilsen, Czech Republic, 2.NTIS - New technologies for information society, Czech Republic）

[SY-F14] Hydrogen Transport and Thermal Desorption in Multiphase Steels
○Andrej Turk[1], Pedro E.J. Rivera-Díaz-del-Castillo[2], Enrique Galindo-Nava[1] （1.University of Cambridge, UK, 2.Lancaster University, UK）

Room4

Symposium | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[SY-N7] Symposium N-7
Chair: Shotaro Hara(Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan)
9:45 AM - 11:00 AM Room4

[SY-N7] Bridging Time Scales with Variationally Enhanced Sampling
○Omar Valsson （Max Planck Institute for Polymer Research, Germany）

[SY-N7] Simulations of Branched Polyelectrolytes
○Filip Uhlik （Charles University, Czech Republic）

[SY-N7] Adaptive resolution simulations coupling molecular dynamics to dissipative particle dynamic
○Matej Praprotnik （National Institute of Chemistry, Slovenia）

[SY-N7] Using Diffusive Molecular Dynamics Simulations to Investigate Grain Boundary Segregation and Grain Boundary Structural Transformations
Louis Hebrard, ○Chad W Sinclair （Dept. of Materials Engineering, University of British Columbia, Canada）

Room8

[SY-D5] Symposium D-5
Chair: Jörg Neugebauer(MPIE, Germany)
9:45 AM - 11:00 AM Room8

[SY-D5] Computational exploration of strong permanent magnet compounds
○Takashi Miyake[1,2,3] (1.CD-FMat, AIST, Japan, 2.ESICMM, NIMS, Japan, 3.CMI[2], NIMS, Japan)

[SY-D5] A machine-learning approach for finding new hard-magnetic phases
Johannes J. Möller, ○Daniel F. Urban, Christian Elsässer (Fraunhofer IWM, Freiburg, Germany)

[SY-D5] High-throughput optimization of finite temperature phase stabilities of Ce-based hard magnetic materials
○Tilmann Hickel, Halil Soezen, Fritz Koermann, Joerg Neugebauer (Max Planck Institut fur Eisenforschung, Germany)

[SY-D5] Understanding pairwise magnetic interactions in Fe-based materials with machine learning techniques
○Osamu Waseda, Omkar Hegde, Tilmann Hickel, Jörg Neugebauer (MPIE, Germany)

[SY-D6] Symposium D-6
Chair: Daniel Urban(Fraunhofer IWM, Germany)
11:15 AM - 12:30 PM Room8

[SY-D6] Novel two-dimensional materials: Materials discovery, data provenance, and workflow reproducibility.
○Nicola Marzari (EPFL, Switzerland)

[SY-D6] In silico screening of Metal-Organic Frameworks for adsorption driven heat pumps and chillers
○Mate Erdos[1], Martijn F. de Lange[1], Freek Kapteijn[2], Othonas A. Moultos[1], Thijs J. H. Vlugt[1] (1.Engineering Thermodynamics, Process &Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Netherlands, 2.Catalysis Engineering, Chemical Engineering Department, Delft University of Technology, Netherlands)

[SY-D6] Machine learning assisted by first-principles calculations for designing intermetallic-typed

metallic glasses
○Tokuteru Uesugi, Manami Sakai, Yorinobu Takigawa, Kenji Higashi (Dep. of Materials Science, Osaka Prefecture Univ., Japan)

Room9

[SY-H11] Symposium H-11
Chair: Erik Van der Giessen(University of Groningen, Netherlands)
9:45 AM - 11:00 AM Room9

[SY-H11] A Hierarchical Multiscale Simulations Approach for Modeling Failure in Polymer Matrix Composites
Xiawa Wu[1], Amin Aramoon[1], Christopher Woodward[2], ○Jaafar A. El-Awady[1] (1.Johns Hopkins University, United States of America, 2.Air Force Research Laboratory, United States of America)

[SY-H11] Some Positive Aspect of Structural Defects in Graphene/Polymer Nanocomposites Studied by Abinitio,Molecular Dynamics, and Continuum Approaches
○Seunghwa Yang[1], Janghyuk Moon[1], Maenghyo Cho[2] (1.School of Energy Systems Engineering, Chung-Ang University, Korea, 2.School of Mechanical and Aerospace Engineering, Seoul National University, Korea)

[SY-H11] Linear and non-linear viscoelastic properties of model fractal-like aggregates polymer nanocomposites
○Samy MERABIA[1], Yang WANG[1], François DETCHEVERRY[1], Marc COUTY[2], Gaëtan MAUREL[2] (1.CNRS and Universite Lyon 1, France, 2.MFP Michelin, Clermont-Ferrand , France)

[SY-H11] **Topological defect structure in the self-assembly of semiflexible polymers under spherical confinement**
○Mihir Khadilkar, Arash Nikoubashman (Johannes GutenBerg University Mainz, Germany, Germany)

[SY-H11] Molecular dynamics simulation of the detachment force between graphene and epoxy resin
○Kazuki Mori[1], Makoto Yabe[2], Yuji Kohno[2], Jun Koyanagi[3] (1.ITOCHU Techno-Solutions Corporation, Japan, 2.Yokohama National University, Japan,

3.Tokyo University of Science, Japan）

[SY-H11] Relation between deformation and electrical
conductivity for electroconductive polymer
nanocomposites with highly segregated
structure
○Oleg V. Lebedev[1], Sergey Abaimov[1], Alexander
Ozerin[2], Anton Trofimov[1], Iskander Akhatov[1]
（1.Center for Design, Manufacturing and Materials,
Skolkovo Institute of Science and Technology, Russia,
2.Laboratory of the Structure of Polymer Materials,
N.S. Enikolopov Institute of Synthetic Polymer
Materials of RAS, Russia）

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and
Network Materials

[SY-H12] Symposium H-12
11:15 AM - 12:00 PM Room9

Room10

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects
in Nuclear Materials

[SY-B9] Symposium B-9
Chair: Michael Tonks(University of Florida, United States of
America)
9:45 AM - 11:00 AM Room10

[SY-B9] Ab Initio Modeling of Self-Interstitial and Vacancy
Migration in Zirconium
○Emmanuel Clouet[1], Céline Varvenne[2] （1.CEA Saclay,
France, 2.CNRS - Aix-Marseille University, France）

[SY-B9] Atomistic modelling of point defect clusters in
zirconium and impact on the microstructure
evolution and crystal growth under irradiation
Benjamin CHRISTIAEN[3], Christophe DOMAIN[3,2], ○L
udovic THUINET[1,2], Antoine AMBARD[3,2], Alexandre
LEGRIS[1,2] （1.UMET, UMR CNRS 8207, Lille university,
F-59655 Villeneuve d'Ascq, France, 2.EM2VM, EDF-
CNRS, France, 3.EDF R&D, MMC, Les Renardieres, F-
77810 Moret-sur-Loing, France）

[SY-B9] Modeling of dislocation climb assisted glide in
crystal plasticity models
○Alankar Alankar, Vikram Phalke, Ritesh Dadhich, Ashish
Mishra （IIT Bombay, India）

[SY-B9] The role of oxide grain boundaries in the
oxidation of zirconium alloy fuel cladding
○Maria S Yankova[1], Felicity Baxter[1,2], Alistair Garner[1],
Philipp Frankel[1], Christopher P Race[1] （1.Materials

Performance Centre, School of Materials, University of
Manchester, UK, 2.Corrosion and Materials Science,
Wood. PLC, UK）

[SY-B9] Advances in X-ray Diffraction Line Profile Analysis
of Dislocation Loops in Zr - Insights from Atomistic
Modelling.
○Chris P Race, Rory Hulse, Tamas Ungar （University of
Manchester, UK）

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects
in Nuclear Materials

[SY-B10] Symposium B-10
Chair: Frederic Soisson(CEA Saclay, France)
11:15 AM - 12:15 PM Room10

[SY-B10] Sink strengths of point defects near tilt grain
boundaries: A phase field model
○Pengchuang Liu[1], Songlin Zheng[2], Pengcheng
Zhang[1], Sanqiang Shi[3], Kaiguo Chen[2] （1.Institute of
Materials, China academy of engineering physics,
China, 2.Institute of Fluid Physics, China academy of
engineering physics, China, 3.Department of
Mechanical Engineering, The Hong Kong Polytechnic
University, Hong Kong）

[SY-B10] Modelling swelling and growth under irradiation
using the phase field method
○Daniel Schwen, Andea M. Jokisaari （Dept. of Fuels
Modeling and Simulation, Idaho National Laboratory,
United States of America）

[SY-B10] Phase-field modelling of dislocation loop
evolution under irradiation : application to
radiation induced segregation prediction near
the dislocation cores
○Gabriel Franck BOUOBDA MOLADJE[1], Ludovic
THUINET[1], Alexandre LEGRIS[1], Charlotte BECQUART[1],
Maylise NASTAR[2], Frédéric SOISSON[2] （1.CNRS,
université de Lille, France, 2.CEA, Université Paris-
Saclay, France）

[SY-B10] **Theoretical derivation of the ABVI model from
cluster expansion Hamiltonian**
○Antonio Fernandez Caballero[1,2], Jan Wrobel[3], Paul
Mummery[1], Duc Nguyen-Manh[2] （1.School of
Mechanical, Aerospace and Civil Engineering,
University of Manchester, UK, 2.Department of
Materials Science and Scientific Computing, CCFE,
United Kingdom Atomic Energy Authority, Abingdon
OX14 3DB, UK, UK, 3.Faculty of Materials Science and
Engineering, Warsaw University of Technology, UI.

Wołoska 141, 02-507 Warsaw, Poland, Poland）

Room11

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K4] Symposium K-4

Chairs: Tetsuo Mohri(IMR, Tohoku University, Japan), Akihiro Nakatani(Dept. of Adaptive Machine Systems, Osaka Univ., Japan)
9:45 AM - 11:00 AM Room11

[SY-K4] Disclination dipole model of kink deformation in layered solid
○Akihiro Nakatani[1], Xiao-Wen Lei[2] （1.Dept. of Adaptive Machine Systems, Osaka Univ., Japan, 2.Dept. of Mechanical Engineering, Univ. of Fukui, Japan）

[SY-K4] Large-scale coarse-grained molecular dynamics simulations on fracture processes of lamellar structure in crystalline polymers
○Yuji Higuchi （The University of Tokyo , Japan）

[SY-K4] Grain boundary sliding within the entropy production rate theory
○Tetsuo Mohri （IMR, Tohoku University, Japan）

[SY-K4] Molecular Dynamics Simulation on Intergranular Cracking Mechanism of Iron Material in High Temperature Pressurized Water Environment
○Qian Chen, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Materials Research, Tohoku University, Japan）

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K5] Symposium K-5

Chairs: Masanori Kohyama(AIST, Japan), Masatake Yamaguchi(Japan Atomic Energy Agency, Japan)
11:15 AM - 12:15 PM Room11

[SY-K5] Effects of a bulk-region size in the first-principles tensile test of a grain boundary
○Masanori Kohyama[1], Hao Wang[2], Shingo Tanaka[1] （1.AIST, Japan, 2.Shanghai Univ., China）

[SY-K5] Combined analysis of first-principles calculations and fracture mechanics experiments on intergranular embrittlement of an alloy steel
○Masatake Yamaguchi （Center for Computational Science and e-Systems, Japan Atomic Energy Agency, Japan）

[SY-K5] First-principles local energy analysis of grain boundary segregation of sp-elements on bcc Fe
○Kazuma Ito[1,2], Somesh Kr. Bhattacharya[3], Shingo

Tanaka[3], Masanori Kohyama[3], Hideaki Sawada[2], Shigenobu Ogata[1] （1.Osaka University, Japan, 2.Nippon Steel &Sumitomo Metal Corporation, Japan, 3.National Institute of Advanced Industrial Science and Technology, Japan）

[SY-K5] Fast and scalable prediction of local energy at grain boundaries: Machine-learning based modeling of first-principles calculations
○Tomoyuki Tamura[1,2], Masayuki Karasuyama[1,2,3], Ryo Kobayashi[1,2], Ryuichi Arakawa[1], Yoshinori Shiihara[4], Ichiro Takeuchi[1,2,5] （1.Nagoya Institute of Technology, Japan, 2.Center for Materials Research by Information Integration (CMI2), Research and Services Division of Materials Data and Integrated System (MaDIS), National Institute for Materials Science (NIMS), Japan, 3.PRESTO, JST, Japan, 4.Toyota Technological Institute, Japan, 5.RIKEN Center for Advanced Intelligence Project, Japan）

Plenary Talk | Plenary Talk

[PL1] Plenary Talk 1

Amorphous materials on the meso-scale: achieving experimental length and timescales

Chair: Ju Li(MIT, USA)

Mon. Oct 29, 2018 10:10 AM - 11:00 AM Room1

Christopher A. Schuh

[PL1] Plenary Talk 1

○Christopher A. Schuh （Department of Materials Science and Engineering, MIT, USA）

(Mon. Oct 29, 2018 10:10 AM - 11:00 AM Room1)

[PL1] Plenary Talk 1

Amorphous materials on the meso-scale: achieving experimental length and timescales

○Christopher A. Schuh （Department of Materials Science and Engineering, MIT, USA）

The defining characteristic of metallic glass is disorder, with the fundamental unit of metallic glass plasticity being the Shear Transformation Zone (STZ), a local cluster of 20-100 atoms rearranging to accommodate shear strain. While the energy scales of STZs are well understood, deterministic relationships between disordered atomic structures and their respective mechanical responses have proven elusive (in stark contrast to, for example, the predictable response of a dislocation to a stress field). In lieu of such detailed deterministic relationships, we turn to stochastic modeling based on the energetics of STZ activation. This talk will review the development and current status of the class of meso-scale models referred to as Shear Transformation Zone Dynamics. These models calculate STZ activation rates by transition state theory with energy barriers modeled using Eshelby's continuum solutions for isotropic inclusions. In these models individual STZs interact through their elastic fields, which are evaluated by the finite element method, and the sample is evolved under the control of a kinetic Monte Carlo algorithm. We particularly review our most recent developments incorporating dynamic structural state variables and improved numerical methods into a new generation of STZ dynamics simulations. With these advances, STZ dynamics simulations are now approaching the level where they can be compared one-to-one (both in terms of length and time scales) with physical nanomechanical experiments.

Plenary Talk | Plenary Talk

[PL2] Plenary Talk 2

Multiscale modeling and realization of photo-responsive polymers

Chair: Alexey Lyulin(Technische Universiteit Eindhoven, The Netherlands)

Mon. Oct 29, 2018 11:00 AM - 11:50 AM Room1

Maenghyo Cho

[PL2] Plenary Talk 2

○Maenghyo Cho （School of Mechanical and Aerospace Engineering, Seoul National University, Korea）

(Mon. Oct 29, 2018 11:00 AM - 11:50 AM Room1)

[PL2] Plenary Talk 2

Multiscale modeling and realization of photo-responsive polymers

○Maenghyo Cho （School of Mechanical and Aerospace Engineering, Seoul National University, Korea）

Liquid crystalline polymers which contain photochromic chromophores can show macroscopic mechanical deformation under light irradiations. The light-induced shape change of the photo-responsive polymers (PRPs) comes from the trans-to-cis, or cis-to-trans isomerization of the mesogens, and it can be utilized to the microscale opto-mechanical actuation device. However, it is difficult to analyze and precisely predict the deformation because the theoretical approach requires a comprehensive knowledge of broad, interdisciplinary physical regimes that range from photochemical reaction kinetics to manipulating continuum scale deformations. Here, we develop a new multiscale model which integrates light input conditions, mesogen alignment, and continuum polymer deformations through sequential multiscale framework combining the DFT(density functional theory), MD(molecular dynamics), and continuum FE(finite element) method. In addition, the multiscale approach is applied to design the photo-mechanical behavior of the PRP nanocomposites with the consideration of the opto-mechanical coupling effect and microscopic interaction between the PRP matrix and fillers. This integrated framework can help to design the PRP and its composites.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C1] Symposium C-1

Chair: Emmanuel Clouet(CEA Saclay, SRMP, France)
Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room1

[SY-C1] Kinetic Monte Carlo model of screw dislocation-solute coevolution in W-Re alloys

Yue Zhao[1], Lucile Dezerald[3], ○Jaime Marian[1,2] （1.Dept. of Materials Science and Engineering, University of California Los Angeles, United States of America, 2.Dept. of Mechanical and Aerospace Engineering, University of California Los Angeles, United States of America, 3.Institut Jean Lamour, University of Lorraine, France）

[SY-C1] Thermally activated solute-drag strengthening by interstitial impurities in BCC Cr

○Christian Brandl （Karlsruhe Institute of Technology, Germany）

[SY-C1] Generalized yield criterion in BCC metals from first principles

○Antoine Kraych[1], Lucile Dezerald[2], Emmanuel Clouet[3], Lisa Ventelon[3], François Willaime[3], David Rodney[1] （1.Institut Lumière Matière, Université Lyon 1, France, 2.Institut Jean Lamour, Université de Lorraine, France, 3.DEN-Département des Matériaux pour le Nucléaire, CEA, Université Paris-Saclay, France）

[SY-C1] Dislocation Motion in High Entropy Alloys

○Luchan Zhang[1], Yang Xiang[2], Jian Han[3], David Srolovitz[3] （1.National University of Singapore, Singapore, 2.Hong Kong University of Science and Technology , Hong Kong, 3.University of Pennsylvania, United States of America）

[SY-C1] A random walk model of screw dislocation cross-slip in face-centered cubic solid solution alloys

○Wolfram Georg Noehring[1,2], William Arthur Curtin[2] （1. Department of Microsystems Engineering, University of Freiburg, Germany, 2. Institute of Mechanical Engineering, École Polytechnique Fédérale de Lausanne, Switzerland)）

[SY-C1] Modeling the climb-assisted glide of edge dislocations through a random distribution of nanosized vacancy clusters

○Marie Landeiro Dos Reis[1], Laurent Proville[1], Maxime Sauzay[2], Mihai Cosmin Marinica[1], Normand Mousseau[3] （1.SRMP-CEA Saclay, France, 2.SRMA-CEA Saclay, France, 3.Département de Physique, Université de Montréal , Canada）

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room1)

[SY-C1] Kinetic Monte Carlo model of screw dislocation-solute coevolution in W-Re alloys

Invited

Yue Zhao[1], Lucile Dezerald[3], ○Jaime Marian[1,2]　(1.Dept. of Materials Science and Engineering, University of California Los Angeles, United States of America, 2.Dept. of Mechanical and Aerospace Engineering, University of California Los Angeles, United States of America, 3.Institut Jean Lamour, University of Lorraine, France）

Dislocation-solute interactions are at the heart of many important processes in materials science and metallurgy, such as solid solution strengthening, dynamic strain ageing, pipe diffusion, etc. In body-centered cubic (bcc) metals, plastic flow at low-to-intermediate homologous temperatures is controlled by screw dislocation glide. In this temperature range, both solute diffusion and dislocation motion are thermally activated processes sensitive to stress, and the overall plastic behavior can be reduced to the study of a single screw dislocation interacting with solutes. This interaction is complex, and can result in material softening and/or hardening depending on temperature and solute concentration. Here, we solve this coupled transport problem for W-Re alloys in three dimensions using kinetic Monte Carlo simulations. The interaction between Re solutes and dislocation segments is captured via the elastic dipole tensor, parameterized with electronic structure calculations, while dislocation segment-segment interactions are described using nonsingular elasticity theory. We find that there are two clearly defined regimes as a function of Re concentration. For low values, the softening effect on kink-pair nucleation energy overcomes kink-solute collisions, leading to an overall reduction in alloy strength compared to pure W. The situation is reversed at higher concentrations, resulting in overall hardening. Our results are in reasonable agreement with several experimental measurements, and point to the intrinsic nature of the softening/hardening transition in W-Re alloys. We also report on preliminary simulations of dislocation-impurity interactions in the W-Cu system, where the basic mechanisms behind dynamic strain aging in substitutional bcc solid solutions starts to manifest itself in a specific temperature range.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room1)

[SY-C1] Thermally activated solute-drag strengthening by interstitial impurities in BCC Cr

○Christian Brandl　(Karlsruhe Institute of Technology, Germany）

The application of body centered cubic (BCC) refractory metals is usually limited by the low temperature brittleness, which is intrinsically linked to the limited screw dislocation mobility. We present a combined ab-initio and molecular dynamics study on the role of impurity interstitials on the dislocation mobility and the implications on the brittle-ductile transition.

The interaction forces between dislocation and impurities are computed for the kink-pair nucleation and kink-drift to predict strengthening contribution additionally to the kink-pair nucleation limited mobility below the Knee temperature. Continuum solute-drag models informed by atomistic simulations with semi-empirical potentials and with the chemically accurate ab-initio simulation are both used to predict experimental temperature regime for solute-drag strengthening. The role of dislocation core contribution compared to the elastic interaction is discussed and compared to recent nanoindentation experiments of high purity Cr with

temperature-dependent hardness, activation volume and activation energies.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room1)

[SY-C1] Generalized yield criterion in BCC metals from first principles

○Antoine Kraych[1], Lucile Dezerald[2], Emmanuel Clouet[3], Lisa Ventelon[3], François Willaime[3], David Rodney[1]　（1.Institut Lumière Matière, Université Lyon 1, France, 2.Institut Jean Lamour, Université de Lorraine, France, 3.DEN-Département des Matériaux pour le Nucléaire, CEA, Université Paris-Saclay, France）

At low-temperature, the plastic deformation of tungsten and other body-centered cubic (BCC) metals is anisotropic, and does not follow the Schmid law applicable to most other metals. This feature arises from the behavior of $1/2<111>$ screw dislocations, which control the plasticity of BCC materials. Under the application of a simple shear stress, the dislocation trajectory undergoes microscopic deviations that are directly linked to the so-called twinning/antitwinning asymmetry (Dezerald et al. 2016). However, other components of the applied stress tensor, the non-glide stresses, are also known to influence the dislocation mobility (Duesbery &Vitek 1998). In this work we use first principles calculations to explore the influence of non-glide stresses on the mobility of screw dislocations in BCC tungsten and determine a generalized yield criterion.

DFT calculations and nudged elastic band method are used in order to determine the Peierls potential of screw dislocations under stress. Different stress tensors are applied to the simulation cells, allowing to calculate the sensibility of the Peierls potential to non-glide stresses, and obtain the dependence of the dislocation Peierls stress on these stresses. These calculations are used to adjust a yield criterion, predicting the response of a single crystal to a tensile test, and the corresponding activated glide systems. Implications regarding non-Schmid slip on weakly stressed systems will be discussed.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room1)

[SY-C1] Dislocation Motion in High Entropy Alloys

○Luchan Zhang[1], Yang Xiang[2], Jian Han[3], David Srolovitz[3]　（1.National University of Singapore, Singapore, 2.Hong Kong University of Science and Technology , Hong Kong, 3.University of Pennsylvania, United States of America）

We propose a stochastic model for dislocation motion in high entropy alloys (HEAs) that focuses on the atomic scale composition disorder. Our model is based upon how atomic-scale variations in composition effect dislocation motion through the variability of the core, rather than long range stress fields. Our model is constructed within the relatively simple Peierls-Nabarro (PN) framework, where the site occupancy disorder produces random variations in the amplitude of the interplanar potential. This in turn leads to stochastic variations in the dislocation core width, Peierls stress, and Peierls energy. Since truly random alloys are not thermodynamically stable except in the extreme high temperature limit, we also consider the effects of short range spatial correlations in the randomness. We then introduce a homogenization procedure that allows for simple incorporation of correlation. We then extend our homogenized PN results to the entire slip plane to predict the effect of randomness on the strength of the material.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room1)

[SY-C1] A random walk model of screw dislocation cross-slip in face-centered cubic solid solution alloys

○Wolfram Georg Noehring[1,2], William Arthur Curtin[2]　(1. Department of Microsystems Engineering, University of Freiburg, Germany, 2. Institute of Mechanical Engineering, École Polytechnique Fédérale de Lausanne, Switzerland))

The energy barrier for cross-slip of screw dislocations in FCC solid solution alloys is controlled by local fluctuations in the solute distribution [1]. Here, a random-walk-like model of cross-slip in solid solution alloys is presented. Cross-slip is treated as a discrete process, where on each step a one Burgers vector long dislocation segment moves from the glide to the cross-slip plane. Each step causes (i) a random energy change due to the random change in solute-dislocation and solute-solute binding energies, and (ii) a deterministic energy change due to constriction formation and stress effects. The random walk model allows to calculate the distribution of cross-slip activation energies for long (several 100 to 1000 Burgers vector long) dislocations, which is relevant for deformation of real materials, but not easily accessible by direct atomistic calculations. At zero stress, thermally activated cross-slip of long dislocations is unlikely because high activation energies become more frequent with increasing length. However, at moderate stresses (few MPa), these barriers disappear; the remaining barriers are typically well below the average barrier that one would expect if considering only average alloying effects (average change in stacking fault energy, elastic constants, etc.). Moreover, cross-slip becomes a weakest-link problem, meaning that the activation energy distribution for a long dislocation under stress can be estimated from a reference distribution for a short (40 Burgers vectors) dislocation at zero stress, whose determination is computationally inexpensive and needs to be done only once.

[1] Nö hring, W.G.; Curtin, W.A. Acta Materialia 2017, 128, 135–148.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room1)

[SY-C1] Modeling the climb-assisted glide of edge dislocations through a random distribution of nanosized vacancy clusters

○Marie Landeiro Dos Reis[1], Laurent Proville[1], Maxime Sauzay[2], Mihai Cosmin Marinica[1], Normand Mousseau[3]　(1.SRMP-CEA Saclay, France, 2.SRMA-CEA Saclay, France, 3.Département de Physique, Université de Montréal , Canada)

A multi-scale model is developed to simulate the climb-assisted glide of edge dislocations anchored by a random distribution of nanosized vacancy clusters. For a shear stress much smaller than the critical stress beyond which dislocations cross the obstacles by simple glide, we found that dislocations remain anchored for a waiting time sufficient to allow the diffusion-controlled absorption of vacancies. Then the dislocations climb perpendicularly to their glide planes up to circumvent the obstacles and subsequently glide until they encounter a different anchoring configuration. Atomic-scale simulations allowed us to characterize the interactions between an edge dislocation and nano-voids as a function of their sizes and shapes. Our atomic-scale data served to calibrate an elastic-line model which we used to evaluate the glide distance of a dislocation with realistic dimensions through a random distribution of obstacles. To complete our scheme, a standard diffusion-based model for the climb velocity of edge dislocations was used to determine the deformation rate expected through the climb-assisted glide. Our predictions made for the archetypical case

of Al are in good agreement with experiments of different types, i.e. tensile deformation tests and steady-creep tests, although no parameter was adjusted in the theory to recover experimental data.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C2] Symposium C-2

Chair: Stefan Sandfeld(Chair of Micromechanical Materials Modelling, TU Bergakademie Freiberg, Germany)
Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room1

[SY-C2] Finite deformation Mesoscale Field Dislocation Mechanics

Rajat Arora[1], Xiaohan Zhang[2], ○Amit Acharya[1] （1.Carnegie Mellon University, United States of America, 2.Stanford University, United States of America）

[SY-C2] Anisotropic and non-symmetric continuum dislocation dynamics

○Thomas Hochrainer （TU Graz, Austria）

[SY-C2] Numerical simulation of model problems in Plasticity based on Field Dislocation Mechanics

○Leo Morin[1,2], Renald Brenner[3], Pierre Suquet[2] （1.PIMM, Arts et Métiers-ParisTech, CNAM, CNRS, UMR 8006, 151 bd de l'Hopital, 75013 Paris, France, 2.Laboratoire de Mécanique et d'Acoustique, Aix-Marseille Univ, CNRS UMR 7031, Centrale Marseille, 4 impasse Nikola Tesla, CS 40006, 13453 Marseille Cedex 13, France, 3.Sorbonne Université, CNRS, UMR 7190, Institut Jean Le Rond d'Alembert, 75005 Paris, France）

[SY-C2] Direct computation of the stress field due to geometrically necessary dislocation densities

○Yichao Zhu[1], Yang Xiang[2] （1.Dalian University of Technology, China, 2.The Hong Kong University of Science and Technology, Hong Kong）

[SY-C2] Meshfree Analysis for Kink Band Formation in Mg-based LPSO Phase Based on Crystal Plasticity Cosserat Model Considering Disclination Density

○Yuichi Kimura[1], Yuichi Tadano[2], Kazuyuki Shizawa[3] （1.Grad. School of Science and Technology, Keio Univ., Japan, 2.Dept. of Mechanical Engineering, Saga Univ., Japan, 3.Dept. of Mechanical Engineering, Keio Univ., Japan）

[SY-C2] Dynamic recrystallization model for Mg/LPSO alloys coupling phase-field model and dislocation-based crystal plasticity model

○Sho KUJIRAI[1], Kazuyuki SHIZAWA[2] （1.Grad. School of Science and Technology, Keio Univ., Japan, 2.Dept. of Mechanical Engineering, Keio Univ., Japan）

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room1)

[SY-C2] Finite deformation Mesoscale Field Dislocation Mechanics

Invited

Rajat Arora[1], Xiaohan Zhang[2], ○Amit Acharya[1] (1.Carnegie Mellon University, United States of America, 2.Stanford University, United States of America)

We will describe a model of dislocation mechanics based (crystal) plasticity of unrestricted geometric and material nonlinearity that, when exercised on a sufficiently fine scale, can rigorously predict fields of arbitrary dislocation distributions in finite bodies of arbitrary anisotropy, and when exercised at larger scales of resolution adequate for meso/macro scale structural response, suitably adapting established macroscale phenonemology related to kinetics of plastic flow, makes predictions up to finite strains of size and rate-dependent mechanical behavior, texture, and mesoscale dislocation microstructure evolution in polycrystalline aggregates and single crystals. The phenonemology used to go to the mesoscale can be systematically improved as the need arises, as can the geometric fields involved along with their governing equations.

The framework will be demonstrated by results on size-effects, effects of boundary constraints on plastic flow, volume change due to dislocations, polygonization fields, evolution of lattice rotations, normal stress-effects-in-shear dependent plastic flow instabilities, all up to large strains (sometimes 100%) and with a focus on effects not predictable within linear dislocation statics or dynamics, or geometrically linear or nonlinear phenomenological plasticity theories.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room1)

[SY-C2] Anisotropic and non-symmetric continuum dislocation dynamics

○Thomas Hochrainer (TU Graz, Austria)

Continuum dislocation dynamics (CDD) is a recently developed crystal plasticity theory based on the kinematics and kinetics of dislocations as moving flexible lines in crystals. In CDD the dislocation state may be characterized in varying levels of details by considering alignment tensors of different order [1]. Constitutive laws for the lowest level CDD theory yield microscopic stresses which determine the average dislocation velocity. Such a constitutive law was recently derived for the lowest order CDD variant [2] from an energy functional.

In the lowest order theory, the average dislocation velocity is assumed to be independent of dislocation character and orientation. However, edge and screw dislocations may have different mobilities, which requires the consideration of anisotropic dislocation velocities. Moreover, two recent papers on continuum modelling of simplified systems of straight parallel edge dislocations found a new microscopic stress contribution which is related to a possible asymmetry between the average velocities of edge dislocations of opposite sign [3,4].

In the current talk we show how the kinematic equations may consider asymmetric and anisotropic dislocation velocities and how these modified evolution equations yield new microscopic stress contributions in the driving force for thermodynamically consistent CDD theory. The influence of selected terms is highlighted in small example problems.

References

[1] T. Hochrainer, 2015. Philos. Mag., 95(12), 1321-1367.

[2] T. Hochrainer, 2016. J. Mech. Phys. Solids 88, 12-22.

[3] I. Groma, M. Zaiser and P. D. Ispánovity, 2016. Phys. Rev. B, 93(21) 214110.

[4] P.-L. Valdenaire, Y. Le Bouar, B. Appolaire and A. Finel, 2016. Phys. Rev. B, 93(21) 214111.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room1)

[SY-C2] Numerical simulation of model problems in Plasticity based on Field Dislocation Mechanics

○Leo Morin[1,2], Renald Brenner[3], Pierre Suquet[2] （1.PIMM, Arts et Métiers-ParisTech, CNAM, CNRS, UMR 8006, 151 bd de l'Hopital, 75013 Paris, France, 2.Laboratoire de Mécanique et d'Acoustique, Aix-Marseille Univ, CNRS UMR 7031, Centrale Marseille, 4 impasse Nikola Tesla, CS 40006, 13453 Marseille Cedex 13, France, 3.Sorbonne Université, CNRS, UMR 7190, Institut Jean Le Rond d'Alembert, 75005 Paris, France）

The aim of this work is to investigate the numerical implementation of the Field Dislocation Mechanics (FDM) theory for the simulation of dislocation-mediated plasticity. First, a revisited elastoplastic formulation of the FDM theory is derived which permits to express the set of equations under the form of a static problem, corresponding to the determination of the local stress field for a given dislocation density distribution, completed by an evolution problem, corresponding to the transport of the dislocation density. The static problem is classically solved using FFT-based techniques (Brenner et al., 2014), while an efficient numerical scheme based on high resolution Godunov-type solvers is implemented to solve the evolution problem. Model problems of dislocation-mediated plasticity are finally considered in a simplified 2D case. First, uncoupled problems with constant velocity are considered, which permits to reproduce annihilation of dislocations and expansion of dislocation loops. Then, coupled problems with several constitutive laws for the dislocation velocity are considered. Various mechanical behaviors such as perfect plasticity and linear kinematic hardening are reproduced by the theory.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room1)

[SY-C2] Direct computation of the stress field due to geometrically necessary dislocation densities

○Yichao Zhu[1], Yang Xiang[2] （1.Dalian University of Technology, China, 2.The Hong Kong University of Science and Technology, Hong Kong）

Computation of the stress field due to geometrically necessary dislocations (GNDs) is widely believed to be typical and straightforward, if compared to other challenging issues in modelling with continuum descriptions of dislocation microstrutures. A common treatment is to adopt the Kroener's formulation which relates the dislocation density field to plastic distortion (or the eigenstrain). Then the internal stress field can be computed by using the corresponding Green's formulae subject to particular loading conditions, e.g. periodic boundary conditions or in R^3. For arbitrary loading conditions, complementary finite element (FE) analysis is needed in analogy with Van Der Giessen and Needleman's superposition method for discrete dislocation

dynamics. In this talk, however, we will show that the stress field due to GNDs subject to arbitrary loading conditions can be resolved even more directly. With the introduction of a set of dislocation density potential functions (DDPFs), one simply needs to do one step of FE analysis, while the time for eigenstrain calculation is fully saved. Other advantages of adopting DDPFs, e.g., its capability of accommodating the anisotropic dislocation motion (e.g. glide v.s. climb) will also be addressed in the proposed presentation.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room1)

[SY-C2] Meshfree Analysis for Kink Band Formation in Mg-based LPSO Phase Based on Crystal Plasticity Cosserat Model Considering Disclination Density

○Yuichi Kimura[1], Yuichi Tadano[2], Kazuyuki Shizawa[3] (1.Grad. School of Science and Technology, Keio Univ., Japan, 2.Dept. of Mechanical Engineering, Saga Univ., Japan, 3.Dept. of Mechanical Engineering, Keio Univ., Japan)

Mg alloys with a long period stacking ordered structure (LPSO) phase has attracted attention as a next-generation structural material due to its high strength and low specific weight. The strength of this alloy is mainly attributed to the kink deformation in LPSO phase. Since the boundary between the kink and matrix has a large misorientation similar to that of a grain boundary, dislocation glides are prevented at the kink boundary. The clarification of detailed behavior of kink formation through numerical simulation is highly expected. Whereas the mechanism of kink band formation has conventionally been explained by the motion and accumulation of dislocations, it is recently attempted to express its process from the point of view of a rotational crystal defect called the disclination. The authors have developed a crystal plasticity Cosserat model classified into couple stress theory with a microscopic rotational degree of freedom to describe the disclination, and carried out FE analyses on a single crystal of LPSO phase. However, the FEM using C^0 continuous shape function is not applicable for the Cosserat model because such function cannot ensure the continuity of higher-order gradient of displacement field peculiar to the Cosserat model and the analysis is limited to the infinitesimal deformation.

In this study, a meshfree method is introduced into our numerical scheme instead of the FEM and it is shown that this method can express the continuous higher-order gradient of displacement field and can be adapted to boundary conditions for microscopic rotation originating in the disclination. Also, a new boundary value analysis suitable for the crystal plasticity couple stress model is presented in the category of finite deformation theory. Then, a meshfree analysis based on the present model considering disclination density is conducted to reproduce the kink formation based on disclination behaviors, and it is shown that this model can predict the kink deformation through a quadrupole structure of disclination and array structures of GN dislocation formed around the kink band. Furthermore, the size effect on the deformation response and the mesh independence of kink band width of the present model are investigated and the influence of the boundary condition for microscopic rotation on the kink deformation is discussed.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room1)

[SY-C2] Dynamic recrystallization model for Mg/LPSO alloys coupling phase-field model and dislocation-based crystal plasticity model

○Sho KUJIRAI[1], Kazuyuki SHIZAWA[2] （1.Grad. School of Science and Technology, Keio Univ., Japan, 2.Dept. of Mechanical Engineering, Keio Univ., Japan）

Magnesium alloy with LPSO (Long-Period Stacking Ordered Structure) phase has been developed and attracted much attention for a next-generation structural material because of its outstanding mechanical properties, i.e., high yield strength, light specific weight and flame retardance. This alloy is mainly composed of α-Mg and LPSO phases. The strengthening mechanism of this alloy is attributed to a kink band formulation in LPSO phase and a grain refinement of α-Mg phase in the vicinity of LPSO phase. The deformation kink, which is one of plastic buckling in laminated materials, is formed by dislocation glide in basal slip systems. The grain refinement of α-Mg phase occurs through the dynamic recrystallization in a warm plastic work. The dynamic recrystallization is a self-organization phenomenon that recrystallized nuclei grow in the deformation process of α-Mg phase. Mechanical properties of structural metals are mainly determined by microstructures generated in the deformation process. Our research group recently developed a dynamic recrystallization model for FCC crystals by coupling the multi-phase-field (MPF) model with the dislocation-based crystal plasticity model as a strain gradient theory. In this report, we extend the above multiphysics model to that for HCP crystals so that we can predict the strengthening behavior of Mg/LPSO alloys. It is known that additional elements prevent the nucleus growth in α-Mg phase. Such effect is called the pinning effect and it is introduced into the present model. The grain boundary segregation of additional elements is also considered. We conduct multiphysics FE analyses for Mg/LPSO alloys and then reproduce the dynamic recrystallization along the deformation kink bands numerically. From the results obtained in this study, it is revealed that Mg/LPSO alloys are strengthened by the deformation kink in the LPSO phase, the grain refinement in the α-Mg phase and the interaction between those effects in the alloys.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E1] Symposium E-1

Chairs: William A. Curtin(LAMMM, EPFL, Switzerland), Liang Qi(University of Michigan, United States of America)

Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room2

[SY-E1] Mechanism of Enhanced Ductility in Mg Alloys

○W. Curtin[1], Z. Wu[2], R. Ahmad[1], B. Yin[1]　(1.EPFL, Switzerland, 2.IHPC, Singapore)

[SY-E1] **Interaction of screw dislocations with interfaces during multiaxial loading: large scale 3D simulations**

○maxime Dupraz[1], S.I. Rao[2], Helena Van Swygenhoven[1,3]　(1.PEM-LSC-PSD, Paul Scherrer Institute, Villigen, Switzerland, 2.Materials Directorate, Air Force Research Laboratory, WPAFB,, United States of America, 3.NXMM-IMX-STI, École Polytechnique Fédérale de Lausanne, Switzerland)

[SY-E1] **The Multiscale calculations on the behaviors of some nuclear fuels and cladding materials**

○shiyu du　(Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, China)

[SY-E1] The connection between ideal strengths and deformation mechanisms in BCC Refractory Metals

○Liang Qi, Chaoming Yang　(University of Michigan, United States of America)

[SY-E1] **Nanoscaled Matrix-Inclusions-Composites**

○Konrad Schneider[1], Swantje Bargmann[2]　(1.Institute of Continuum and Material Mechanics, Hamburg University of Technology, Germany, 2.Chair of Solid Mechanics, University of Wuppertal, Germany)

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room2)

[SY-E1] Mechanism of Enhanced Ductility in Mg Alloys

Invited

○W. Curtin[1], Z. Wu[2], R. Ahmad[1], B. Yin[1] (1.EPFL, Switzerland, 2.IHPC, Singapore)

Pure Mg has low ductility due to strong plastic anisotropy and due to a transition of pyramidal dislocations to a sessile basal-oriented structure [1]. Alloying generally improves ductility; for instance, Mg-3wt.%RE (RE=Y, Tb, Dy, Ho, Er) alloys show relatively high ductility [2], and typically larger than most commercial Mg-Al-Zn alloys at similar grain sizes. Possible concepts for ductility in alloys include the reduction of plastic anisotropy due to solute strengthening of basal slip, the nucleation of from basal I1 stacking faults, the prevention of the detrimental transformation to sessile structures, and the weakening of strong basal texture by some solute/particle mechanisms. Experiments and modeling do not strongly support these concepts, however. Here, we introduce a new mechanism of pyramidal cross-slip from the lower-energy Pyr. II plane to the higher energy Pyr. I plane as the key to ductility in Mg and alloys [3]. Certain alloying elements reduce the energy difference between Pyr. I and II screw dislocations, accelerating cross-slip that then leads to rapid dislocation multiplication and alleviates the effects of the undesirable pyramidal-to-basal dissociation. A theory for the cross-slip energy barrier is presented, and first-principles density functional theory (DFT) calculations, following methods in [4], are used to compute the necessary pyramidal stacking fault energies as a function of solute type for many solutes in the dilute concentration limit. Predictions of the theory then demonstrate why Rare Earth solutes are highly effective at very low concentrations, and generally capture the trends in ductility and texture evolution across the full range of Mg alloys studied to date. The new mechanism then points in directions for achieving enhanced ductility across a range of non-RE alloys.

[1] Z. Wu, W.A. Curtin, Nature 526 (2015) 62-67
[2] S. Sandlobes, et al., Acta Materialia 59 (2011) 429-439; Acta Materialia 70 (2014) 92-104
[3] Z. Wu, R. Ahmad, B. Yin, S. Sandlobes, and W. A. Curtin, Science 359, 447-452 (2018).
[4] B. Yin, Z. Wu, and W. A. Curtin, Acta Materialia 136 (2017) 249-261.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room2)

[SY-E1] Interaction of screw dislocations with interfaces during multiaxial loading: large scale 3D simulations

Invited

○maxime Dupraz[1], S.I. Rao[2], Helena Van Swygenhoven[1,3] (1.PEM-LSC-PSD, Paul Scherrer Institute, Villigen, Switzerland, 2.Materials Directorate, Air Force Research Laboratory, WPAFB,, United States of America, 3.NXMM-IMX-STI, École Polytechnique Fédérale de Lausanne, Switzerland)

In spite of extensive numerical and experimental studies, there are still many open questions related to the interaction of dislocations with interfaces. Large scale 3D Molecular Dynamics simulations of a screw dislocation interacting with Coherent Twin Boundaries (CTB) are presented for Al, Cu and Ni bi-crystals modeled with 6 different embedded atom (EAM) potentials. The simulation cell containing approximately 7.2 million atoms mimics a bi-pillar geometry subjected to compression. Two scenarii were investigated for the interaction between the screw dislocation and the CTB. In the first one, we consider the case of a single arm source: the dislocation is pinned at one end of the sample while interacting with the CTB. In the second one, the dislocation is free to propagate into the incoming grain and to interact with the twin boundary over its

entire length. It is shown that both the reaction mechanism and reaction stress depend on the material, the sign of the dislocation, the stacking fault energy, the potential chosen and can differ significantly from the results reported for quasi-2D simulations. In Cu and Ni, screw dislocations can overcome the CTB at a much lower resolved shear stress than in the quasi-2D case by cross-slip using the Friedel-Escaig (FE) mechanism. In Al, the transmission of the screw dislocation into the twinned grain occurs at a much larger stress and is achieved by a sequential mechanism using both Fleischer (FL) and FE mechanism. For all materials, the critical stress for transmission is affected by the dislocation line length and curvature. Our results highlight the importance of directly modeling the slip transfer reactions using full 3D-models.

Following these first results, we extended this study on two fronts. First, we evaluated the impact of the boundary structure on the interaction mechanism and on the critical stress for transmission, by considering the case of Incoherent Twin Boundaries containing ledges. Second, we investigated the influence of complex loading conditions on the GB-dislocation interactions. In particular we simulated intergranular interaction by applying shear stress on the bi-crystal, and performing multiaxial loading tests with different load ratios.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room2)

[SY-E1] The Multiscale calculations on the behaviors of some nuclear fuels and cladding materials

○shiyu du （Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, China）

For the nuclear plants, the safety and efficiency of the reactors are the most conerned issues mainly determined by the performance of the applied materials. Hence, the structural design of new nuclear fuels and the development of new generation cladding materials have been the research focus for years. In our works, we have studied the crystalline structures of different members of uranium silicides by first principle calculations. The impact of defects on the stability and lattice structure of uranium silicide from microscopic scale is investigated and predictions on the performance in the reactor are discussed. As the promising cladding materials, SiC/SiC composite is studied in our group as well. Non-equilibrium Molecular Dynamics simulations are performed to study the mechanism for the mechanical failure of the coating-matrix and coating-fiber interfaces. It is found that the mechanical strength of interface is strongly dependent on the temperature of the system. At 700-1000K, the shear strength is significantly reduced due to the phase transition of the pyrolysis carbon coatings. Furthermore, the implanted He atoms are also determined as a major factor that influence the mechanical behavior. The exsitence of He atoms in the coating materials may cause a significant increase in shear strength and have a delaying effect on the high temperature failure. The phase field formulation has been employed to investigate the abnormal grain growth behaviors for UO_2 with pores in the final stage of sintering from mesoscale. The microstructure evolution is found dependent on the total volume fraction and individual sizes of pores. The grain growth rate is evidently suppressed when the porosity is high and it is found independent of pore size at low porosity. Moreover, the smaller pores may cause worse abnormal grain growth at low porosities and more significant stagnation effect at high porosities in the sintering of UO_2.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room2)

[SY-E1] The connection between ideal strengths and deformation mechanisms in BCC Refractory Metals

○Liang Qi, Chaoming Yang （University of Michigan, United States of America）

An important theoretical criterion to evaluate the ductility of body-centered cubic (bcc) refractory metals is the mechanical failure mode of their perfect crystals under tension along [100] directions. When the tensile stress reaches the ideal tensile strength, a perfect crystal of a group-6 element (Mo or W) fails by a cleavage fracture along (100) plane so that it is intrinsically brittle, but a perfect crystal of a group-5 element (V, Nb or Ta) fails by a shear deformation along certain slip plane so that it is intrinsically ductile. We have applied first-principles calculations and linear elastic fracture mechanics to find the alloying strategy to change their intrinsic ductility/brittleness. However, how these ideal strength properties affect the realistic deformation and fracture mechanisms of these refractory alloys are still unclear. Thus, we construct and find different modified embedded atom method (MEAM) interatomic potentials, which can duplicate the ideal strength behavior of those bcc refractory metals under multiple deformation modes. Then we apply atomistic simulations based on these interatomic potentials to investigate the dislocation and fracture behaviors near the crack tips for refractory metals with different ideal tensile strength properties, such as Mo and Nb. The results indeed show that the competitions between dislocation activities and fracture propagations in different refractory metals indeed are controlled by their ideal strength behavior in the corresponding perfect crystals. These results bring us new physical insights on the ductility-brittle mechanisms of bcc refractory metals under extreme stress conditions.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room2)

[SY-E1] Nanoscaled Matrix-Inclusions-Composites

○Konrad Schneider[1], Swantje Bargmann[2]　(1.Institute of Continuum and Material Mechanics, Hamburg University of Technology, Germany, 2.Chair of Solid Mechanics, University of Wuppertal, Germany）

Tailor-Made Multi-Scale Materials Systems are predicted to achieve ultimate properties such as scratch-proof surfaces, ultra lightweight stable structures or resistance against extreme heat. However, the origin of theses exceptional characteristics most likely emerges from the hierarchal structure of these substances. Starting at the nano-scale hard, stiff, strong and at the same time very lightweight structures are obtainable, cf. [1]. Often it is a vague procedure to explore the many unknown adjustment options like morphology, material combination etc. which would result in desired properties.

This contribution focuses on so called matrix-inclusion nano-composites. Herein state of the art generation procedures of randomized representative volume elements, featuring a fast, robust and highly automatable algorithm with fully periodic finite element models, are employed [2,3]. Super stiff nano-particles and a soft cross-linked matrix material are considered. We investigate non-linear effects of macroscopic responses which are directly linked to the employed material laws at the micro-scale and might therefore lead to a more conclusive relation between the different scales.

[1] Georgopanos, Prokopios, Gerold A. Schneider, Axel Dreyer, Ulrich A. Handge, Volkan Filiz, Artur Feld, Ezgi D. Yilmaz et al. "Exceptionally strong, stiff and hard hybrid material based on an elastomer and isotropically

shaped ceramic nanoparticles." *Scientific reports* 7, no. 1 (2017): 7314.

[2] Schneider, Konrad, Benjamin Klusemann, and Swantje Bargmann. "Automatic three-dimensional geometry and mesh generation of periodic representative volume elements for matrix-inclusion composites." *Advances in Engineering Software* 99 (2016): 177-188.

[3] Bargmann, Swantje, Benjamin Klusemann, Jürgen Markmann, Jan Eike Schnabel, Konrad Schneider, Celal Soyarslan, and Jana Wilmers. "Generation of 3D representative volume elements for heterogeneous materials: a review." *Progress in Materials Science* (2018).

[SY-E2] Symposium E-2

Chairs: Ya-Fang Guo(Beijing Jiaotong University, China), Flemming JH Ehlers(University Paris Diderot, France)
Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room2

[SY-E2] Using IM3D to simulate nano-beam and nano-target effects in ion radiation
$\circ$Ju Li （Massachusetts Institute of Technology, United States of America）

[SY-E2] First principles studies of H interaction with the face-centred cubic Al Σ5 [100] twist grain boundary during a uniaxial tensile test
Flemming JH Ehlers[2,1], Mahamadou Seydou[2], David Tingaud[1], Francois Maurel[2], Yann Charles[1], $\circ$ Sylvain Queyreau[1] （1.Universite Paris XIII, Sorbonne Paris Cite, Laboratoire des Sciences des Procedes et des Materiaux, LSPM UPR 3407, France, 2.University Paris Diderot, Sorbonne Paris Cite, ITODYS, UMR 7086, France）

[SY-E2] **Investigation of the {10-11} twin boundary migration in Magnesium**
Qun Zu[1], Xiao-Zhi Tang[2], $\circ$Ya-Fang Guo[2] （1.School of Mechanical Engineering, Hebei University of Technology, China, 2.Institute of Engineering Mechanics, Beijing Jiaotong University, China）

[SY-E2] Effect of Twins on Mechanical Properties of Silicon Nanowires
$\circ$Zheng Qin （Tianjin Univ., China）

[SY-E2] Intrinsic Ductility of Alloys from Nonlinear Elasticity
$\circ$Ian Winter[1,2], Maarten de Jong[1,3], Daryl Chrzan[1,2] （1.University of California, Berkeley, United States of America, 2.Lawrence Berkeley National Laboratory, United States of America, 3.SpaceX, United States of America）

[SY-E2] **Tailoring the stability of {10-12} twin in magnesium with solute segregation at the twin boundary and strain path control**
Heyu Zhu, $\circ$Ziran Liu （Dept. of Phyiscs, Hunan Normal University, Changsha, Hunan, China）

[SY-E2] Contribution of defects on the anisotropic diffusion behaviour of hydrogen in nickel single crystals
$\circ$Arnaud Metsue, Guillaume Hachet, Abdelali Oudriss, Xavier Feaugas （LaSIE UMR 7356 CNRS, France）

[SY-E2] Development of simplified model for one-sided mechanical joining of dissimilar materials
$\circ$Jaeho Kim, Heungjae Choi, Dongchoul Kim （Dept. of Mechanical Engineering, Sogang Univ, Korea）

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room2)

[SY-E2] Using IM3D to simulate nano-beam and nano-target effects in ion radiation

○Ju Li （Massachusetts Institute of Technology, United States of America）

Full 3D simulations of ion irradiation are necessary in a wide range of applications to capture the increasing effect of ion leakage out of surfaces or interfaces [Nuclear Fusion 57 (2017) 016038]. Using a recently developed 3D Monte Carlo simulation code IM3D [Scientific Reports 5 (2015) 18130], we first quantify the relative error of the 1D approach in three applications of nano-scale ion implantation: (1) nano-beam for nitrogen-vacancy (NV) center creation, (2) implantation of nanowires to fabricate pn junctions, and (3) irradiation of nano-pillars for small-scale mechanical testing of irradiated materials. Because the 1D approach fails to consider the exchange and leakage of ions from boundaries, its relative error increases dramatically as the beam/target size shrinks. Lastly, the "Bragg peak" phenomenon, where the maximum radiation dose occurs at a finite depth away from the surface, relies on the assumption of broad beams. We discovered a topological transition of the point-defect or defect-cluster distribution isosurface when one varies the beam width, in agreement with a previous focused helium ion beam irradiation experiment. We conclude that full 3D simulations are necessary if either the beam or the target size is comparable or below the SRIM longitudinal ion range. [Nanoscale 10 (2018) 1598]

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room2)

[SY-E2] First principles studies of H interaction with the face-centred cubic Al Σ5 [100] twist grain boundary during a uniaxial tensile test

Flemming JH Ehlers[2,1], Mahamadou Seydou[2], David Tingaud[1], Francois Maurel[2], Yann Charles[1], ○Sylvain Queyreau[1] （1.Universite Paris XIII, Sorbonne Paris Cite, Laboratoire des Sciences des Procedes et des Materiaux, LSPM UPR 3407, France, 2.University Paris Diderot, Sorbonne Paris Cite, ITODYS, UMR 7086, France）

For the theoretical examination of intergranular fracture, ab initio investigations of grain boundaries (GBs) subjected to loading play a central role. While the modelling of material failure is an inherently multi-scale task, a first principles framework often provides unmatched accuracy for the description of atomic rearrangements and bond breakage at the heart of the region of key interest. At the same time, it is integral to a meaningful analysis that the atomistic traction-separation curve emerging from density functional theory (DFT) based studies be coupled self-consistently to the stress field of the surrounding bulk grain. The absence of a robust solution to this challenge has manifested itself as a "cell size convergence problem" for the computed atomistic GB properties. In this talk, we first show how this obstacle may be entirely circumvented for the modelling of metal GBs within a standard DFT framework. (F. J. H. Ehlers et al., Comput. Mater. Sci. 139, 39 (2017)) In the procedure, we delimit a GB "local region" outside which the system response to deformation bears no significant evidence of the presence of a nearby GB. Then, we show through the example of H decoration of the fcc Al Σ5 36.87° [100] twist GB how this platform may be used efficiently for quantifying the influence of impurities on a metal GB in a multi-scale modelling scenario. The H formation energies at the various unequivalent sites in the vicinity of the GB evolve differently with the increase of tensile strain. Finally, the H impact on the full TSL curve assuming fast diffusion of H atoms at the

most stable sites during elongation is assessed.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room2)

[SY-E2] Investigation of the {10-11} twin boundary migration in M agnesium

Qun Zu[1], Xiao-Zhi Tang[2], ○Ya-Fang Guo[2]   (1.School of Mechanical Engineering, Hebei University of Technology, China, 2.Institute of Engineering Mechanics, Beijing Jiaotong University, China)

Due to the low symmetry and limited slip systems, deformation twinning plays an important role in the plastic deformation of hexagonal close-packed (hcp) metals. In this work, the {10-11} twin boundary migration under different directions of shear is studied by molecular dynamics simulations. The twin boundary migration is found to be fulfilled by the two-layer twinning dislocation movement on the twin boundary, with both screw and edge components. The implementation of the TD-mediated migration relies on the <1-210> screw component, while the direction of TB migration is determined by the <10-12> edge component. The two-layer twinning dislocation structure is further compared with the experimental observation.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room2)

[SY-E2] Effect of Twins on Mechanical Properties of Silicon Nanowires

○Zheng Qin   (Tianjin Univ., China)

The yield strength and tensile ductility of metals can be effectively increased by the existence of nano twins, leading to a significant ductile-to-brittle transition in Au, for example. Similarly, in experiments, silicon nanorods or nanowires containing twins have also been reported. Using molecular dynamics (MD) simulations, a modified embedded-atom-method (MEAM) potential was used to systematically study twinned silicon nanowires (SiNWs) with different shapes, in order to characterize the effect of twins on their mechanical properties. Our results indicate that twins improve the yield strength and tensile ductility of SiNWs, which contribute to the further understanding of mechanical responses of low-dimensional silicon materials, and certify that they have promising potential applications in the design and manufacture of silicon-based nano devices.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room2)

[SY-E2] Intrinsic Ductility of Alloys from Nonlinear Elasticity

○Ian Winter[1,2], Maarten de Jong[1,3], Daryl Chrzan[1,2]   (1.University of California, Berkeley, United States of America, 2.Lawrence Berkeley National Laboratory, United States of America, 3.SpaceX, United States of America)

The direct computation of the ideal strength of an alloy is confounded by the lack of formal crystalline symmetry. A simple analytical method to estimate the ideal strength and to study intrinsic ductility of a crystalline solid using higher-order elastic constants is presented. Since the method is rooted in parameters that are easily calculated, even for disordered systems, it can be applied to study the properties of alloys.

This method estimates the stress and strain associated with elastic instability and yields the detailed mode of the instability. It is noted that ductility and brittleness are relative. A parameter gauging the relative intrinsic ductility of a material is introduced, and is shown to be consistent with experimental measurements of elongation for a number of materials. Finally, the model is applied to the study of a chemically complex alloy, W-Nb-Mo-Ta-V, and is used to suggest shifts in composition that will increase the ductility of the alloy. The work is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05-CH11231 (Materials Project program KC23MP).

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room2)

[SY-E2] Tailoring the stability of {10-12} twin in magnesium with solute segregation at the twin boundary and strain path control

Heyu Zhu, ○Ziran Liu （Dept. of Phyiscs, Hunan Normal University, Changsha, Hunan, China）

{10-12} twinning in magnesium is commonly activated at the room temperature under mechanical loading to accommodate arbitrary deformation. Effect of solute segregation at twinning boundary on the stability of {10-12} twinning which is dependent on the strain path was investigated by employing first-principles calculations. A model of simulating twinning under external stress is proposed to predict the stability of twinning with solid solutes under strains. The calculations reveal that the stability of {10-12} twinning could be tailored by applying external stress on twinning with or without solid solutes at boundary. The modeling well match the previous experimental results. Effective solute could be selected based on the electron work function to substitute a certain position along the {10-12} twinning boundary in order to stabilize the twinning.

Reference:
1. Z.R. Liu, D.Y. Li, Acta Materialia 2015;89:225.
2. Z.R. Liu, D.Y. Li, Computational Materials Science 2015;103:90.
3. H. Zhu, Z. R. Liu, Submitted to Computational Materials Science, 2018.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room2)

[SY-E2] Contribution of defects on the anisotropic diffusion behaviour of hydrogen in nickel single crystals

○Arnaud Metsue, Guillaume Hachet, Abdelali Oudriss, Xavier Feaugas （LaSIE UMR 7356 CNRS, France）

It has been proven that hydrogen contributes significantly to the embrittlement of metals. In particular, several experimental studies have shown that hydrogen promotes the formation of superabundant vacancies, which can act as an embrittlement mechanism. Recently, anisotropic hydrogen diffusion behaviour has been put in forward experimentally in external stress-free Ni single crystals [1]. Therefore, it has been suggested that defects, including superabundant vacancies and vacancy clusters, and their elastic displacement fields may be responsible to the observed anisotropic diffusion behaviour.

In this study, we conduct DFT-based *ab initio* calculations to study hydrogen diffusion in an elastic strain field induced by the solute, vacancies and vacancy clusters in Ni single crystal. Temperature effects have

been taken into account from the extension of the calculations to the free energy including vibration and electronic excitations contributions. The diffusion tensor in the solid under stress is determined from the hydrogen elastic dipole and the total strain field induced by the defect. The latter is calculated in an anisotropic elasticity media according to the previous work of Larché and Cahn [2]. We found that the elastic displacement fields induced by the solute and the vacancies are not strong enough to reproduce the anisotropic diffusion behaviour observed experimentally. Therefore, we turn our study to the effect of the vacancy clusters, which can act as gas bubbles. These vacancy clusters have been observed using TEM on H-charged Ni single crystals [3]. The presence of such clusters and their elastic displacement fields can reproduce the diffusion coefficient tensor observed experimentally and suggests the large contribution of these defects on the anisotropic diffusion of hydrogen in Ni single crystal. Finally, we discuss some implications of the presence of vacancy clusters on the initiation of embrittlement based on the instability of such defects according to the work of Bockris and Reddy [4].

[1] J. Li, et al., Sci Rep, vol 7, 45041, 2017
[2] F. C Larché et J. W Cahn, Acta Metall, vol 30, p 1835-1845, 1982
[3] G. Hachet, et al., Acta Mater, vol 148, p 280-288, 2018
[4] J. O'M Bockris and S. U. M. Khan, Surface Electrochemistry: A Molecular Level Approach, Plenum Press, 1993

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room2)

[SY-E2] Development of simplified model for one-sided mechanical joining of dissimilar materials

○Jaeho Kim, Heungjae Choi, Dongchoul Kim （Dept. of Mechanical Engineering, Sogang Univ, Korea）

There are needs for one-sided mechanical joining dissimilar materials in automotive industry because it is efficient to fasten dissimilar materials for manufacturing light-weight vehicles. The full car crash model applying the joining technology with solid elements leads to an impractical computational cost due to the complexity of the model. Thus, we develop a simplified model with shell elements of the joining technology, which is efficient enough to simulate a full car model. We analyze and optimize the parameters of the simplified model that determine the behavior of the joining technology. The developed model is validated with lap shear and cross tension tests.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F1] Symposium F-1

Chair: Yunzhi Wang(The Ohio State University, United States of America)
Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room3

[SY-F1] **An Integrated Experimental and Computational Approach to Microstructure-Property Relationships in Structural Materials**

Longsheng Feng, Pengyang Zhao, Steve Niezgoda, Mike J Mills, ○Yunzhi Wang （The Ohio State University, United States of America）

[SY-F1] **Development of a multiscale simulation system based on microstructure of fine-grained aluminum**

○ATSUSHI SAGARA, YOSHITERU AOYAGI （Dept. of Finemechanics, Tohoku Univ., Japan）

[SY-F1] **Image-based crystal plasticity analysis on the activities of slip systems in polycrystal alpha-Ti**

○Yoshiki Kawano[1], Tetsuya Ohashi[1], Tsuyoshi Mayama[2], Masaki Tanaka[3], Yelm Okuyama[3], Michihiro Sato[1] （1.Kitami Institute of Technolgy, Japan, 2.Kumamoto University, Japan, 3.Kyushu University, Japan）

[SY-F1] **Micro structure-based Crystal Plasticity Modeling of of Duplex Titanium Alloy During Hot Deformation**

○Jun Zhang[1], Yang Wang[2], Yu Wang[2] （1.Institute of Systems Engineering,China Academy of Engineering Physics, China, 2.Department of Modern Mechanics, CAS Key Laboratory of Mechanical Behavior and Design of Materials, University of Science and Technology of China, China）

[SY-F1] **Nonlocal multiscale modeling of deformation behavior of polycrystalline copper by second-order homogenization method**

○makoto uchida, Akito Taniguchi, yosihisa kaneko （Osaka city Univ., Japan）

[SY-F1] **Residual stress prediction for turning of Ti-6Al-4V considering the microstructure evolution**

Zhipeng Pan[2], ○Donald S Shih[1], Hamid Garmestani[3], Elham Mirkoohi[2], Steven Y Liang[2] （1.Magnesium Research Center, Kumamoto University, Japan, 2.George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, United States of America, 3.School of Materials Science and Engineering, Georgia Institute of Technology, United States of America）

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room3)

[SY-F1] An Integrated Experimental and Computational Approach to Microstructure-Property Relationships in Structural Materials

Invited

Longsheng Feng, Pengyang Zhao, Steve Niezgoda, Mike J Mills, ○Yunzhi Wang （The Ohio State University, United States of America）

Location-specific component design requires modeling capabilities that incorporate specific transformation and deformation mechanisms operating in alloys having different compositions and microstructures under different service conditions. In this presentation, we focus on how to utilize phase-field modeling techniques at different length scales to address this difficult challenge and develop mechanism-based and microstructure-sensitive modeling tools. In particular, using creep deformation in Ni-base superalloys as an example, we demonstrate how to integrate phase-field modeling with experimental characterization and use phase-field method to bridge *ab initio* calculations and crystal plasticity (CP) simulations to (a) identify transformation / deformation mechanisms and quantify activation pathways, (b) provide "mechanism maps" and microstructure-sensitive constitutive laws for dislocation - microstructure interaction and co-evolution, and (c) develop an integrated phase-field + full-field FFT-based CP modeling framework for collective behavior of precipitate and dislocation microstructures during creep deformation. The work is supported by the National Science Foundation under the DMREF program.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room3)

[SY-F1] Development of a multiscale simulation system based on microstructure of fine-grained aluminum

○ATSUSHI SAGARA, YOSHITERU AOYAGI （Dept. of Finemechanics, Tohoku Univ., Japan）

In plastic working of metal plates, spring back and generation of cracks and sticks cause defective products. The finite element method is widely used to predict and control behavior of plastic working. Since press forming that is a sort of plastic working consists of various processes such as deep drawing, stretching, and bending, a multiaxial stress state dominates plastic deformation. The von Mises yield function is well known as a theory to express yielding behavior of mechanical isotropic metals under a multiaxial stress state. The mechanical properties for the von Mises yield function are usually identified by a uniaxial tensile test. In the case of ultrafine-grained metals produced by severe plastic deformation, they have strong orientation in mechanical properties due to a rolling texture. Therefore, the isotropic yield function cannot fully express the yielding behavior of ultrafine-grained metals. Some models such as Hill yield function, Barlat Yld-2000, etc. are proposed to express the mechanical anisotropy of metals. However, a large number of material parameters are required for determination of yield function and it is difficult to determine these parameters only by uniaxial tensile test. Tests reproducing a multiaxial stress state such as a biaxial tensile test and a compression-torsion test, which requires a tremendous labor, are necessary to obtain a yield surface identifying the material parameters. Numerical prediction of yield surface is anticipated on the basis of multiscale simulation considering information of microstructure of metals.

In this study, we aim at seamless bridging of design, development, and practical use of mechanical anisotropic metals with CAE system. Mechanical anisotropy of severe rolled aluminum is predicted by crystal plasticity analyses reflecting information of rolling texture. Furthermore, biaxial tensile tests were conducted and the mechanical anisotropy was evaluated by comparison of the experimental and numerical results. We

developed a user subroutine for a commercial CAE software. Simulation result calculated by the CAE software was compared with microscopic deformation behavior of practical plastic working to evaluate the effect of predicted anisotropic yield function.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room3)

[SY-F1] Image-based crystal plasticity analysis on the activities of slip systems in polycrystal alpha-Ti

○Yoshiki Kawano[1], Tetsuya Ohashi[1], Tsuyoshi Mayama[2], Masaki Tanaka[3], Yelm Okuyama[3], Michihiro Sato[1]
（1.Kitami Institute of Technolgy, Japan, 2.Kumamoto University, Japan, 3.Kyushu University, Japan）

It has been pointed out that the activation of basal slip systems in alpha-Ti leads to fatigue failure under fatigue loading. Thus, it is important to quantitatively evaluate the activity of basal slip systems in alpha -Ti for ensuring the safety and reliability and predicting the fatigue lifetime with higher accuracy. However, the deformation mechanisms are still incompletely understood, and the activity of basal slip systems under the deformation is also not clarified.

When forced displacement is applied to polycrystal alpha-Ti, decreases in the amount of deformation in crystal grains would lead to those of increases in the other crystal grains because the reduction of the deformation in a crystal grain must be compensated by increases in those in the other crystal grains. That is, there is a possibility that changes in the activity of slip systems of crystal grains influence those of the basal slip systems of the other crystal grains.

In this study, a crystal orientation map obtained by Electron Back Scatter Diffraction (EBSD) patterns of a pure titanium (alpha-Ti) specimen was converted into a geometric model for finite element method using an interface developed by authors, and Crystal Plasticity Finite Element (CPFE) analysis was conducted. The crystal orientations in the specimen showed that (0001) planes of almost crystal grains declined in the direction from ND to RD, and the microstructure has a texture so-called RD-Split. A dislocation density dependent constitutive equation was employed and unidirectional tensile loading was applied to the geometric model by the forced displacement. Several sets of initial Critical Resolved Shear Stress (CRSS) were employed for the simulation. The relationship between the initial CRSS of each slip system and the activity of basal slip systems was investigated.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room3)

[SY-F1] Micro structure-based Crystal Plasticity Modeling of of Duplex Titanium Alloy During Hot Deformation

○Jun Zhang[1], Yang Wang[2], Yu Wang[2]　（1.Institute of Systems Engineering,China Academy of Engineering Physics, China, 2.Department of Modern Mechanics, CAS Key Laboratory of Mechanical Behavior and Design of Materials, University of Science and Technology of China, China）

A crystal plasticity finite element model (CPFE) is presented to describe the hot deformation of titanium alloy with a duplex microstructure. The model accounts for the individual plasticity slips within both primary α grains and lamellar Widmanstatten grains using a isostress homogenization approach. The finite element model is initial by a random program. The material parameters considering the scale of singal crystal are determined by the combination of interpolation optimization method and the experiment data published in

the literature. The numerical results are in good agreement with the experimental tension stress-strain curve at high temperature, indicating that the numerical model is suitable to describe the hot deformation of duplex titanium alloy. The corresponding results give a deep insight into the relationship between the microstructure and macro-mechanical behavior, and provide richer clues for the optimization design of titanium alloy.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room3)

[SY-F1] Nonlocal multiscale modeling of deformation behavior of polycrystalline copper by second-order homogenization method

○makoto uchida, Akito Taniguchi, yosihisa kaneko （Osaka city Univ., Japan）

The macroscopic mechanical property of metal materials relates to the microscopic polycrystalline structure. In the present study, micro- to macroscopic nonuniform deformation of the polycrystalline pure copper is evaluated by experimental and numerical studies. The uniaxial tension of the specimen having curved gage section was performed. The effects of the curvature and the grain size on the deformation localization in the specimen were experimentally evaluated by digital image correlation method. The strain localization around the curvature is modulated for the specimen with larger crystal grain. The computational simulations of the tensile tests were then performed using the second-order homogenization method. A series of the numerical simulation clarified the size-depended strain localization in the macroscopic scale.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room3)

[SY-F1] Residual stress prediction for turning of Ti-6Al-4V considering the microstructure evolution

Zhipeng Pan[2], ○Donald S Shih[1], Hamid Garmestani[3], Elham Mirkoohi[2], Steven Y Liang[2] （1.Magnesium Research Center, Kumamoto University, Japan, 2.George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, United States of America, 3.School of Materials Science and Engineering, Georgia Institute of Technology, United States of America）

An analytical model for residual stress prediction considering the effects of material dynamic recrystallization under process-induced mechanical and thermal stresses is proposed. The effect of microstructure evolution on residual stress generation during the turning process is considered. The Johnson-Mehl-Avrami-Kolmogorov model is used to calculate grain size evolution due to thermal mechanical effects in the machining process. A modified Johnson-Cook flow stress model is developed by introducing a material grain growth-induced softening term. The classic Oxley's cutting mechanics theories are implemented for machining forces calculation. A hybrid algorithm accounting for thermal, mechanical, and microstructure evolution effects is used to predict the residual stress profile on a machined workpiece surface. The proposed method is implemented for the orthogonal turning of Ti-6Al-4V material. Comparison is conducted between the model prediction and the measured residual stress data in the literature. The general trend of the machining-induced residual stress on the machining surface is accurately captured by the proposed model. Moreover, the parametric study is conducted to investigate the effect of rake angle and depth of cut on the residual stress profile.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F2] Symposium F-2

Chair: Selim Esedoglu(University of Michigan, United States of America)

Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room3

[SY-F2] New algorithms for simulating grain boundary motion

○Selim Esedoglu （University of Michigan, United States of America）

[SY-F2] The Role of Grain Shape in Discrete Element Modeling of Snow Mechanics

○Carolin Willibald, Thiemo Theile, Martin Schneebeli （Institute for Snow and Avalanche Research (SLF, ETH), Switzerland）

[SY-F2] Experimental-Computational Analysis of Primary Static Recrystallizazion in DC04 Steel

○Martin Diehl, Markus Kühbach, Dierk Raabe （Max-Planck-Institut fuer Eisenforschung GmbH, Germany）

[SY-F2] Large scale phase-field simulations of solid state sintering

○Johannes Hoetzer[1,2], Marco Seiz[2], Michael Kellner[2], Wolfgang Rheinheimer[3], Hernik Hierl[1], Britta Nestler[2,1] （1.Karlsruhe University of Applied Sciences, Germany, 2.Karlsruhe Institute of Technology, Germany, 3.Purdue University, United States of America）

[SY-F2] Phase-field simulations of coupled dendritic-eutectic growth

○Marco Seiz[1], Michael Kellner[1,2], Johannes Hötzer[1,2], Philipp Steinmetz[3], Britta Nestler[1,2] （1.Institute of Applied Materials - Computational Materials Science, Karlsruhe Institute of Techology, Germany, 2.Institute of Digital Materials Science, Karlsruhe University of Applied Sciences, Germany, 3.Department of Materials Science and Engineering, University of Alabama at Birmingham, United States of America）

[SY-F2] The use of thermodynamic tensor models for phase-field simulations of spinodal decomposition in quaternary alloys coupled with CALPHAD data.

○Yuri Amorim Coutinho[1], Nico Vervliet[2], Lieven De Lathauwer[2,3], Nele Moelans[1] （1.Dept. of Materials Engineering, KU Leuven, Belgium, 2.Dept. of Electrical Engineering, KU Leuven, Belgium, 3.Group Science, Engineering and Technology, KU Leuven - Kulak, Belgium）

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room3)

[SY-F2] New algorithms for simulating grain boundary motion

Invited

○Selim Esedoglu （University of Michigan, United States of America）

I will describe the latest developments in a class of algorithms known as threshold dynamics for simulating the motion of interfaces under curvature and related flows, as appears in many models of grain boundary motion. These are remarkably elegant algorithms that generate the desired evolution, along with all the correct boundary conditions along junctions, by alternating two very simple and efficient procedures: Convolution with a kernel and thresholding. They allow arbitrarily large time steps, and handle topological changes automatically. The most recent versions allow specifying N-choose-2 anisotropic (normal dependent) surface tensions and anisotropic (normal dependent) mobilities for a network of N grains. We will describe simple and explicit formulas that tell us how to bake in the desired set of mobility and surface tension functions into the algorithm.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room3)

[SY-F2] The Role of Grain Shape in Discrete Element Modeling of Snow Mechanics

○Carolin Willibald, Thiemo Theile, Martin Schneebeli （Institute for Snow and Avalanche Research (SLF, ETH), Switzerland）

The macro-mechanical properties of the heterogeneous material snow are determined by its microstructure. Single ice crystals are connected by sintering and form a complex ice skeleton. In this microstructure fracture occurs under high strain rate deformations, which are relevant for applications such as avalanche risk forecasting or snow mobility. During such a deformation snow transforms from a porous sintered into a granular material. Both states can be represented by the discrete element method, which is well suited for the mechanical description of snow. However, a convenient but strongly simplified assumption is a spherical shape of the snow particles. The grain shape is important in both structural states: it affects the granular dynamics and controls the number and size of inter-particle contacts, which are crucial for the strength and fracturing behavior of the structure. Yet, a detailed reconstruction of the snow grains with discrete elements is neither preferable for the computational efforts nor necessary for most applications. In laboratory experiments, we investigate the mechanical properties of ice beads and two natural snow types, differing in crystal shape and size. The ice beads allow one-to-one comparison with the DEM simulations and are used as a well-defined intermediate step to later adapt the model to the natural snow types. Compression tests were performed under variation of the sintering time, which is related to the bond size and therefore critical for the strength of the snow microstructure. By means of 3D computed tomography images, the number and size of bonds between the ice beads are quantified and simulations can be performed with the same bead configuration as in the experiments. The relation of the sintering state and the macroscopic strength of the sample is examined in experiments and simulations. Once the simulations perform well in the bead case, the model is modified in terms of bond number and size, to match the mechanical behavior of the natural snow types. Accounting for the grain shape in our DEM snow model remarkably improves the simulations of snow micro- as well as macro-mechanical processes.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room3)

[SY-F2] Experimental-Computational Analysis of Primary Static Recrystallizazion in DC04 Steel

○Martin Diehl, Markus Kühbach, Dierk Raabe （Max-Planck-Institut fuer Eisenforschung GmbH, Germany）

Low-alloyed steels with body-centered cubic crystal structure (bcc, ferrite) are a material class which is widely used in automotive sheet metal forming applications. When produced with an adequate crystallographic texture, the mechanical behavior of steels for forming applications is characterized by an isotropic in-plane flow behavior in combination with a low yield strength. To obtain these beneficial mechanical properties, an adequate cold rolling strategy in terms of the number of passes, deformation rates, and total reduction needs to be followed by an annealing procedure with a time-temperature profile that facilitates primary static recrystallization. The most fundamental connection between cold rolling and heat treatment consists in the reduction of the dislocation-related free energy stored during deformation by the formation of new grains with a very small dislocation content. Hence, the local variation in crystallographic orientation and defect population lead to very inhomogeneous grain boundary migration velocities.

We present here results of a coupled experimental-computational approach for studying microstructure evolution in industrially cold rolled DC04 steel under quasi-isothermal conditions. For the experimental characterization, quasi in-situ experiments consisting of interrupted isothermal holding at 600°C and subsequent Electron Backscatter Diffraction (EBSD) orientation imaging were conducted. The results reveal a strong correlation between local dislocation density, quantified via the Kernel Average Misorientation (KAM), and the local increase of recrystallized volume fraction. To complement the experimental findings and gain further insights into the influence of the sub-surface microstructure, a Cellular Automata (CA) model was utilized. The employed three-dimensional microstructure model was directly built from the experimentally characterized deformation microstructure. Different approaches of scaling the KAM into dislocation density values, i.e. the driving force for recrystallization, are employed. Similarities and deviations between experimental and computational results are discussed with the aim at increasing the understanding the mechanisms of static primary recrystallization.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room3)

[SY-F2] Large scale phase-field simulations of solid state sintering

○Johannes Hoetzer[1,2], Marco Seiz[2], Michael Kellner[2], Wolfgang Rheinheimer[3], Hernik Hierl[1], Britta Nestler[2,1] （1.Karlsruhe University of Applied Sciences, Germany, 2.Karlsruhe Institute of Technology, Germany, 3.Purdue University, United States of America）

Ceramic materials are of high interest for technical applications due to their excellent material properties regarding hardness, strength, density, wear resistance or corrosion resistance.
Due to the dependence of the material properties on the microstructure, a deep understanding of the sintering process is needed to produce advanced ceramics with tailored properties.
During the solid state sintering process the initially loose powder of green body densifies and particles coarsen.
This process is driven by the reduction of the interfacial energy from the surface as well as the grain boundaries.
Depending on the different mechanisms, volume, surface and grain boundary diffusion, the densification and

grain growth rate in the microstructure can be influenced.

However, due to the complex interplay of the material and process parameters, it is challenging to predict the microstructure evolution.

In this talk, a phase-field model is presented to investigate the microstructure evolution during solid state sintering.

The model is based on the grand potential approach and considers the different diffusion mechanisms which can vary by multiple magnitudes.

To resolve realistic green bodies with multiple thousand particles and different partial size distributions, large scale domains are required.

To efficiently investigate such systems, the model is implemented in a highly optimized manner in the massive parallel phase-field solver framework PACE3D.

Therefore the solver is optimized on various levels and the kernels are explicitly vectorized using intrinsics.

In the first part of this talk, the influence of the different diffusion mechanisms on the microstructure evolution for two and four particle settings are validated.

In the second part, the densification and grain growth depending on the active diffusion mechanisms are investigated using realistic green bodies with multiple thousand grains.

Also the effect of different initial densities and partial size distributions are investigated.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room3)

[SY-F2] Phase-field simulations of coupled dendritic-eutectic growth

°Marco Seiz[1], Michael Kellner[1,2], Johannes Hötzer[1,2], Philipp Steinmetz[3], Britta Nestler[1,2] (1.Institute of Applied Materials - Computational Materials Science, Karlsruhe Institute of Techology, Germany, 2.Institute of Digital Materials Science, Karlsruhe University of Applied Sciences, Germany, 3.Department of Materials Science and Engineering, University of Alabama at Birmingham, United States of America)

The solidification of alloys shows a large variety of different microstructures depending on the material system and processing conditions. Since material properties such as tensile strength are dependent on the microstructure, its prediction is a topic of high interest in order to produce materials with tailored properties. Whereas theory is capable of investigating simple geometries, simulations are necessary in order to ascertain the influence of complex evolving geometries. An example of this is the coupled growth of dendrites and eutectics, which typically grow at different length scales.

One way to simulate such problems is the phase-field method which has been established as a versatile tool to investigate microstructural evolution. The used phase-field model is based on a grand potential approach with parabolic free energies approximating thermodynamic CALPHAD data of the system Al-Cu. Additionally, an ad-hoc nucleation mechanism is implemented.

Validation is done by comparison to analytical theories of pure dendritic and eutectic growth. Following the validation, the coupled growth of coarse dendrites and fine eutectics during directional solidification is investigated in two as well as three dimensions. Depending on the process parameters, observations include closely-spaced dendrites turning into cells, stable coupled growth of dendrites and eutectics, nucleation of eutectic on dendritic sidebranches as well as transitions to a completely eutectic state. Based on these results a tentative microstructure map is established.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room3)

[SY-F2] The use of thermodynamic tensor models for phase-field simulations of spinodal decomposition in quaternary alloys coupled with CALPHAD data.

○Yuri Amorim Coutinho[1], Nico Vervliet[2], Lieven De Lathauwer[2,3], Nele Moelans[1] (1.Dept. of Materials Engineering, KU Leuven, Belgium, 2.Dept. of Electrical Engineering, KU Leuven, Belgium, 3.Group Science, Engineering and Technology, KU Leuven - Kulak, Belgium)

The successful coupling of the phase-field and CALPHAD methods for a thermodynamic consistent description of the system free energy in a phase-field model is challenging for multicomponent alloys. The many coupling schemes presented in the literature all tend to suffer from inefficiencies and limitations when applied to higher-order systems. When collecting calculated thermodynamic data in a multiway array or a tensor, we can observe that the number of entries grows exponentially as a function of the number of components and thus the direct use of tensors to provide thermodynamic information to a phase-field simulation is not feasible for quaternary or higher order systems. However, when a canonical polyadic decomposition is applied, we can represent the data contained in the tensor with a small number of coefficients, which grows only linearly if new components are included. This approach allows the construction of thermodynamic tensor models, which can be efficiently used to approximate individual entries of the original tensor with good accuracy. Furthermore, the gains in data reduction obtained with the tensor decomposition technique increases when more elements are considered in the simulations. The efficiency of this novel coupling scheme is verified with spinodal decomposition simulations of quaternary alloys.

Symposium | M. Time- and History-Dependent Material Properties

[SY-M1] Symposium M-1

Chair: Thomas Voigtmann(German Aerospace Center, Cologne, Germany)

Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room4

[SY-M1] Structure-property Relations in Sheared Dense Flocculated Suspensions

○Jan Vermant （ETH Zurich, Switzerland）

[SY-M1] Soft deformable colloids make strong liquids with stress-driven relaxation

Nicoletta Gnan, ○Emanuela Zaccarelli （CNR Institute for Complex Systems, Rome, Italy）

[SY-M1] Linear viscoelasticity on matter out of equilibrium

○Leticia Lopez-Flores[1], Magdaleno Medina-Noyola[1], Jose Manuel Olais-Govea[1,2], Martin Chavez-Paez[1] （1.Universidad Autonoma de San Luis Potosi, Mexico, 2.Instituto Tecnologico y de Estudios Superiores de Monterrey, Mexico）

[SY-M1] Memory effects in functional polymers: The interplay between entropic elasticity and kinetic arrest

○Fathollah Varnik, Elias M. Zirdehi （Ruhr-University Bochum, Germany）

[SY-M1] Modelling and Experimental Verified Coupled Visco hyper electro-elastic Behaviour of Dielectric Elastomer Circular Actuator

○ARPIT SRIVASTAVA, Sumit Basu （IIT KANPUR, INDIA -208016, India）

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room4)

[SY-M1] Structure-property Relations in Sheared Dense Flocculated Suspensions

Invited

○Jan Vermant （ETH Zurich, Switzerland）

Rheological properties of dense attractive colloidal suspensions are characterized by time and deformation history dependent phenomena, which when reversible, are know as thixotropy. In the present work we will use a series of advanced characterization tools to elucidate the structure property relations in such systems. High frequency rheology is used to investigate the details of the colloidal interactions betweenthe particles and aggregates. Superposition rheology and 2D small amplitude oscilatory strain are used to investigate the mechanical properties, combined with stress jumps. Finally, high speed confocal rheoscopy is used to provide structural information on length scales of up to several 100 particles. The experiments show the role of microstructural anisotropy and and heterogeneity of the structure are caused by hydrodynamic stresses as particles and aggregates go on a "colloidal merry go round" during shear flow. The evolution of microstructural descriptors as a function of rate and strain is discussed. Comparison with recent simulation result on large scale structures will be included.
the goal is to give a hollistic view of the structure property relations in such systems.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room4)

[SY-M1] Soft deformable colloids make strong liquids with stress-driven relaxation

Invited

Nicoletta Gnan, ○Emanuela Zaccarelli （CNR Institute for Complex Systems, Rome, Italy）

Fragility is a key concept in the glass transition which describes the dependence of the structural relaxation time on the control parameter (packing fraction ϕ or temperature) upon approaching dynamical arrest. Recently, Mattson et al[1] showed a connection between softness and fragility in colloidal systems, but a deep understanding of its microscopic origin still remains elusive. Numerical simulations represents a strong ally to elucidate this problem, but in most cases softness is tuned by modifying the pair-potential parameters allowing particles to overlap to a certain extent, while neglecting crucial aspects that contribute to the elastic properties of realistic particles. On the other hand, more refined numerical models of soft particles are challenging to simulate due to the presence of internal degrees of freedom of high computational cost. As a consequence simple models like the Hertzian potential cannot capture mechanisms such as particle deformations, making the concept of "softness" in simulations and experiments very different.
To fill this gap, I will discuss a new model of 2D polymer rings with tunable softness which undergo substantial deformation at high densities. The ability to deform has a strong impact on the dependence of the relaxation time on ϕ which change from fragile-to-strong behavior. In addition, at high packing fractions, dynamics is controlled by an intermittent particle motion which gives rise to a compressed exponential decay of the self-intermediate scattering function. This behavior can be rationalized in terms of deformed rings that act as stress dipoles[2,3]. This simple model thus provides microscopic insights into two mechanisms which are of a deep interest in soft matter: the fragility dependence on softness and the occurrence of a compressed exponential decay in dynamical correlation functions.
[1] J. Mattsson, H. M. Wyss, A. Fernandez-Nieves, K. Miyazaki, Z. Hu, D. R. Reichman and D. A. Weitz, Nature

462, 83 (2009).

[2] L. Cipelletti, S. Manley, R. C. Ball and D. A. Weitz, PRL 84, 2275 (2000).

[3] E. E. Ferrero, K. Martens and J.-L. Barrat, PRL 113, 248301 (2014).

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room4)

[SY-M1] Linear viscoelasticity on matter out of equilibrium

○Leticia Lopez-Flores[1], Magdaleno Medina-Noyola[1], Jose Manuel Olais-Govea[1,2], Martin Chavez-Paez[1]
（1.Universidad Autonoma de San Luis Potosi, Mexico, 2.Instituto Tecnologico y de Estudios Superiores de Monterrey, Mexico）

The recent non equilibrium self consistent generalized Langevin equation (NE-SCGLE) theory of irreversible process in liquids has permitted to obtain a description of non- equilibrium processes involved in the arrested spinodal decomposition due to sudden and deep quenches inside the spinodal region. For a simple model liquid, where the system could be modeling by a hard sphere plus an attractive Yukawa tail, this theoretical approach predicts that the spinodal line is the borderline between the ergodic and the arrested states. Also, by means of this approach has been determined a border between phase separation and gelation, besides providing the corresponding dynamic properties to each phase. This work addresses a general method to obtain the linear viscoelastic properties of non- equilibrium processes involved in the spinodal decomposition when the system has been quenching inside the spinodal region. We show an example of the normalized shear viscosity as a function of the waiting time. This scheme offers the opportunity to describe the linear viscoelasticity and the diffusion mechanics as the waiting time elapses. Furthermore this approach is able to describe gelation effects, it leads naturally to a diverging shear viscosity at glass and gelation transition points.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room4)

[SY-M1] Memory effects in functional polymers: The interplay between entropic elasticity and kinetic arrest

○Fathollah Varnik, Elias M. Zirdehi （Ruhr-University Bochum, Germany）

In contrast to metallic alloys, the shape memory effect in polymers is not based on a change of crystalline phases but on the interplay between entropic elasticity and kinetic arrest. Consequently, the shape recovery process, during which chains start to recover their entropically most favorable conformation, strongly depends on preparation protocol, frozen stresses and the selected recovery temperature. In this work, we study these issues via molecular dynamics simulations with a special focus on aging processes and the effects arising from the presence of small molecules. It is shown that aging leads to irreversible plastic rearrangements and a resulting increase of residual strain during shape recovery. At a fixed temperature, this process is enhanced if small molecules are added to the system. Interestingly, the triggering temperature depends in a non-monotonic way on the size of added molecules. This observation is rationalized in terms of diffusion coefficient of added molecules and the strength of their coupling to the polymer matrix.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room4)

[SY-M1] Modelling and Experimental Verified Coupled Visco hyper electro-elastic Behaviour of Dielectric Elastomer Circular Actuator

○ARPIT SRIVASTAVA, Sumit Basu （IIT KANPUR, INDIA -208016, India）

Soft dielectric elastomers, with very low stiffness and high permittivity and electric breakdown strength, hold promise as candidate materials for a variety of applications including, in energy harvesting, as actuators and biological muscles. As actuators in particular, a number of applications have emerged where, utilising coupled electro-hyperelasticity under very high electric fields in thin, membrane-like structures, large actuation has been achieved. Moreover, the theoretical framework for electro-hyperelasticity of these materials has also been established. But long time durability of these devices, is still a matter of concern. The concern arises primarily from the fact that these soft elastomers not only physically age with time, but are also highly rate dependent. We have used an equi-biaxially pre-stretched circular dielectric elastomer membrane attached to a rigid frame with a load hung at the centre to demonstrate the effects of viscoelasticity. The membrane is then loaded with oscillating voltage and the motion of the center of the membrane is tracked with a laser displacement sensor, over many time periods. As the membrane is taken through a large number of cycles,the response slowly drifts. For a very soft elastomer like VHB, the drift can be sometimes discerned in as few as 20-30 cycles of operation. To model the deformation and the drift with time, a coupled electrostatic, visco-hyperelastic large deformation model for the elastomer has been incorporated into an explicit Finite Element framework. We have been able to reproduce the experimental response of the VHB membrane fixed to a rigid frame very accurately. Though the modelling has been verified for VHB only, the framework is general enough to be used to assess the effectiveness of any dielectric elastomeric material, used as a membrane under any three dimensional electro-mechanically loaded configuration.

[SY-M2] Symposium M-2

Chair: Emanuela Zaccarelli(University of Rome I, Italy)
Mon. Oct 29, 2018 3:45 PM - 5:45 PM Room4

[SY-M2] MMM in aircraft industries: use cases for simulation of additive manufacturing

○Annett Seide[1], Thomas Goehler[1], Roman Sowa[2]　（1.MTU Aero Engines AG, Germany, 2.MTU Aero Engines Polska Sp. z o. o., Poland）

[SY-M2] VISCOELASTIC BEHAVIOUR OF HETEROGENEOUS MATERIALS STUDIED THANKS TO AN EXTENSION OF CRAFT SOFTWARE IN HARMONIC REGIME

○Julien Boisse , Stéphane André, Laurent Farge　（University of Lorraine, France, France）

[SY-M2] Multi-scale modelling of Zener Pinning during the solid solution treatment of a Nickel-based Superalloy

○Magnus Jack Anderson[1], Jonathan Benson[1], Christos Argyrakis[2], Jeffery William Brooks[1], Hector Christian Basoalto[1]　（1.The University of Birmingham, UK, 2.Rolls-Royce plc, UK）

[SY-M2] Assessment of residual stresses in welds made of multiphase alloys

○Victor De rancourt[1], Sylvain Flouriot[1], Benjamin Sarre[2], Benoit Panicaud[2], Guillaume Geandier[3]　（1.Commissariat a l'energie atomique, France, 2.Universite de Technologie de Troyes, France, 3.Universite de Lorraine - CNRS, France）

[SY-M2] Atomic analysis of crystalline nucleation and growth in the supercooled liquid of glass-forming binary alloy

○Masato Wakeda[1], Shigenobu Ogata[2,3]　（1.Research Center for Structural Materials, National Institute for Materials Science, Japan, 2.Graduate school of engineering science, Osaka Univ., Japan, 3.Center for Elements Strategy Initiative for Structural Materials (ESISM), Kyoto Univ., Japan）

[SY-M2] Crystal growth in fluid flow: Nonlinear response effects

○Hailong Peng[1,2], Dieter Herlach[1], Thomas Voigtmann[1]　（1.German Aerospace Center, Germany, 2.Central South University, China）

[SY-M2] Time-dependent active microrheology in dilute colloidal suspensions

Sebastian Leitmann[1], Suvendu Mandal[4,1], Matthias Fuchs[2], Antonio M. Puertas[3], ○Thomas Franosch[1]　（1.Innsbruck Univ., Austria, 2.Konstanz Univ. , Germany, 3.University of Almeria, Spain, 4.Heinrich-Heine University Düsseldorf , Germany）

(Mon. Oct 29, 2018 3:45 PM - 5:45 PM Room4)

[SY-M2] MMM in aircraft industries: use cases for simulation of additive manufacturing

○Annett Seide[1], Thomas Goehler[1], Roman Sowa[2] （1.MTU Aero Engines AG, Germany, 2.MTU Aero Engines Polska Sp. z o. o., Poland）

MTU Aero Engines is Germany's leading engine manufacturer and an established global player in the industry. Computational Materials Engineering and Additive Manufacturing (AM) of high temperature alloys are only two of the forward-looking techniques MTU is working with. To represent industrial application of MMM it will be displayed how MTU uses Materials Simulation techniques for AM process.

For a materials engineer some of the key aspects of the AM process are texture, microstructure (e.g. precipitate size and phase fraction) and mechanical properties (e.g. yield stress). Consequentially, the AM simulation includes laser/electron beam scanning strategy, interaction of beam and powder, microstructure evolution and crystal plasticity.

AM simulation at MTU covers amongst others the following typical use cases: (1) description of the influence of chemical composition on microstructure and mechanical properties, (2) determination of surface roughness depending on scanning strategy and (3) heat treatment optimization with regard to yield strength and texture. All of those show the strong coupling between material/manufacturing history and resulting material properties.
The main focus will be on the use case regarding determination of surface roughness as a function of scanning strategy. The goal will be to present requirements and methods related to the specific use case as well as an insight into the industrial application itself. We will give one example of successful integration of materials modeling and simulation as tools to tailor materials properties through process parameter optimization.

(Mon. Oct 29, 2018 3:45 PM - 5:45 PM Room4)

[SY-M2] VISCOELASTIC BEHAVIOUR OF HETEROGENEOUS MATERIALS STUDIED THANKS TO AN EXTENSION OF CRAFT SOFTWARE IN HARMONIC REGIME

○Julien Boisse , Stéphane André, Laurent Farge （University of Lorraine, France, France）

Following the routes opened by the resort to spectral solvers applied on real composite microstructures to analyse the homogenization problem in elasticity, we extended a FFT approach implemented in the CRAFT solver [1] to viscoelastic materials. The idea is to propose a virtual Dynamical Mechanical Analysis experiment applied on heterogeneous microstructures. DMA performs a frequency analysis of the transfer function of the material by applying a sinusoidal harmonic steady-state regime. The transfer function (modulus, relaxation, compliance... quantities) is complex with classical storage and loss components (real and imaginary parts) [2]. It offers a full frequency characterization of the material constitutive law which can be applied afterwards in all cases of temporal excitations. CRAFT code and its central Lippmann-Schwinger equation are then solved in complex variables.
Examples will be given of various microstructures made of two individual viscoelastic constituents assumed

to behave according to a standard 3-parameter Voigt rheological model (spring connected in series with a Voigt unit [2]). As already shown [3], the key resulting effect on the homogenized effective material is the appearance of an additional fading memory term i.e. of a transfer function with broadened spectrum of relaxation times. Following this fact and connections established with fractional rheological models, we will show that a very efficient effective model can describe the mesoscopic behaviour of a great variety of microstructures.

REFERENCES

[1] H. Moulinec, P. Suquet, A numerical method for computing the overall response of nonlinear composites with complex microstructure, Comput. Methods Appl. Mech. Engrg., 157, 69-94, 1998.
[2] N.W. Tschoegl, The Phenomenological Theory of Linear Viscoelastic Behavior, An Introduction, Springer Verlag, 1989.
[3] R. Brenner, P. Suquet, Overall response of viscoelastic composites and polycrystals: exact asymptotic relations and approximate estimates. Int. J. Sol. Struct., 50(10), 1824-1838, 2013.
[4] S. Andre, Y. Meshaka, C.Cunat, Rheological constitutive equation of solids: a link between models based on irreversible thermodynamics and on fractional order derivative
equations, Rheologica Acta, 42, 500-515.

(Mon. Oct 29, 2018 3:45 PM - 5:45 PM Room4)

[SY-M2] Multi-scale modelling of Zener Pinning during the solid solution treatment of a Nickel-based Superalloy

○Magnus Jack Anderson[1], Jonathan Benson[1], Christos Argyrakis[2], Jeffery William Brooks[1], Hector Christian Basoalto[1]　(1.The University of Birmingham, UK, 2.Rolls-Royce plc, UK)

The ability to manufacture components to provide location specific properties is needed to improve component performance, increase component life and reduce cost. In Ni-base superalloys, the grain size and the strengthening precipitate dispersion have a large impact upon creep and fatigue behaviour. It is possible to obtain dual microstructures across turbine discs through careful design of the solid solution treatment process, optimising mechanical properties where needed.

A simulation tool has been developed to assist in the design of such heat treatments, modelling grain growth with Zener pinning precipitates that evolve during thermal processing. The work focuses on modelling grain growth in the Ni-based Superalloy RR1000, containing a tri-modal γ' particle dispersion where the largest particles pin grain boundary movement. A multi-scale approach has been developed to capture the evolution of the precipitates, using a statistical approach to capture the kinetics of the secondary and tertiary particle populations.

The grain growth is described using a two-dimensional model, including the evolution of primary γ' precipitates. The level-set method is used to model the grain boundaries and precipitate-matrix interfaces implicitly. A multi-component mean-field description has been applied to simulate the kinetics of the precipitates. A morphologically explicit mean-field growth rate has been developed to describe the kinetics of the primary particles, consistent with the description of the secondary and tertiary particles.

The proposed model shows good potential in capturing grain growth kinetics and may serve as a useful tool for simulating solid solution treatments in multi-modal nickel-based superalloys.

(Mon. Oct 29, 2018 3:45 PM - 5:45 PM Room4)

[SY-M2] Assessment of residual stresses in welds made of multiphase alloys

○Victor De rancourt[1], Sylvain Flouriot[1], Benjamin Sarre[2], Benoit Panicaud[2], Guillaume Geandier[3] （1.Commissariat a l'energie atomique, France, 2.Universite de Technologie de Troyes, France, 3.Universite de Lorraine - CNRS, France）

Welding can induce strong changes in the parent metal so that the mechanical behavior of a welded structure often remains unclear. Mechanical tests are therefore directly performed on welds to assess the mechanical performance of a welded structure. The purpose of such mechanical tests consists in showing evidences of safety margins. In the future, the growing knowledge on the physics of welding accompanied with better welding monitoring tools may replace the need for such tests. Such developments need enhanced multiphysics and multiscale models validated against experimental measurements. Nevertheless, the complexity of such models is highly increased in the case of multiphase materials

The present work introduces a modelling framework accounting for coupled phase transformations and stresses. The modelling framework is weakly coupled with temperature which is introduced as an external parameter in the simulations. The mechanical behavior features an homogenization scheme, chosen as the β-rule, which accounts for the multiphase nature of the material. The mechanical behavior of each phase accounts for viscoplasticity. Finally, plasticity is coupled with phase transformation to account for dislocation inheritance. The model is then calibrated on a two-phase α-β titanium alloy, namely Ti-6Al-4V.

Finite element simulations of welding are then performed. Such simulations are compared with characterizations of residual stress fields obtained from X-ray diffraction experiments, which have been performed recently at the European Synchrontron Radiation Facility. The qualitative comparison between the experimental characterization and the numerical results is quite good as well as the quantitave comparison of stress extrema. A more detailed comparison is then made including a comprehensive parameter analysis. Finally, the discussion will underline the main role of the β-rule homogenization method on the assessment of residual stresses.

(Mon. Oct 29, 2018 3:45 PM - 5:45 PM Room4)

[SY-M2] Atomic analysis of crystalline nucleation and growth in the supercooled liquid of glass-forming binary alloy

○Masato Wakeda[1], Shigenobu Ogata[2,3]　（1.Research Center for Structural Materials, National Institute for Materials Science, Japan, 2.Graduate school of engineering science, Osaka Univ., Japan, 3.Center for Elements Strategy Initiative for Structural Materials (ESISM), Kyoto Univ., Japan）

Microstructures of solid metals is significantly affected by solidification process from liquid melts. In special, nucleation and growth of crystalline nucleus in supercooled liquid dominates the glass forming ability of amorphous metals or microstructures of crystalline metals. However, key factors affecting nucleation and growth of crystalline nucleus are still under discussion. In experiments, unveiling the nucleation and growth

processes is difficult due to limitation of observable time- and space-scale resolution. On the other hand, atomic simulation such as molecular dynamics (MD) has a difficulty to investigate the crystallization of alloys from liquid state, because the time-scale of the crystallization of alloys is generally beyond the time-scale of atomic simulation. In order to provide atomistic knowledge of the solidification of liquid metal, we in this study focus on the feature of crystalline nucleus in the supercooled liquid metals. First, we prepared atomic models of glass-forming binary alloy, in which a spherical crystal nucleus is embedded in advance. The size of embedded nucleus is smaller than the critical nucleus size. Then we conducted MD simulation under the NPT condition at supercooled liquid temperature under the constraint of nucleus radius: the constraint is realized by adding a boost potential to the liquid-crystal composite model. During MD simulations, we evaluated the crystal nucleus from geometrical and statistical aspects. The obtained results provide the atomistic insight into the early stage of crystallization of metal.

(Mon. Oct 29, 2018 3:45 PM - 5:45 PM Room4)

[SY-M2] Crystal growth in fluid flow: Nonlinear response effects

○Hailong Peng[1,2], Dieter Herlach[1], Thomas Voigtmann[1] (1.German Aerospace Center, Germany, 2.Central South University, China)

Mechanism of solidification is of great interest both to experimentalist and theorist, as it determines the mechanical and thermophysical properties of formed crystalline structures. Many materials, for example, most polymeric and metallic materials of daily life, are produced from the liquid state as their parent phase, in the presence of strong flow (e.g., in extrusion or casting processes). Since crystal growth governs the evolution of the microstructure, detailed knowledge of how crystallization is affected by the processing conditions offers an effective way to design and control material properties in applications.

We investigate crystal-growth kinetics in the presence of strong shear flow in the liquid, using molecular-dynamics simulations of a binary-alloy model. Close to the equilibrium melting point, shear flow always suppresses the growth of the crystal-liquid interface. For lower temperatures, we find that the growth velocity of the crystal depends nonmonotonically on the shear rate. Slow enough flow enhances the crystal growth, due to an increased particle mobility in the liquid. Stronger flow causes a growth regime that is nearly temperature-independent, in striking contrast to what one expects from the thermodynamic and equilibrium kinetic properties of the system, which both depend strongly on temperature. We rationalize these effects of flow on crystal growth as resulting from the nonlinear response of the fluid to strong shearing forces.

(Mon. Oct 29, 2018 3:45 PM - 5:45 PM Room4)

[SY-M2] Time-dependent active microrheology in dilute colloidal suspensions

Invited

Sebastian Leitmann[1], Suvendu Mandal[4,1], Matthias Fuchs[2], Antonio M. Puertas[3], ○Thomas Franosch[1]
 (1.Innsbruck Univ., Austria, 2.Konstanz Univ. , Germany, 3.University of Almeria, Spain, 4.Heinrich-Heine University Düsseldorf , Germany)

In a microrheological set-up a single probe particle immersed in a complex fluid is exposed to
a strong external force driving the system out of equilibrium. Here, we elaborate analytically the time-dependent response of a probe particle in a dilute suspension of Brownian particles to a large step-force, exact in first order of the density of the bath particles. The time-dependent drift velocity approaches its stationary state value exponentially fast for arbitrarily small driving
in striking contrast to the power-law prediction of linear response encoded in the long-time tails of the velocity autocorrelation function. We show that the stationary-state behavior depends nonanalytically on the driving force and connect this behavior to the persistent correlations in the equilibrium state. We argue that this relation holds generically. Furthermore, we elaborate that
the fluctuations in the direction of the force display transient superdiffusive behavior.

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O1] Symposium O-1

Chairs: Lars Pastewka(University of Freiburg, Germany), Izabela Szlufarska(University of Wisconsin, United States of America)

Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room5

[SY-O1] A numerical insight into third body flow regimes within dry contacts
　　○Guilhem Mollon （INSA Lyon - LaMCoS, France）

[SY-O1] A novel multiscale framework for modeling of diamond tools wearA novel multiscale framework for modeling of diamond tools wear
　　○Adriana Quacquarelli[1], Nicolas Fillot[1], Guilhem Mollon[1], Thierry Commeau[2], Aurelie Nouveau[2] （1.Université de Lyon, LaMCoS, INSA-Lyon, CNRS UMR5259, F-69621, France, 2.Umicore Specialty Powders France, France）

[SY-O1] **Thermodynamics of sliding contact: Joule-Thomson effect**
　　○Vera Deeva[1], Stepan Slobodyan[2] （1.Tomsk Polytechnic University, Russia, 2.Tver State Technical University, Russia）

[SY-O1] Molecular Simulation of adsorption process of anti-corrosion additives
　　○Kohei Nishikawa[1], Hirotoshi Akiyama[1], Kazuhiro Yagishita[2], Hitoshi Washizu[1] （1.University of Hyogo, Japan, 2.JX Nippon Oil &Energy Corporation, Japan）

[SY-O1] **The adhesive behavior of elastic contacts in the presence of interfacial shear stresses**
　　Nicola Menga[1,2], ○Giuseppe Carbone[1,2], Daniele Dini[2] （1.Department of Mechanics, Mathematics and Management - Polytechnic University of Bari, Italy, 2.Department of Mechanical Engineering, Imperial College London, UK）

[SY-O1] Soft Matter Mechanics: numerical and experimental methodologies for dry and lubricated tribological problems
　　○Carmine Putignano [1,2], Giuseppe Carbone[1,2] （1.Polytechnic University of Bari, Italy, 2.Imperial College London, UK）

[SY-O1] Two simple models for pull-off decay of self-affine rough surfaces
　　○Antonio Papangelo[1,2], Michele Ciavarella[1,2] （1.Politecnico di Bari, Italy, 2.Hamburg University of Technology, Germany）

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room5)

[SY-O1] A numerical insight into third body flow regimes within dry contacts

○Guilhem Mollon （INSA Lyon - LaMCoS, France）

In this communication we present new results related to the mechanical behavior of the solid interfacial material that is present within a dry sliding interface, and that transmits the load while accommodating the relative displacement between the surfaces - the so-called third body. To reach this purpose, an innovative numerical method is employed, based on the multibody meshfree framework. In this approach, the solid matter composing the third body is represented as a large collection of individual grains interacting by contact and adhesion, much like in the Discrete Element Modelling (DEM) framework, commonly applied in this case for the last fifteen years. However, in contrast with DEM, this new framework allows to consider each grain as highly deformable, which relaxes the assumption of a purely granular third body. In the simulations we present, 2000 such grains are placed between two rigid rough surfaces with periodic lateral boundary conditions, and these surfaces are submitted to typical tribological loadings (pressure and shear). While playing on a limited number of parameters of the third body (deformability, adhesion, damping), we observe the emergence of a very wide range of mechanical behaviors in the interface, such as granular flow, quasi-fluid Couette regime, fragile cracking, agglomeration, rolling, wall-slip, etc. The consequences of these regimes on the local friction coefficient and on the fluctuations of the loading on the surfaces in space and time (which ultimately control the degradation and the wear of these surfaces) are evaluated. Finally, comments are addressed on the possible application of such knowledge in multi-scale approaches in order to relate these results to experimental measurements.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room5)

[SY-O1] A novel multiscale framework for modeling of diamond tools wearA novel multiscale framework for modeling of diamond tools wear

○Adriana Quacquarelli[1], Nicolas Fillot[1], Guilhem Mollon[1], Thierry Commeau[2], Aurelie Nouveau[2]
 （1.Université de Lyon, LaMCoS, INSA-Lyon, CNRS UMR5259, F-69621, France, 2.Umicore Specialty Powders France, France）

Stone cutting involves diamond impregnated tools (DIT) consisting in microdiamonds embedded into a metallic binder. Diamond Tools lifetime is influenced by the wear mechanism of the metallic matrix due to the abrasive debris flow generated during cutting process. Both diamonds, stone debris and the metallic matrix have different dimensions. Therefore, different mechanical and physical process, somehow related, are involved at different scales. Experimental tests are necessary but not sufficient to predict the overall behaviour of diamond tools. A numerical multiscale approach is then initiated to extend the experimental approach.

As DIT performance is influenced by the microstructure properties of the binders (porosity, grains size, bulk properties and composition of metallic powder), a microscopic 2D model representative of metal microstructure has been built. A multibody meshfree technique coupled with a Discrete Element Method (DEM) approach is used. The granular swarf is described by rigid grains with realistic shape, while the

metallic matrix is represented by a collection of degradable grains which fails by fatigue due to the continuous generation and flow of rock debris. Cracking initialization and propagation can be monitored. In typical sections far from diamond, an empirical local wear law can be written, proposed and compared to experiments.

At another scale, the flow of stone debris is studied and assimilated to a viscous flow of continuous material.

Then, A 3D continuous model is implemented to monitor wear close to diamond. The pressure field is obtained by solving Reynolds equation and used in a global wear law. The microgeometry evolution is then compared to experiments.

Finally, the whole set of numerical models at the different scale can be used as a tool to anticipate the performance of the metallic matrix of diamond tools.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room5)

[SY-O1] Thermodynamics of sliding contact: Joule-Thomson effect

ᴼVera Deeva[1], Stepan Slobodyan[2] (1.Tomsk Polytechnic University, Russia, 2.Tver State Technical University, Russia)

The structure and properties (physical, thermal, mechanical, etc.) of complex materials during its formation process have strong correlation with the surrounding medium. Each of the material particles interacts with surroundings randomly, independently of each other, resulting from a probabilistic nature. This fact leads to the rich material properties with small changes in parameters.
An electrical contact pair in the commutator and brush assembly of the electric machine is of interest from the point of view of its structure due to material multivariance (carbon, metal, nanostructure, and others), which have a correlation with environment formed by wear particles or lubricant under sliding interaction. These elements exemplify the strong correlations between mechanical fluctuations of the wear particles and temperature behavior of the contact area (air with wear particles or lubricant), in particular, the non-equilibrium thermodynamics. In our paper we consider the abundance of wear particles as the porous plug. To study this throttling process, we shall concern with the stream as a two-phase system, in particular, gas medium and wear particles in the sliding contact. After due calculation, we receive the expression showing that measure of the strength of association between Joule-Thompson effect and the surrounding medium following a parabolic law, likewise under a temperature gradient, the temperature in contact area is not constant, it varies linearly with the coordinate of the entry end of the contact area. Furthermore, we consider two cases: $k_c = 1$ and $k_c = 0.2$. The comparison indicated a maximum difference of 30 percent of the thermal effects between the entry and outlet ends of the contact area. This means that the strong correlations that are responsible for mechanical fluctuation leads to the increase in the dispersion of the temperature fluctuations in the outlet end of the contact area caused by the corresponding susceptibility to the surrounding medium. The Joule-Thompson effect is probably one of the most important factors determining the different interaction conditions and accordingly material properties of the entry and outlet ends of the contact area between commutator and brush.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room5)

[SY-O1] Molecular Simulation of adsorption process of anti-corrosion additives

○Kohei Nishikawa[1], Hirotoshi Akiyama[1], Kazuhiro Yagishita[2], Hitoshi Washizu[1]　(1.University of Hyogo, Japan, 2.JX Nippon Oil &Energy Corporation, Japan)

Newly formed metal surface is often unstable and becomes stable when it is terminated with another molecule, but the original color and properties may be diminished when it is covered with oxygen or gasses in atmosphere. To prevent this phenomenon, anti-copper-corrosion additives adsorb onto the surface of cupper and save copper`s color and properties from oxygen or other substances. In spite of the many property, there are few molecular findings about anti-copper-corrosion additive and the mechanism of adsorption onto the surface of copper and prevent corrosion. For anti-copper-corrosion, we use benzotriazole C6H5N3 (BTA) which used for a long time.

The method of simulation is molecular dynamics method and for parameter we use reax force field (reaxFF) potential which involves chemical reaction to analyze the mechanism of the adsorption and the properties of the anti-copper-corrosion additive of copper (Cu) and oxidized copper (Cu2O) surface. For this large-scale computing, we use molecular dynamics calculations software LAMMPS which is good at parallelized efficiency. Outline for this simulation model, we make a slab composed with copper (Cu) and oxidized copper (Cu2O), and put 60 anti-copper-corrosion additives foreside of it, randomly. Then calculate time development of this system to replicate the real system.

We analyze destination, orientation and direction, and charge transfer of anti-copper-corrosion additives BTA to the slab. When we compare the adsorption destination of BTA molecules on copper (Cu) to oxidized cupper (Cu2O), 5 times as many BTA molecules adsorbed onto the copper (Cu) than the oxide copper (Cu2O). Orientation and direction also show a difference, BTA molecules adhesion on oxidized copper (Cu2O) were horizontal and that adhesion on copper (Cu) were slightly verticality. In addition, a lot of BTA molecules adsorbed on copper (Cu) toward N to bottom of it, and transfer the charge from Cu atoms of top layer of the copper (Cu) part. This selective deposition is thought that the mechanism that few of the anti-copper-corrosion additives are able to protect copper`s new surface.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room5)

[SY-O1] The adhesive behavior of elastic contacts in the presence of interfacial shear stresses

Nicola Menga[1,2], ○Giuseppe Carbone[1,2], Daniele Dini[2]　(1.Department of Mechanics, Mathematics and Management - Polytechnic University of Bari, Italy, 2.Department of Mechanical Engineering, Imperial College London, UK)

Among the many factors influencing the contact behavior of two mating surfaces, the interplay between shear stresses (and associated frictional response) and adhesion in elastic contacts is still a long-standing tribological problem. Most of the theoretical models focusing on this phenomenon seem to indicate that the presence of frictional stresses at the sliding interface tend to mask adhesion, thus leading to a reduction of the contact area. This is usually explained by invoking the only theory available in the literature (by Savkoor and Briggs in 1977) to study the interrelation between contact tangential stresses and adhesion, which, however, holds true only in the case of full stick conditions between the mating surfaces, i.e. when slip at the contact interface is totally prevented from taking place. Moreover, on the contrary, some experimental

investigations have shown that, under gross slip conditions between almost perfectly smooth surfaces no contact area reduction is observed as long as the sliding velocity is moderate, and in some cases, even an increase of the contact size is reported. Aiming at shedding light on this behaviour, we focus on the adhesive sliding contact between two perfectly smooth surfaces under the condition that gross slip takes place at moderate velocities. We treat the exemplar case of a smooth rigid sphere sliding on a soft elastic half-space. We developed a theoretical model, which, by relying on the theory of contact mechanics and on arguments borrowed from thermodynamics, shows that an increase of the contact area, compared to the classical JKR case, may be caused by the presence of constant uniform shear stress at the interface. This is specifically true at low velocity, before the onset of stick-slip. In fact, at low-speed sliding, the shear stress fluctuations at the interface, which produce an apparent repulsive surface energy term, are negligible compared to the average stress. However, when the contact moves into the stick-slip regime the shear stress fluctuations may become comparable to the average interfacial stress leading to a strong repulsive surface energy, which may also justify why adhesion is instead almost completely masked at relatively large sliding velocities.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room5)

[SY-O1] Soft Matter Mechanics: numerical and experimental methodologies for dry and lubricated tribological problems

○Carmine Putignano [1,2], Giuseppe Carbone[1,2] (1.Polytechnic University of Bari, Italy, 2.Imperial College London, UK)

Assessing the mechanics of soft matter is a crucial point in modern research, involving, at the same time, engineering, physics and material science. Indeed, modelling soft materials is particularly challenging given the strongly time-dependent and usually nonlinear constitutive stress-strain relations that govern their response. Further complexity is embedded in the modelling analysis when soft solids are into contact and the problem is exacerbated by the geometry of the intimately mating surfaces. In this work, we focus specifically on the contact mechanics of linear viscoelastic materials and we present a variety of Boundary elements methods developed to determine the mechanical solution in terms of stresses, strains and, ultimately, friction. In particular, we describe the main features of viscoelastic contact mechanics under different contact conditions, involving steady-state, reciprocating and generalized motion laws. Each configuration is different since the solution is dramatically influenced by the relaxation of the different regions into contact. In all these analyses, a fundamental role is played by the surface roughness, which introduces a huge number of space and, consequently, time scales. Such a scenario is furtherly complicated when the presence of a fluid is considered at the contact interface: indeed, the fluid viscosity, coupled with the material viscoelasticity, determines tremendous variations in comparison with the classical elasto-hydrodynamic theory. In detail, the pressure and the film thickness distributions show strongly non-symmetrical trends at the contact inlet and outlet. All this entails a friction curve strongly different from the Stribeck curve, usually predicted for elastic solids, and demonstrates the necessity of ad hoc developed modelling strategies for soft materials.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room5)

[SY-O1] Two simple models for pull-off decay of self-affine rough surfaces

○Antonio Papangelo[1,2], Michele Ciavarella[1,2] （1.Politecnico di Bari, Italy, 2.Hamburg University of Technology, Germany）

Predicting the adhesive behaviour of randomly rough multiscale surfaces nowadays remains a tough task. The classical asperity model of Fuller and Tabor (1975) reduces the rough surface to a set of independent asperities, which behave accordingly to the JKR model for adhesion of spheres (Jonshon et al. 1971). Fuller and Tabor showed that the pull-off force is strongly affected by the height root mean square (rms), so that a tiny variation in height rms leads to order of magnitudes reduction in surface stickiness. Nevertheless, the present understanding of rough contact as "fractals" poses serious questions about the validity of asperity models. Recent large numerical calculations by Pastewka and Robbins show that "slopes and curvatures" may play an important role, which is in contrast with asperity model predictions. We propose and discuss here two simple models for pull-off decay, namely the Bearing Area Model (BAM, Ciavarella, 2017) belonging to a DMT class of models, and Generalized Johnson Parameter (GJP, Ciavarella &Papangelo, 2018) model. BAM starts from the observation that the entire DMT solution for "hard" spheres (Tabor parameter tending to zero) assuming the Maugis law of attraction, is very easily obtained using the Hertzian load-indentation law and estimating the area of attraction as the increase of the bearing area geometrical intersection when the indentation is increased by the Maugis range of attraction. GJP instead postulates that stickiness of randomly rough multiscale surfaces depends on a generalization of the classical Johnson parameter valid for the single sinusoid. The GJP is obtained as the ratio between the adhesive energy and the elastic energy needed to flatten the surface. We make extensive comparisons of GJP and BAM predictions with respect to Pastewka and Robbins (2014) and Persson and Scaraggi (2014) numerical calculations showing reasonable agreement. We show that for low fractal dimensions, BAM and GJP are insensitive to rms slopes and curvatures, so being independent on "small-scale features", which are difficult to define for fractal surfaces.

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O2] Symposium O-2

Chairs: Mark Owen Robbins(Johns Hopkins University, United States of America), Tasuku Onodera(Hitachi, Ltd., Japan)

Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room5

[SY-O2] Droplet Spreading on a Surface Exhibiting Solid-liquid Interfacial Premelting

○Yang Yang[1], Brian B Laird[2] (1.East China Normal University, China, 2.University of Kansas, United States of America)

[SY-O2] **Comparative Study on the Adsorption of Violate Organic Compounds on the Surfaces of Two-Dimensional Materials: Toward the Early Lung Cancer Detection**

○Van An Dinh[1,2] (1.Nanotechnology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan)

[SY-O2] Adsorption of the Volatile Organic Compounds on Graphene including Van de Waals Interaction

○Thi Viet Bac Phung[1], Trong Lam Pham[1], Yoji Shibutani[1,2], Van An Dinh[1,2] (1.Nanotechnology Program, Vietnam Japan University - Vietnam National University, Viet Nam, 2.Center for Atomic and Molecular Technologies, Graduate School of Engineering, Osaka University, Japan)

[SY-O2] **Diffusion of a Cu nanodroplet on an amorphous carbon surface**

Yong-Long Chen[1], ○Yu-Chen Chiu[1], Kai Chen[2], Yu-Chieh Lo[1] (1.National Chiao Tung University, Taiwan, 2.Xi'an Jiaotong University, China)

[SY-O2] First principal modeling of oxygen and carbon adsorption on Fe (110) surface with symmetrical tilt Sigma3(111) grain boundary

○Ivan Lobzenko, Yuki Uchiyama, Yoshinori Shiihara (Toyota Technological Institute, Japan)

[SY-O2] Theoretical study of the effects of boron doping on the electronic structure of g-C_3N_4/TiO_2(001) heterojunction

○Jianhong Dai, Yan Song (Harbin Institute of Technology at weihai, China)

[SY-O2] Atomistic Simulations that Reach Anthropological Timescale and Beyond

○Ju Li (Massachusetts Institute of Technology, United States of America)

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room5)

[SY-O2] Droplet Spreading on a Surface Exhibiting Solid-liquid Interfacial Premelting

○Yang Yang[1], Brian B Laird[2] （1.East China Normal University, China, 2.University of Kansas, United States of America）

We study the spreading kinetics of Pb(l) droplets on an Al(111) substrate using MD simulation. The Al-Pb solid-liquid interface was found [Phys. Rev. Lett, **110**, 096102 (2013)] to exhibit premelting below the T_m(Al). Because the Al(111) free surface does not premelt, the spreading of the droplet is accompanied by a transition from a faceted to a premelted surface. We examine the effect of this premelting on the droplet spreading kinetics and compare the results to two standard mechanisms of droplet spreading: *hydrodynamic spreading*, in which energy dissipates through viscous relaxation, and *kinetic spreading*, where friction dominates. When premelting is present, kinetic spreading is observed at intermediate times, with exponential relaxation at long times. For two non-premelting Al/Pb interfaces (one faceted surface at 625K and one where premelting was suppressed) hydrodynamic spreading is seen instead at intermediate times. We also examine the effect of premelting on the droplet equilibrium contact angle.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room5)

[SY-O2] Comparative Study on the Adsorption of Violate Organic Compounds on the Surfaces of Two-Dimensional Materials: Toward the Early Lung Cancer Detection

○Van An Dinh[1,2] （1.Nanotechnology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan）

Every year, the large number of death due to lung cancer is reported. 5 years after diagnosis, there is only small number (13% ~ 48% depending on country) of the lung cancer patients are alive. Screening tests to detect lung cancer at an early stage is very important for localizing the cancer cells and significantly improving the possibility of the curability of the disease. Breath contains clinically useful markers [2] such as the violate organic compounds (VOCs), which can be detected by electronic sensors. The two-dimensional (2D) materials such as graphene, silicone, germanene, etc. are expected to be promising materials for the electronic sensors for detecting VOCs because these materials exhibit a very high sensitivity in adsorption of gases.

In this talk, we present a comparative study on the adsorption of various VOCs on the surfaces of the substrate MoS_2 and other 2D materials such as silicene, graphene, borophene and germanene by using the quantum simulation method based on Density Functional Theory (DFT). Scanning images of the adsorption possibility are shown for the six types of VOCs in breath of lung cancer patients on these substrate materials by using *computational DFT-base Nanoscope [2]* to determine the potential adsorption areas and the path of VOCs diffusion on the surfaces of substrates. The adsorption energy is calculated by DFT method combining with the five approaches of van der Waals dispersion: revPBE, optPBE, optB88, optB86b and DFT-D2. Charge transfer between the substrates and VOCs is explored by calculating the Bader charges. In addition, the effect of electric field on the adsorption is also investigated.

[1] Phillips, M. *et al.* Lancet. **353**, 1930-1933 (1999), ib. Chest. **123**, 2115-2123 (2003).
[2] Developed by author (Vietnam Japan University).

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room5)

[SY-O2] Adsorption of the Volatile Organic Compounds on Graphene including Van de Waals Interaction

○Thi Viet Bac Phung[1], Trong Lam Pham[1], Yoji Shibutani[1,2], Van An Dinh[1,2] （1.Nanotechnology Program, Vietnam Japan University - Vietnam National University, Viet Nam, 2.Center for Atomic and Molecular Technologies, Graduate School of Engineering, Osaka University, Japan）

The interactions of some volatile organic compounds (VOCs) such as ethanol, acetone, benzene, toluene, diclomethane with graphene are systematically investigated by using first principles calculations. The VOCs are chosen as selected examples of main VOCs in exhaled breath in lung cancer patients [1, 2]. To evaluate the adsorption sites of VOCs on graphene, we have performed simulation including physical adsorption under the different van de Waals functionals. The global minimum energy configurations and binding energies for VOCs molecules adsorbed on graphene are determined by using *Computational DFT-based Nanoscope* [3] for imaging the binding possibility of the adsorbed molecules on graphene. It is shown that the adsorption energy is highly sensitive to the wDW potentials. We explore the fundamental insights of the interactions between VOCs molecules and graphene. Furthermore, the effects of the external electric field on the charge transfer between the adsorbed molecules and graphene are also discussed.

Keywords: Graphene; VOCs adsorption; Charge transfer; Electric field; First-principles calculations

References

[1] P. Fuchs, C. Loeseken, J. K. Schubert, and W. Miekisch, International Journal of Cancer 126, 11, 2663-2670, 2010.

[2] X. Sun, K. Shao, T. Wang, Anal. Bioanal. Chem. 408, 11, 2759-80, 2016.

[3] Developed by V. A. Dinh, Vietnam Japan University.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room5)

[SY-O2] Diffusion of a Cu nanodroplet on an amorphous carbon surface

Yong-Long Chen[1], ○Yu-Chen Chiu[1], Kai Chen[2], Yu-Chieh Lo[1] （1.National Chiao Tung University, Taiwan, 2.Xi'an Jiaotong University, China）

Due to better electrical and thermal conductivity, copper (Cu) nanowires are promising material for the application in the next-generation transparent conductors, integrated circuits. Recently, there have been few reports on the discovery of single-crystalline metal nanowires growing on a carbon substrate. It is noteworthy

that on amorphous carbon substrates the most productive growth of Cu nanowire can be achieved. The development of such a direct process is important and attractive for the production of Cu nanowires. Amorphous carbon films play an important role in the production of Cu nanowires. However, the influence of amorphous carbon films on Cu still remains unclear. According to our research, because of the roughness of amorphous carbon surface, Cu atoms are difficult to diffuse on an amorphous carbon film. Nevertheless, Cu can diffuse on amorphous carbon surface with the form of cluster. To confirm this, we conducted molecular dynamics (MD) simulations to explore cluster diffusion behaviors of nanoscale Cu on various carbon films with different morphology. The surface effects, including surface roughness and sp^2/sp^3 bond ratio of carbon films. The aim of this work is to understand cluster diffusion of nanoscale Cu on the amorphous carbon films in order to find out the optimal controlling factors for the formation of Cu nanowires.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room5)

[SY-O2] First principal modeling of oxygen and carbon adsorption on Fe (110) surface with symmetrical tilt Sigma3(111) grain boundary

○Ivan Lobzenko, Yuki Uchiyama, Yoshinori Shiihara （Toyota Technological Institute, Japan）

Iron is material of great interest for vast majority of industries. Being a good catalyst, Fe plays an important role in chemical reactions with carbon and oxygen atoms involved. Despite extensive experimental and theoretical studies a complicated process of oxidation and carburization of iron surfaces is not well understood yet [1,2]. In particular, low attention is paid to chemisorption on iron surfaces with grain boundaries. Nowadays with extensive development of methods for production of metals with nano-hetero structure, studies of adsorption on surfaces with high concentration of grain boundaries became an important issue.

In the present work the study of oxygen and carbon atoms adsorption on iron surfaces have been made by means of density functional method. Adsorption on Fe (110) surface with symmetrical tilt Sigma3(111) grain boundary is compared to that on "clean" Fe (100), (110) and (111) surfaces. It is revealed that grain boundary enhances adsorption properties of iron for both oxygen and carbon atoms. In order to explain such effect, modeling of adsorption on clean surfaces under various strains was made. Comparison of electronic properties of structures under study shows correlation of adsorption energies with the electronic density of states at Fermi level.

References

[1] T.Ossowski, A. Kiejna, Surface Science. 637-638, p. 35 (2015);
[2] H. Grabke, Materials at High Temperatures 17, p. 483 (2000).

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room5)

[SY-O2] Theoretical study of the effects of boron doping on the electronic structure of g-C$_3$N$_4$/TiO$_2$(001) heterojunction

○Jianhong Dai, Yan Song （Harbin Institute of Technology at weihai, China）

The formation of g-C$_3$N$_4$/TiO$_2$(001) heterojunction between anatase TiO$_2$ crystal and graphite-like carbon nitride can decrease the recombination of photo-generated electron-hole pairs, and improve the charge transfer properties. The influence of boron doping on the stability and electronic structures of g-C$_3$N$_4$/TiO$_2$

(001) interfaces were studied by first principles calculations. The stable g-C$_3$N$_4$/TiO$_2$(001) interface and possible occupations of boron dopant in the interface were studied by comparing the formation energies of different configurations. The boron was found to be easily doped in the g-C$_3$N$_4$/TiO$_2$(001) interfacial zone. The electronic structures of g-C$_3$N$_4$/TiO$_2$(001) interface and boron doped systems were evaluated. Strong bonding interactions between the g-C$_3$N$_4$ and TiO$_2$(001) were found in the g-C$_3$N$_4$/TiO$_2$(001) interface, and the boron dopant can improve the charge transfers between g-C$_3$N$_4$ and TiO$_2$(001). Therefore, the boron may improve the photocatalytic properties of g-C$_3$N$_4$/TiO$_2$(001) heterojunction.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room5)

[SY-O2] Atomistic Simulations that Reach Anthropological Timescale and Beyond

Invited

$^{\circ}$Ju Li （Massachusetts Institute of Technology, United States of America）

Atomistic and first-principles modeling, which describe the world as assembly of atoms and electrons, provide the most fundamental answer to problems of materials. However, they also suffer the most severe timescale limitations. For instance, in molecular dynamics (MD) simulations, in order to resolve atomic vibrations, the integration time step is limited to hundredth of a picosecond, and therefore the simulation duration is limited to sub-microsecond due to computational cost. Although a nanosecond simulation is often enough (surprisingly) for many physical and chemical properties, it is usually insufficient for predicting microstructural evolution and thermo-mechanical properties of materials. In this invited talk I will discuss recent attempts at overcoming the timescale challenges of atomic-resolution simulations: (a) strain-boost hyperdynamics [Phys. Rev. B 82 (2010) 184114] for simulating primarily displacive events and associated issues of activation entropy and the Meyer-Neldel compensation rule, (b) diffusive molecular dynamics (DMD) [Phys. Rev. B 84 (2011) 054103] for microstructural evolution driven by repetitive diffusion events and coupled displacive-diffusive processes.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A1] Symposium A-1

Chair: Anton Van der Ven(University of California Santa Barbara, United States of America)

Mon. Oct 29, 2018 1:30 PM - 3:00 PM Room6

[SY-A1] Atomistic to continuum: coarse-graining in and out of equilibrium
      ○Celia Reina[1], Xiaoguai Li[1], Peter Embacher[2], Nicolas Dirr[2], Johannes Zimmer[3] （1.University of Pennsylvania, United States of America, 2.Cardiff University, UK, 3.University of Bath, UK）

[SY-A1] **Finite-temperature Localized Stress and Strain for Atomic Models**
      ○Ranganathan Parthasarathy[1], Anil Misra[2], Lizhi Ouyang[1] （1.Tennessee State University, United States of America, 2.University of Kansas, United States of America）

[SY-A1] Uncertainty Quantification for Classical Effective Potentials
      ○Sarah Longbottom, Peter Brommer （School of Engineering, University of Warwick, UK）

[SY-A1] The role of null-lagrangians in the continuum interpolation of the linear chain with hyper-pre-stress
      ○Alexandre Danescu （Ecole Centrale de Lyon, France）

[SY-A1] Practical Time Averaging of nonlinear dynamics
      Sabyasachi Chatterjee[1], ○Amit Acharya[1], Zvi Artstein[2] （1.Carnegie Mellon University, United States of America, 2.The Weizmann Institute of Science, Israel）

(Mon. Oct 29, 2018 1:30 PM - 3:00 PM Room6)

[SY-A1] Atomistic to continuum: coarse-graining in and out of equilibrium

Invited

○Celia Reina[1], Xiaoguai Li[1], Peter Embacher[2], Nicolas Dirr[2], Johannes Zimmer[3]　(1.University of Pennsylvania, United States of America, 2.Cardiff University, UK, 3.University of Bath, UK)

We will describe various spatio-temporal coarse-graining procedures to understand the thermodynamic behavior and evolution of general atomistic/particle models. We will first revisit the equilibrium setting, providing further insights into the thermodynamic potentials and the interplay between temperature and the mechanical behavior. Then, we will move to the non-equilibrium setting, where we will discuss how to compute macroscopic dissipative evolutions, in particular parameters. In all cases, the results will be validated with full resolution particle simulations.

(Mon. Oct 29, 2018 1:30 PM - 3:00 PM Room6)

[SY-A1] Finite-temperature Localized Stress and Strain for Atomic Models

○Ranganathan Parthasarathy[1], Anil Misra[2], Lizhi Ouyang[1]　(1.Tennessee State University, United States of America, 2.University of Kansas, United States of America)

Homogeneous deformation of an ordered crystalline solid at finite temperature can cause non-affine transformation of atomic trajectories, particularly when the inter-atomic potential is anharmonic. In such a case, continuum measures based on affine transformation of trajectories are insufficient to ensure energetic equivalence between the atomic and continuum scales and non-classical stress measures are required. These measures also need to be localizable to obtain continuum stress and strain spatially resolvable to atomistic scales. To this end, the total work done on an atom under deformation is decomposed into the work corresponding to changing its equilibrium position and work corresponding to changing its second moment about equilibrium position. Correspondingly, we define two kinematic variables: a deformation gradient tensor and a vibration tensor, and derive their stress conjugates, termed here as static and vibration stresses, respectively. The proposed approach is validated using MD simulation in NVT ensembles for fcc aluminum subjected to uniaxial strain at high temperatures up to 0.9Tm. Highly non-linear and non-affine evolution of second moments are observed in the elastic portion of the high temperature-high tensile strain regime, in which the conjugate pair of vibration stress and vibration tensor contribute significantly to free energy change, particularly as the material approaches elastic instability through violation of the Cauchy-Born rule. In the elastic portion of the compressive regime, the non-affinity of the second moments point to anomalous phonon dispersion and non-monotonic variation of average group velocities with strain, which resembles experimental observations in certain crystalline solids. The results are strongly relevant for developing finite temperature continuum theories based on discrete simulations or inter-atomic potentials.

(Mon. Oct 29, 2018 1:30 PM - 3:00 PM Room6)

[SY-A1] Uncertainty Quantification for Classical Effective Potentials

○Sarah Longbottom, Peter Brommer （School of Engineering, University of Warwick, UK）

Effective potentials are an essential ingredient of classical molecular dynamics (MD) simulations. Little is understood of the errors incurred in representing the complex energy landscape of an atomic configuration by an effective potential containing considerably fewer parameters. The probabilistic sloppy model method [1] has been implemented in the *potfit* force matching code [2]. This introduces uncertainty quantification into the interatomic potential generation process. Uncertainties in the effective potential are propagated through MD to obtain uncertainties in quantities of interest, which are a measure of the confidence in the model predictions.

We demonstrate the technique using three potentials for nickel: two simple pair potentials, Lennard-Jones and Morse, and a local density dependant EAM potential. A sloppy model fit to DFT reference data is constructed for each potential to calculate the uncertainties in lattice constants, elastic constants and thermal expansion. These can be used to show the unsuitability of pair potentials for nickel. In contrast, with EAM we observe a decreased uncertainty in the model predictions. This shows that our method can capture the effects of the error incurred in the potential generation process without resorting to comparison with experiment or DFT, which is an essential part to assess the predictive power of MD simulations.

Further work is in progress to create a new potential, with uncertainty quantification, for silicon heterostructures. The potential is tailored to describe thermal transport in specific morphologies which are of interest as thermoelectric devices [3, 4].

[1] S. L. Frederiksen, et al., Phys. Rev. Lett., 93(16), 2004.
[2] P. Brommer, et al., Modell. Simul. Mater. Sci. Eng., 23(7), 2015.
[3] H. Karamitaheri, et al., J. Appl. Phys., 113(20), 2013.
[4] H. Karamitaheri, et al., J. Appl. Phys., 115(2), 2014.

(Mon. Oct 29, 2018 1:30 PM - 3:00 PM Room6)

[SY-A1] The role of null-lagrangians in the continuum interpolation of the linear chain with hyper-pre-stress

○Alexandre Danescu （Ecole Centrale de Lyon, France）

The simplest discrete one-dimensional model including elastic bulk and surface energy is the linear chain with hyper-pre-stress. It is known that when NN and NNN "geometrically incompatible" interactions are taken into account the qualitative behavior of the chain can fall into three generic cases depending on the ratio of the stiffnesses of the NN and NNN interactions. We adress here the general question of finding an exact continuum interpolant of the discrete solution. Guided by the qualitative aspects of the characteristic equation we chose the Mindlin model is an appropriate candidate. Starting from a general form of the elastic energy in the continuum we show that null-lagrangians are mandatory in order to obtain an exact interpolant.

(Mon. Oct 29, 2018 1:30 PM - 3:00 PM Room6)

[SY-A1] Practical Time Averaging of nonlinear dynamics

Sabyasachi Chatterjee[1], ○Amit Acharya[1], Zvi Artstein[2]　(1.Carnegie Mellon University, United States of America, 2.The Weizmann Institute of Science, Israel)

This talk aims to understand and exploit the slow time-scale behavior of rapidly evolving microscopic dynamics. The microscopic systems considered are posed in terms of systems of non-linear ordinary differential equations, not necessarily containing an a priori split into fast and slow variables. Such a question arises naturally and ubiquitously in efforts to understand macroscopic dynamics, on engineering time-scales, of well-accepted models of microscopic dynamics that, however, are not amenable to practical computing over the much, much larger macroscopic time-scales of interest. This is because there is a vast separation of time scales involved between the dynamics of the macroscopic variables of interest and the microscopic dynamics, and evolving the microscopic dynamics directly fails to address the question of the macroscopic dynamics.

The methodology employed involves a computational scheme based on fundamental mathematical theory that a) defines appropriate `coarse' variables corresponding to the microscopic dynamics that evolve in a stable manner on the coarse time scale; b) determines the equation of evolution for such variables; and c) defines a practically useful strategy for accurately initializing short bursts of microscopic runs for the evolution of the slow variables, without special requirements on the nature of the microscopic dynamics.

We will illustrate the theory with examples that violate ergodicity and include both conservative and dissipative behavior. Depending on research progress between submission of this abstract and the conference, the coarse graining of discrete dislocation dynamics to a pde-based plasticity model without relying on constitutive assumptions will be demonstrated. This latter effort is ongoing joint work with Giacomo Po (UCLA), Xiaohan Zhang (Stanford) and Nasr Ghoniem (UCLA).

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A2] Symposium A-2

Chair: Kenjiro Sugio(Hiroshima Univ., Japan)
Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room6

[SY-A2] Bridging the chasm between phenomenological theories and electronic structure

○Anton Van der Ven（University of California Santa Barbara, United States of America）

[SY-A2] Two-component Dirac-Kohn-Sham calculation for multiscale modeling of materials

○Koichi Nakamura[1,2]（1.Kyoto Univ., Japan, 2.E-JUST, Egypt）

[SY-A2] Combination of Kinetic Monte Carlo Method and First Principles Calculation to Explore Stable Structure of Solute Cluster in Al-Si Based Alloys

○Kenjiro Sugio, Hiroshi Mito, Yongbum Choi, Gen Sasaki（Hiroshima Univ., Japan）

[SY-A2] Electronic structure analysis of Fermi level instability in Fe-rich Si alloy

○Chen Ying[1], Arkapol Saengdeejing[1], Tetsuo Mohri[2]（1.School of Engineering, Tohoku University, Japan, 2.Institute for Materials Research, Tohoku University, Japan）

[SY-A2] **From first-principles defect chemistry to device damage models of radiation effects in III-V semiconductors**

○Peter A Schultz, Harold P Hjalmarson（Sandia National Laboratories, United States of America）

[SY-A2] How to model ordering processes in metallic hydrides? A Tight-Binding Ising modeling proposal and its application to Zr-H

Paul Eymeoud[1], ○Fabienne Ribeiro[1], Remy Besson[3], Guy Tréglia[2]（1.Institut de Radioprotection et de Sûreté Nucléaire/PSN-RES/SEMIA/LPTM, France, 2.Centre Interdisciplinaire de Nanoscience de Marseille, CNRS, France, 3.Unité Matériaux Et Transformations (UMET), CNRS UMR 8207, Université de Lille, 59655 Villeneuve D'Ascq, France）

[SY-A2] Bridging the chasm between phenomenological theories and electronic structure

Invited

○Anton Van der Ven （University of California Santa Barbara, United States of America）

The first-principles prediction of non-equilibrium materials processes remains a major challenge. The evolution of a solid out of equilibrium is affected by intrinsic thermodynamic, mechanical and kinetic properties that are often difficult if not impossible to measure accurately in isolation. Nevertheless, there are many successful phenomenological theories of phase transformations and microstructure evolution that have been formulated in terms of thermodynamic free energies and kinetic transport coefficients. One approach to treating non-equilibrium materials processes from first principles, therefore, is to predict intrinsic thermodynamic, kinetic and mechanical properties starting with electronic structure theory. However, the crucial role of temperature and entropy in most materials processes requires a rigorous statistical mechanics approach. In this talk I will describe our recent efforts at bridging the gap between phenomenological theories of materials and first-principles electronic structure predictions. The approach relies on statistical mechanics methods that utilize effective Hamiltonians expressed in terms of mathematically rigorous local descriptors to treat configurational, vibrational and electronic degrees of freedom. Effective Hamiltonians are capable of extrapolating first-principles electronic structure calculations within (kinetic) Monte Carlo simulations, thereby enabling the calculation of equilibrium and non-equilibrium materials properties at finite temperature. I will illustrate how these approaches can be used to predict the dynamic evolution of battery electrodes and high temperature structural materials.

[SY-A2] Two-component Dirac-Kohn-Sham calculation for multiscale modeling of materials

○Koichi Nakamura[1,2] （1.Kyoto Univ., Japan, 2.E-JUST, Egypt）

It is known well that some specific properties and characteristics of materials cannot be exactly simulated without considering the relativistic effect, whereas general first-principles electronic-state calculation technique for material systems has been established on the basis of the Schrödinger equation under non-relativistic limit. The most fundamental idea to treat the relativistic effect is the electronic-state calculation based on the Dirac equation from the viewpoint of the relativistic quantum mechanics, and the effective methodologies, such as multiconfiguration Dirac-Fock and Dirac-Kohn-Sham (DKS) methods, have been developed for leading to exact electronic states. The relativistic calculation based on the Dirac equation originally uses 4-component spinors, which consist of 2 large components and 2 small components. However, the calculation with 4-component spinors is computationally too expensive to perform for material systems practically. To avoid the calculation with 4-component spinors, some theoretical treatments of calculation with 2-component spinors, such as zeroth-order regular approximation (ZORA), infinite-order regular approximation (IORA), relativistic scheme by elimination of small components (RESC), and high-order Douglas-Kroll transformation, have been developed in the field of molecular physics and chemistry. For the application of these methods to material systems under the periodic boundary condition, some special techniques should be required to adopt the elimination of small components to the basis set by plane wave or projector augmented wave. In this study, examples of the DKS calculation with 2-component spinors by

ZORA, IORA, and RESC methods shall be presented for some typical material systems. The details of techniques how to eliminate small components of spinors and the differences in specific properties and characteristics of target materials according to relativistic methodologies will be discussed in the conference.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room6)

[SY-A2] Combination of Kinetic Monte Carlo Method and First Principles Calculation to Explore Stable Structure of Solute Cluster in Al-Si Based Alloys

○Kenjiro Sugio, Hiroshi Mito, Yongbum Choi, Gen Sasaki （Hiroshima Univ., Japan）

Stable structure of solute cluster in Al-Si based alloys was investigated by combining Kinetic Monte Carlo (KMC) method and first principle calculation. The new KMC code was developed to simulate the behavior of the added impurities in aluminum at finite temperature. The size of KMC cell was $20a_0 \times 20a_0 \times 20a_0$ or $20a_0 \times 20a_0 \times 40a_0$, where a_0 is lattice constant of aluminum. Aluminum atoms were arranged in FCC structure and the impurity atoms of 3at.% or 4at.% was introduced. Diffusion of impurities was performed by swapping two neighbor atoms which was selected randomly. After the swapping, total energy of the KMC cell was calculated and compared with the total energy before the swapping. The stable structure of the impurity cluster was explored with repeating this process. The total energy was calculated by adding up the atom energies which was calculated by dividing the total energy by number of atoms in the cluster. The total energy of the cluster was calculated by the first principle method. Because the atom energy calculated once was recorded in the database, the number of the first principle calculation was reduced. Quantum ESPRESSO was used to carry out the first principle calculation. The pseudopotential file of Becke-Lee-Yang-Parr function was used for Al, Si, Mg, Cu, Zn, Zr, Ti and Ag. The k-point mesh based on Monk horst-Pack (4×4×4) was used to integrate Brillouin zone and the cut off energy of plane wave was 30 Ry. The size of supercell was $2a_0 \times 2a_0 \times 2a_0$, where a_0 is 0.404 nm. The cluster consisted of a central atom and the first neighbor atoms in FCC was arranged in the center of the supercell. The energy of an isolated cluster was calculated. Calculations for binary system (Al-Si, Al-Mg, Al-Cu, Al-Zn, Al-Zr, Al-Ti, Al-Ag), ternary system (Al-Si-Mg, Al-Zn-Mg, Al-Si-Cu, Al-Mg-Cu,Al-Mg-Zr) and quaternary system (Al-Si-Mg-Cu, Al-Si-Mg-Zr, Al-Cu-Mg-Ag) were carried out.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room6)

[SY-A2] Electronic structure analysis of Fermi level instability in Fe-rich Si alloy

○Chen Ying[1], Arkapol Saengdeejing[1], Tetsuo Mohri[2] （1.School of Engineering, Tohoku University, Japan, 2.Institute for Materials Research, Tohoku University, Japan）

Fe-Si binary alloy has a variety of applications due to its excellent magnetic and mechanical properties. Some drastic change in mechanical properties as Si concentration increasing to 9-10at.% has been intriguing since a long time ago. We have conducted an integrated study on elastic properties in Fe-rich Si alloy based on the electronic structure calculations incorporated with phonon vibration effect and thermal electrons excitation for a Si-doped bcc-Fe alloy up to 12.5at.%Si [1,2], as a part of a multiscale simulation of the mechanical properties of Fe-Si [3]. Our calculations reproduced a non-monotonic change of the elastic properties with Si

concentration, showed a ductile to brittle transition behavior as the Si content increases beyond 9.4at.%, which is agree with the well know experimental results, The calculation further revealed that the Si concentration dependence of the elastic properties is originated from a combination of magnetovolume effect at a low Si concentration up to 8.0 at.%, $D0_3$ ordering on the recovery of elastic properties at Si concentration's being over 10.9at.%, and the instability of density of states at the Fermi energy right at the Si concentration with drastic degradation of elastic properties. The present work aims at a thorough understanding on this Fermi level instability. We calculated the Fermi surfaces at 9.4, 10.9 and 12.5at.%Si, and found that at 10.9 at.%Si, the Fermi surface just touches the boundary of the Brillouin zone which leads to a decrease of the energy of the electrons, further deceases the elastic properties. This founding suggests that the Fermi lever stability/instability is related to the local atomic configuration of doped atoms, then the re-distribution of band structure and furthermore the relative position of Fermi surface to the Brillouin zone, which might be the electronic structural origin of the drastic change of the mechanical properties at some subtle Si concentrations in Fe-rich Si alloy.

References

[1] A.Saengdeejing, Ying Chen, Ken Suzuki, Hideo Miura, Tetsuo Mohri, Computational Materials Science, 70, 100-106, 2013.

[2] S. Bhattacharya, M. Kohyama1, S. Tanaka1, Y. Shiihara, A. Saengdeejing, Ying Chen and T. Mohri, Mater. Res. Express 4, 116518 (2017)

[3] T. Mohri, Y. Chen, A. Saengdeejing, et al., npj Computational Materials - Nature 3, 10 (2017)

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room6)

[SY-A2] From first-principles defect chemistry to device damage models of radiation effects in III-V semiconductors

○Peter A Schultz, Harold P Hjalmarson （Sandia National Laboratories, United States of America）

An atoms-to-circuits assessment of radiation damage in microelectronics begins with understanding atomic displacement damage in a semiconductor material, the subsequent evolution of the radiation-induced defect populations in the material, and propagating this understanding into defect-aware damage models for continuum-scale device simulations. The foundation of a multiscale modeling framework to understand long-time, device-scale response is a quantitative description of the dominant atomic processes using quantum mechanical modeling. We describe the development of a comprehensive radiation-induced defect reaction network in Si-doped (n-type) and C-doped (p-type) GaAs using density functional theory (DFT), identifying mobile species and consequent defect reactions, characterizing defect properties needed to formulate the chemistry needed in defect physics models for device simulations. In turn, the device simulations solve a set of drift-diffusion equations to evolve a model chemistry, and predict the electrical response of device of a specified configuration and operating conditions. The upscaling bridge from the atomistic description given by DFT and experimental defect spectroscopies to a device description of radiation response proves to have many challenges. We describe the successes and also the remaining outstanding challenges in standing up a full first-principles motivated hierarchical multiscale model of radiation damage in electronic devices. --- Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room6)

[SY-A2] How to model ordering processes in metallic hydrides? A Tight-Binding Ising modeling proposal and its application to Zr-H

Paul Eymeoud[1], ○Fabienne Ribeiro[1], Remy Besson[3], Guy Tréglia[2]   (1.Institut de Radioprotection et de Sûreté Nucléaire/PSN-RES/SEMIA/LPTM, France, 2.Centre Interdisciplinaire de Nanoscience de Marseille, CNRS, France, 3.Unité Matériaux Et Transformations (UMET), CNRS UMR 8207, Université de Lille, 59655 Villeneuve D'Ascq, France)

Modeling metal hydrides is of prime interest in the field of materials for energy, due to these material potential uses as hydrogen storage devices or to their potential formation in nuclear reactors. In particular, zirconium alloys are used in water-cooled nuclear reactor and can be embrittled by hydride precipitation. This motivates developing theoretical tools to model, understand and predict the behavior of zirconium hydrides, and to precise their links to local stresses and mechanical properties. In order to explore the Zr-H phase diagram and to clarify dissolution/precipitation mechanisms and kinetic, one needs thermodynamic simulations such as Monte Carlo approaches. They have to be grounded on an energetic model with a good compromise between precision and numerical cost, and in particular, which is able to characterize order-disorder phenomena on the interstitial H-gap subnetwork of metal hydrides.

To this aim, using the Generalized Perturbation Method based on Tight-Binding Coherent Potential Approximation, we have derived an effective Ising Model, which describes the order energy of the FCC zirconium hydride systems as a sum of interactions of HH pairs. We present here this general approach through the example of Zr-H. The process revealed the predominance of pairwise interaction between third-order hydrogen neighbors. Ability of the pairwise interactions model to characterize hydrogen-vacancy sublattice order has been then established by confrontation to first-principle approaches.

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I1] Symposium I-1

Chairs: David Sroloviz(University of Pennsylvania, USA), Enrique Martinez Saez(Los Alamos National Laboratory, USA)

Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room7

[SY-I1] **Grain Growth at the Nanoscale: The Coupling of Stress and Grain Boundary Motion**

○Peter Voorhees[1], Kevin McReynolds[1,3], Akinori Yamanaka[2]　(1.Northwestern University, United States of America, 2.Tokyo University of Agriculture and Technology, Japan, 3.National Institute for Standards and Technology, United States of America)

[SY-I1] Verification of grain growth models by time-resolved 3D experiments in pure iron

○Jin Zhang[1,2], Yubin Zhang[2], Wolfgang Ludwig[3], David Rowenhorst[4], Henning F Poulsen[2], Peter W Voorhees[1]　(1.Northwestern University, United States of America, 2.Technical University of Denmark, Denmark, 3.European Synchrotron Radiation Facility, France, 4.The US Naval Research Laboratory, United States of America)

[SY-I1] Coarse-grained, three-dimensional modeling of defects at low-angle grain boundaries with the amplitude expansion of the phase field crystal model

○Marco Salvalaglio[1], Rainer Backofen[1], Ken R. Elder[2], Axel Voigt[1]　(1.Institute of Scientific Computing, Technische Universität Dresden, 01062 Dresden , Germany, 2.Department of Physics, Oakland University, Rochester, 48309 Michigan , United States of America)

[SY-I1] **Estimation of Grain Boundary Anisotropy using Multi-phase-field Model based on the Ensemble Kalman Filter**

○Akinori Yamanaka, Yuri Maeda, Kengo Sasaki　(Tokyo University of Agriculture and Technology, Japan)

[SY-I1] Multiscale Modelling of Graphene from Nano to Micron Scales

○Tapio Ala-Nissila　(Aalto and Loughborough University, Finland)

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room7)

[SY-I1] Grain Growth at the Nanoscale: The Coupling of Stress and Grain Boundary Motion

Invited

○Peter Voorhees[1], Kevin McReynolds[1,3], Akinori Yamanaka[2]　(1.Northwestern University, United States of America, 2.Tokyo University of Agriculture and Technology, Japan, 3.National Institute for Standards and Technology, United States of America)

Phase field crystal (PFC) models have been used to describe a wide range of phenomena from grain growth to solidification and dislocation motion in crystals. The method allows the atomic scale motion and defect formation to be determined on diffusive timescales. Following a brief introduction to the PFC method, the structure and dynamics of grain boundaries will be discussed. Using two-dimensional and three-dimension PFC simulations, we find that the atomic-scale structure of the boundary gives rise to qualitatively new grain growth kinetics as well as to grain rotation and grain translation. These new modes of growth can give rise to periodic changes in the morphologies of the grains as they grow or shrink. We find that grain translation is a result of the climb, glide, and elastic interactions of the dislocations that comprise the grain boundary, as well as dislocation interactions at trijunctions. We also find conditions where the stress generated during grain boundary motion can lead to a cessation of grain growth.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room7)

[SY-I1] Verification of grain growth models by time-resolved 3D experiments in pure iron

○Jin Zhang[1,2], Yubin Zhang[2], Wolfgang Ludwig[3], David Rowenhorst[4], Henning F Poulsen[2], Peter W Voorhees[1]　(1.Northwestern University, United States of America, 2.Technical University of Denmark, Denmark, 3.European Synchrotron Radiation Facility, France, 4.The US Naval Research Laboratory, United States of America)

Predicting the grain growth behavior of polycrystalline materials is important in the design of material properties in many engineering applications. Various analytical models are proposed to predict the growth behavior, *e.g.*, grain size distribution from the Hillert's theory or local growth behavior, *e.g.*, the growth rate from the MacPherson-Srolovitz theory. However, experimental verification of these models is lacking. In this work, we present a unique comprehensive dataset with 1300 grains and 15 annealing time-steps, which allows us to test various models for grain growth. In particular, we focus on the MacPherson-Srolovitz theory and address to what extent various statistical ensembles can be meaningfully described by the model and to what extent it is required to include anisotropy. A comprehensive statistical analysis shows that geometrical properties averaged over the entire grain ensemble are well described by the model, but the properties and evolution of the individual grains exhibit substantial scatter.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room7)

[SY-I1] Coarse-grained, three-dimensional modeling of defects at low-angle grain boundaries with the amplitude expansion of the

phase field crystal model

○Marco Salvalaglio[1], Rainer Backofen[1], Ken R. Elder[2], Axel Voigt[1]　(1.Institute of Scientific Computing, Technische Universität Dresden, 01062 Dresden , Germany, 2.Department of Physics, Oakland University, Rochester, 48309 Michigan , United States of America)

The Phase-Field Crystal (PFC) approach describes the dynamics of the local atomic probability density on atomic length scales and diffusive time scales [1]. It generally requires a fine spatial discretization, which limits the application of the method to small systems. The so-called amplitude expansion of the PFC model (APFC) is known to solve this issue, as it accounts for the evolution of the slowly varying amplitudes of the atomic probability density [2]. However, a limited number of parameters are present in the model and this poses some restrictions in the quantitative description of material properties. Moreover, the application of this model to three-dimensional systems has not been extensively explored.

We illustrate the modeling of defects at low-angle grain boundaries (GBs) forming between tilted crystals by means of the APFC model in two and three dimensions. This is achieved through a Finite Element Method with advanced numerical features such as adaptive mesh refinement exploiting the features of the APFC approach. Moreover, an extension of the model to control the energy of defects and GBs is proposed [3]. The possibility to describe dislocation networks at planar and spherical grain boundaries is illustrated for different lattice symmetries, namely triangular/honeycomb in 2D as well as body-centered cubic and face-centered cubic in 3D. The dynamics of spherical grain boundaries is also addressed in detail. In particular, the anisotropic shrinkage of spherical grain is addressed, revealing general qualitative features independent of the specific rotational axis and crystal symmetry [4] in agreement with recent atomistic calculations.

[1] K. R. Elder, M. Katakowski, M. Haataja, and M. Grant, Phys. Rev. Lett. 88, 245701 (2002)
[2] N. Goldenfeld, B. P. Athreya, and J. A. Dantzip, Phys. Rev. E 72, 020601 (2005)
[3] M. Salvalaglio, R. Backofen, A. Voigt, K. R. Elder, Phys. Rev. E 78, 184104 (2017)
[4] M. Salvalaglio, R. Backofen, K. R. Elder, A. Voigt, arXiv:1803.03233

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room7)

[SY-I1] Estimation of Grain Boundary Anisotropy using Multi-phase-field Model based on the Ensemble Kalman Filter

○Akinori Yamanaka, Yuri Maeda, Kengo Sasaki　(Tokyo University of Agriculture and Technology, Japan)

Grain growth is one of the most fundamental microstructure evolutions in metallic materials. Because the size of crystal grains strongly affects mechanical properties of materials, it is essential to predict the grain growth behavior during polycrystalline grain growth and recrystallization. Recently, the multi-phase-field model has been widely used for simulating the grain growth behavior and predicting average grain size and grain size distribution. In order to simulate a realistic grain growth behavior by the multi-phase-field simulation, we need to use accurate data of grain boundary properties, for example, anisotropic grain boundary mobility and grain boundary energy. However, it is difficult to identify the anisotropic grain boundary properties from experimental results by trial-and-error. This study proposes a data assimilation methodology for estimating grain boundary properties by incorporating experimental results into the multi-phase-field simulation of polycrystalline grain growth. We construct the data assimilation methodology using the Ensemble Kalman filter. We demonstrate that the anisotropic grain boundary energy can be successfully estimated from three-dimensional distributions of polycrystalline microstructure by the data assimilation method proposed in this

study.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room7)

[SY-I1] Multiscale Modelling of Graphene from Nano to Micron Scales

Invited

○Tapio Ala-Nissila （Aalto and Loughborough University, Finland）

Over the last few years novel 2D materials and thin heteroepitaxial overlayers have attracted intense attention due to their unusual properties and important technological applications. Many properties such as thermal conductivity and electrical transport are intimately coupled to the large scale mechanical and structural properties of the materials whose modeling is a formidable challenge due to a wide span of scales involved. In this talk, I will review progress in structural multi-scale modeling of 2D materials and thin overlayers [1], and graphene in particular [2], based on the Phase Field Crystal (PFC) model combined with standard microscopic modeling methods (classical MD and Quantum DFT). The PFC framework allows one to reach diffusive time scales for structural relaxation of the materials at the atomic scale, which facilitates quantitative characterisation of domain walls, dislocations, grain boundaries, and strain-driven self-organisation up to almost micron length scales. This allows one to study e.g. thermal conduction and electrical transport in multi-grain systems [3]. References: 1. Elder et al., PRL vol. 108, 226102 (2012); PRB vol. 88, 075423 (2013); JCP 144, 174703 (2016). 2. Hirvonen et al., PRB 94, 035414 (2016). 3. Fan et al., PRB vol. 95, 144309 (2017); Hirvonen et al., Sci. Reps. 7, 4754 (2017); Azizi et al., Carbon 125, 384 (2017); Fan et al., Nano Lett. 7b1072 (2017).

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I2] Symposium I-2

Chair: Elizabeth Holm(Carnegie Mellon University, United States of America)
Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room7

[SY-I2] Energy and dynamics of grain boundaries based on underlying mircrostructure

○Yang Xiang （Hong Kong University of Science and Technology, Hong Kong）

[SY-I2] **Grain growth in ultrafine-grained thin films: A 3D problem**

○Ahu Oencue[1], Thorsten Halle[2], Dana Zoellner[3] （1.Institute of Experimental Physics, Otto-von-Guericke University, Magdeburg, Germany, 2.Institute of Materials and Joining Technology, Otto-von-Guericke University, Magdeburg, Germany, 3.B CUBE Center for Molecular Bioengineering, TU Dresden, Dresden, Germany）

[SY-I2] The Kinetics of Ideal Grain Growth: A Large Scale Monte Carlo Simulation

○Xiangge Qin （School of Materials Science and Engineering, Jiamusi University, China）

[SY-I2] Understanding the energetics of grain boundary motion in terms of compatible transformations and optimal transport theory

○Ian W Chesser[1], Brandon Runnels[2], Elizabeth Holm[1] （1.Carnegie Mellon University, United States of America, 2.University of Colorado Colorado Springs, United States of America）

[SY-I2] **Microstructure Stabilization and the Herring Condition**

○Jeremy K Mason, Erdem Eren （University of California, Davis, United States of America）

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room7)

[SY-I2] Energy and dynamics of grain boundaries based on underlying mircrostructure

Invited
○Yang Xiang （Hong Kong University of Science and Technology, Hong Kong）

Grain boundaries are the interfaces of grains with different orientations in polycrystalline materials. Energetic and dynamic properties of grain boundaries play essential roles in the mechanical and plastic behaviors of the materials. These properties of grain boundaries strongly depend on their microscopic structures. We present continuum models for the energy and dynamics of grain boundaries based on the continuum distribution of the line defects (dislocations or disconnections) on them. The long-range elastic interaction between the line defects is included in the continuum models to maintain stable microstructure on grain boundaries during the evolution. The continuum models is able to describe both normal motion and tangential translation of the grain boundaries due to both coupling and sliding effects that were observed in atomistic simulations and experiments.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room7)

[SY-I2] Grain growth in ultrafine-grained thin films: A 3D problem

○Ahu Oencue[1], Thorsten Halle[2], Dana Zoellner[3] （1.Institute of Experimental Physics, Otto-von-Guericke University, Magdeburg, Germany, 2.Institute of Materials and Joining Technology, Otto-von-Guericke University, Magdeburg, Germany, 3.B CUBE Center for Molecular Bioengineering, TU Dresden, Dresden, Germany）

Grain microstructures of polycrystalline solids have an massive impact on materials properties. For investigations of bulk materials it is generally assumed that surfaces effects are insignificant. In contrast, in thin films surface effects become non-negligible. If during grain growth in such films the average grain size reaches the order of the layer thickness, grain growth slows down or even comes to a halt.

While analytic theories of nano- and microcrystalline grain growth are often in good agreement with numerical results using computer simulations with respect to, e.g., average growth kinetics, particularly analytic grain size distributions or topological correlations between grains rarely capture the experimental features. One reason of this disagreement can be found in the simple fact that the experimental samples are of 3D nature, but are commonly measured in 2D and compared with 2D simulations and analytic theories.

In the present work, we model grain growth in ultra-fine grained thin films using a three-dimensional Monte Carlo Potts model. In particular, we take into account that a reduction in grain size from micrometer to nanometer increases the importance of higher order grain boundary junctions, namely triple lines. The results are compared to experimental measurements of ultrafine-grained thin metallic films in three dimensions undergoing grain growth.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room7)

[SY-I2] The Kinetics of Ideal Grain Growth: A Large Scale Monte Carlo Simulation

○Xiangge Qin （School of Materials Science and Engineering, Jiamusi University, China）

Most of the metallic materials are polycrystalline aggregates, understanding the grain growth kinetics and controlling the grain size are important for predicting the microstructure of polycrystalline materials and preparing bulk nanomaterials. Although some theoretical equations for the ideal grain growth kinetics have been proposed, it is difficult to achieve an ideal grain growth process experimentally.

A considerable number of Monte Carlo simulations of the grain growth process have been reported, but none of the simulation results accurately match the ideal three-dimensional grain growth kinetics. In this paper, Monte Carlo method was used to simulate the three-dimensional grain growth process of metal. The effect of model temperature and model size on the dynamic simulation results of grain growth was studied. The grain size distribution during grain growth was analyzed. Large-scale simulation results show that the ideal grain growth kinetics accords with the theoretically predicted parabolic law, and the grain size distribution at the steady state stage is consistent with the Weibull distribution function.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room7)

[SY-I2] Understanding the energetics of grain boundary motion in terms of compatible transformations and optimal transport theory

○Ian W Chesser[1], Brandon Runnels[2], Elizabeth Holm[1]　(1.Carnegie Mellon University, United States of America, 2.University of Colorado Colorado Springs, United States of America)

In this study, we investigate two approaches to understanding the complex dependence of grain boundary mobility on temperature, crystallography, and driving force observed in experiments and molecular dynamics simulations. We first calculate energy barriers for unit mechanisms associated with faceted grain boundary migration, and show that although these barriers are useful in understanding trends in grain boundary mobility such as mobility type classification, they are difficult to enumerate for a large number of boundaries. As a second approach to explore the kinetics of grain boundary motion, we model GB mobility using Bain strains and dissipation energy, in the sense of martensitic phase transformations and twinning. This framework provides new insight into faceted grain boundary motion by interpreting it as a competition between compatible transformations at the boundary informed by approximate energy barriers to motion computed in an optimal transport framework. We establish a yield criterion for grain boundary migration via the interplay between optimal transportation energies, temperature, and applied load, and compare our results to existing shear coupling data in the literature.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room7)

[SY-I2] Microstructure Stabilization and the Herring Condition

Invited

○Jeremy K Mason, Erdem Eren　(University of California, Davis, United States of America)

Consistency of properties is critical for materials performance, and fundamentally depends on the stabilization of the microstructure. Existing stabilization techniques often rely on chemical modifications, with the solute preferentially segregating to the interfaces or precipitating as small second phase particles. The idea to instead stabilize a microstructure by modifying the crystallographic degrees of freedom is part of the broader subject known as grain boundary engineering. This has been most successful with materials that form low-energy annealing twins, though this severely restricts the materials to which the concept can be applied.

We propose that, rather than increasing the fraction of low-energy boundaries, grain boundary engineering can most effectively stabilize a microstructure by increasing the fraction of boundaries with boundary plane orientations at cusps in the energy landscape. The resistance of such boundaries to reorientation can pin boundary junction lines in two-dimensional materials and boundary junction points in three-dimensional materials. This is discussed in the context of the two-dimensional Herring condition and the three-dimensional analogue, which is apparently not widely known in the literature.

This leads to the idea that the microstructure of materials with arbitrary chemical compositions could be stabilized by introducing a misorientation distribution that makes many singular boundary plane orientations available; the material would then be allowed to evolve to a local minimum of the overall grain boundary energy, with the junction points pinned in metastable configurations. Simulation of such a process requires the implementation of accurate and general equations of motion for the junction points. We finally describe our ongoing development of a finite element-based microstructure evolution code for this purpose.

Symposium | L. Structure, Statistics and Mechanics in Crystal Dislocation Plasticity

[SY-L1] Symposium L-1

Chairs: Jerome Weiss(CNRS/ University of Grenoble-Alpes, France), Yinan Cui(University of California, Los Angeles, United States of America)

Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room8

[SY-L1] Flow and failure of (amorphous) materials - a nonequilibrium phase transition?

○Peter Schall （University of Amsterdam, Netherlands)

[SY-L1] Reversibility and Criticality in Amorphous and Crystalline Solids

○Charles Reichhardt （Los Alamos National Laboratory , United States of America)

[SY-L1] Exploring Crystal-plastic Constitutive Rules with the OOF Tool

○Andrew Reid[1], Stephen Langer[1], Shahiryar Keshavarz[1,2] （1.NIST, United States of America, 2.Theiss Research, United States of America)

[SY-L1] Objective fusion of multiscale experiments and multiscale models using Bayesian inference

○Surya Raju Kalidindi （Georgia Tech, United States of America)

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room8)

[SY-L1] Flow and failure of (amorphous) materials - a nonequilibrium phase transition?

Invited

○Peter Schall （University of Amsterdam, Netherlands）

Amorphous materials show intriguing mechanical properties that are of fundamental interest and of great importance for applications. While the aging, deformation and failure have been longstanding research questions for conventional glasses, recent soft glasses including colloidal suspensions, foams and emulsions have spawned new interest and new perspectives on glassy flow. In these systems, flow is ubiquitous: it is easily induced by small applied stresses, and the underlying flow and failure mechanisms can be conveniently studied at the particle scale. Simulations and experiments on soft glassy systems have witnessed exciting scaling relations that are believed to underlie the flow of glasses under applied stress. In particular, colloidal and granular systems have been powerful models to directly visualize and measure internal strain fields and their hierarchical organization. The emerging picture is that flow and flow instabilities are related to non-equilibrium phase transitions from a reversible elastic-like to irreversible plastic response of the material. At yielding of the material, plastic regions percolate across the sample, mediating the flow in the otherwise elastic matrix. Flow is therefore neither strongly localized nor homogeneous across the material; instead, system-spanning correlations of plastic activity occur, revealing a novel kind of criticality of the slowly flowing material. Similar long-range correlated flow phenomena have been observed in the deformation of crystals, as bursts of dislocations. Also in these crystalline materials, the internal elastic strain field is believed to be responsible for the highly correlated dislocation activity. I will elucidate this underlying mechanism by detailed investigation of the strain field in colloidal crystals and glasses. Furthermore, I will show that the underlying general mechanism links our soft materials to a far wider range of materials and phenomena including conventional material plasticity, geological flow phenomena, and earth quakes.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room8)

[SY-L1] Reversibility and Criticality in Amorphous and Crystalline Solids

Invited

○Charles Reichhardt （Los Alamos National Laboratory , United States of America）

The physical processes governing the onset of yield, where a material changes its shape permanently under external deformation, are not yet understood for amorphous solids that are intrinsically disordered. Here, using molecular dynamics simulations and mean-field theory, we show that at a critical strain amplitude the sizes of clusters of atoms undergoing cooperative rearrangements of displacements (avalanches) diverges. We compare this non-equilibrium critical behaviour to the prevailing concept of a 'front depinning' transition that has been used to describe steady-state avalanche behaviour in different materials. We explain why a depinning-like process can result in a transition from periodic to chaotic behaviour and why chaotic motion is not possible in pinned systems. These findings suggest that, at least for highly jammed amorphous systems, the irreversibility transition may be a side effect of depinning that occurs in systems where the disorder is not quenched.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room8)

[SY-L1] Exploring Crystal-plastic Constitutive Rules with the OOF Tool

Invited

○Andrew Reid[1], Stephen Langer[1], Shahiryar Keshavarz[1,2] （1.NIST, United States of America, 2.Theiss Research, United States of America）

A focus of the US National Institute of Standards and Technology effort associated with the Materials Genome Initiative is the construction of software tools for exploring structure-property relationships. One of these is the OOF Object-oriented finite-element tool, which is an integrated materials-focused image segmentation, mesh construction, and modeling system, allowing interactive structure-property explorations on meshes modeling realistic microstructures. A crystal-plastic modeling capability has recently been added to the OOF finite-element tool, bringing together OOF's ability to easily create meshes corresponding to real microstructures, and the capability to quickly and easily explore a wide variety of constitutive rules derived from various dislocation activity mechanisms derived. This provides a length-scale bridge from continuum descriptions of dislocations in the bulk to representative volume elements relevant to particular classes of microstructures. Early results of this exploration will be presented. The promise of this effort is that, coupled with suitable reference experiments on small systems, high-fidelity continuum crystal-plastic constitituve rules can be identified, and then employed in larger-scale material models.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room8)

[SY-L1] Objective fusion of multiscale experiments and multiscale models using Bayesian inference

○Surya Raju Kalidindi （Georgia Tech, United States of America）

There is currently no formal framework for fusing the information gathered from multiscale materials modeling and measurement efforts in ways that optimally inform each other. This is mainly because the space of governing physics in any selected multiscale materials phenomenon is extremely large (this includes all potential model forms and the ranges of parameter values needed to identify the governing physics as accurately as possible), and the amount of the relevant experimental data is typically limited, incomplete, and uncertain. Consequently, a direct calibration of the governing physics based on the available measurements using standard regression techniques usually does not produce reliable results. In this paper, we explore the benefits of applying Bayesian inference techniques combined with reduced-order models and higher-throughput experimental assays in establishing a mathematically rigorous framework for addressing the challenge identified above. More specifically, the new framework will be demonstrated with a very simple case study - the identification of the intrinsic single crystal material properties from spherical indentation stress-strain measured on a polycrystalline sample.

[SY-L2] Symposium L-2

Chairs: Charles Reichhardt(Los Alamos National Laboratory , United States of America), Peter Schall(University of Amsterdam, Netherlands)

Mon. Oct 29, 2018 3:45 PM - 5:45 PM Room8

[SY-L2] **The role of system size, internal disorder, and dislocation patterning on the nature of plastic fluctuations**
○Jerome Weiss （CNRS/University of Grenoble-Alpes, France）

[SY-L2] **Dislocations associated with stick-slip friction of lubricants in boundary lubrication**
Rong-Guang Xu[1,2], Hengxu Song[2], Stefanos Papanikolaou[2], ○Yongsheng Leng[1] （1.George Washington Univ, United States of America, 2.West Virginia Univ, United States of America）

[SY-L2] **Comparison of surface-indentation and pillar-compression at the nanoscale of FCC metals: Unification of size effects using 3D Discrete Dislocation Dynamics**
○Hengxu Song[1,2], Stefanos Papanikolaou[1,2] （1.west virginia university, United States of America, 2.johns hopkins university, United States of America）

[SY-L2] **Statistical models for cross slip and reaction rate processes in continuum dislocation dynamics**
○Vignesh Vivekanandan, Peng Lin, Anter El-Azab （Purdue University, United States of America）

[SY-L2] **Designing Interfaces: a combinatorial approach to geometrical manipulation of interfaces**
○Hakan Yavas[1], Alberto Fraile[1], Tomas Polcar[1,2], Ondrej Man[3] （1.Czech Technical University, Czech Republic, 2.University of Southampton, UK, 3.CEITEC, Czech Republic）

(Mon. Oct 29, 2018 3:45 PM - 5:45 PM Room8)

[SY-L2] The role of system size, internal disorder, and dislocation patterning on the nature of plastic fluctuations

Invited

○Jerome Weiss （CNRS/University of Grenoble-Alpes, France）

In classical plasticity theory, plastic *flow* is assumed to be smooth and homogeneous, as illustrated by the Orowan's relation linking the strain-rate to an average mobile dislocation density. However, it has been long recognized that in HCP materials plastic deformation can occur through bursts of activity involving the coordinated motion of numerous dislocations, i.e. dislocation avalanches. More recently, acoustic emission (AE) measurements showed that these avalanches are associated with scale-free properties such as intermittency, power-law statistics and fractal patterns. In the words of Mandelbrot, these plastic fluctuations are wild, thus making tricky the definition of a representative volume element for plasticity. On the other hand, in multi-slip systems such as FCC materials, short-range interactions between dislocations lead to the emergence of dislocation patterns characterized by a well-defined internal length scale, which can be related with the dislocation density and strain-hardening from the similitude principle and Taylor's relation. AE measurements have shown that this patterning frustrate the development of dislocation avalanches. Consequently, plastic deformation occurs essentially through small and uncorrelated, i.e. mild, fluctuations, coexisting however with few larger and intermittent events leading to fundamental rearrangements of the dislocation substructure. When the system size becomes comparable or smaller than the internal length scale mentioned above, dislocation patterning can no longer emerge, leading to a dominance of wild (scale-free) fluctuations even for FCC or BCC materials, and a change in the mechanisms of hardening. In other words, there is size effect on the nature of plastic fluctuations. Such wild fluctuations might be unwelcomed in the context of nanotechnology. Recent works showed that the introduction of disorder (alloying) allows controlling (decreasing) the internal length scale, hence mitigating wild plastic fluctuations at small scales. These different aspects of plastic fluctuations will be reviewed.

(Mon. Oct 29, 2018 3:45 PM - 5:45 PM Room8)

[SY-L2] Dislocations associated with stick-slip friction of lubricants in boundary lubrication

Rong-Guang Xu[1,2], Hengxu Song[2], Stefanos Papanikolaou[2], ○Yongsheng Leng[1] （1.George Washington Univ, United States of America, 2.West Virginia Univ, United States of America）

Improved understanding of squeezing and frictional behaviors of lubricant films under extreme confinement at nanometer scales can lead to strategies for preventing surface failure and efficient energy usage. Shearing of a solidified simple nonpolar film under nanoconfinement is studied by using a liquid-vapor molecular dynamics simulation method. We find that, in contrast with the shear melting and recrystallization behavior of the solidlike phase during the stick-slip motion, interlayer slips within the film and wall slips at the wall-film interface are often observed. The ordered solidified film is well maintained during the slip. However, repeated film dilation and collapse of the lubricant film during the stick-slip friction are observed, which is associated with the nucleation, propagation and annihilation of dislocations found in the solidlike film. These novel observations may provide new insights into the mechanical behaviors of lubricant films and thus improved lubricant design.

(Mon. Oct 29, 2018 3:45 PM - 5:45 PM Room8)

[SY-L2] Comparison of surface-indentation and pillar-compression at the nanoscale of FCC metals: Unification of size effects using 3D Discrete Dislocation Dynamics

○Hengxu Song[1,2], Stefanos Papanikolaou[1,2] （1.west virginia university, United States of America, 2.johns hopkins university, United States of America）

Plasticity of FCC materials at the nanoscale is size dependent, abrupt and stochastic. These features have hindered the predictability of nanoscale plasticity and consequently, engineering at small scales. Surface indentation and pillar compression have been the two major pathways towards developing predictive theories. While surface indentation has strong relevance to engineering, the development of theories has been more efficient for pillar compression studies. In this work, we connect the flat-punch nanoindentation and uniaxial pillar compression size effects under one unified framework. Through three-dimensional Discrete Dislocation Dynamics (3D DDD) simulations, we investigate uniaxial compression of pillars and also flat-punch nanoindentation, for identical pre-existing dislocation densities. We study various pillar/punch sizes (0.25 - 8 μm) and experimentally relevant initial dislocation densities. We demonstrate that Tabor's law, which is valid at the macroscale, also extends at the nanoscale, given that statistical averaging is appropriately considered. We develop the statistical theory behind this nanoscale "Tabor's law" using probabilistic concepts and we confirm its validity using 3D-DDD simulations.

(Mon. Oct 29, 2018 3:45 PM - 5:45 PM Room8)

[SY-L2] Statistical models for cross slip and reaction rate processes in continuum dislocation dynamics

○Vignesh Vivekanandan, Peng Lin, Anter El-Azab （Purdue University, United States of America）

We tackle the question of temporal coarse graining in dislocation dynamics with a special attention to cross slip and dislocation reaction rates. The time series approach was used to analyze the statistical properties of these processes from discrete dislocation dynamics. The statistical data required to perform this analysis is obtained using the method of dislocation dynamics simulation. The temporal correlations and correlation times of cross-slip and short-range reactions were computed. The correlation time was used as a coarse graining time-scale in continuum dislocation dynamics. Using this mesoscopic time-scale, a coarse grained stochastic representation of cross slip and dislocation reactions has been achieved and implemented in continuum dislocation dynamics. We compare the performance of two discrete dislocation dynamics approaches, the microMegas model and ParaDiS, on the results of the coarse grained cross slip and junction formation rates, and, in turn, on the dislocation microstructure predicted by continuum dislocation dynamics.

(Mon. Oct 29, 2018 3:45 PM - 5:45 PM Room8)

[SY-L2] Designing Interfaces: a combinatorial approach to geometrical manipulation of interfaces

○Hakan Yavas[1], Alberto Fraile[1], Tomas Polcar[1,2], Ondrej Man[3] （1.Czech Technical University, Czech Republic, 2.University of Southampton, UK, 3.CEITEC, Czech Republic）

The selection and design of modern high-performance engineering materials are driven by controlling and optimizing varieties of mechanical and thermal properties such as strength, ductility, plasticity, and toughness. Nanoscale metallic multilayers (NMMs) are the relatively new class of materials with a high potential of changing their conventional counterparts that are using in the high-end applications, i.e. nuclear, space and aerospace. The superior properties of the NMMs are mostly correlated with the advanced design and fabrication of the interfaces at a very confined space (2- 20 nm). In this presentation, we will represent a novel nanoscale interface architecture of the Zr-Nb NMMs that are fabricated by following epitaxial and physical vapor deposition based film-growth techniques. Then, we will discuss the effect of polycrystalline, epitaxial and amorphous interfaces on the deformation kinetics. Additionally, we will also present the dynamic response maps of the molecular dynamics simulations and correlate them to dislocation activity.

Symposium | J. Multiscale Modeling of Heterogeneous Layered Media

[SY-J1] Symposium J-1

Chairs: Jinghong Fan(Alfred University, United States of America), Sinan Keten(Northwestern University, United States of America)

Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room10

[SY-J1] **A multiscale failure analysis for layered composites with statistical account of manufacturing defects**

○Ramesh Talreja （Texas A&M University, United States of America）

[SY-J1] Multiscale Modeling of Fiber Reinforced Materials for Future Aerospace Structures

○Anthony M Waas （U. Washington, Seattle, WA 98195; also Univ. of Michigan, Aerospace Engineering, Ann Arbor, MI 48109, United States of America）

[SY-J1] **A-DiSC (Adaptive Discrete-Smeared Crack) Model for Multi-Scale Progressive Damage Analysis of Composite Structures**

○Tong-Earn Tay, Xin Lu, Vincent Beng-Chye Tan （National University of Singapore, Singapore）

[SY-J1] Analysis for the Plane Problem of Layered Magnetoelectric Composite with Collinear Interfacial Cracks

○Wenxiang Tian[1], Zheng Zhong[1,2] （1.School of Aerospace Engineering and Applied Mechanics,Tongji Univ, China, 2.School of Science, Harbin Institute of Technology, China）

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room10)

[SY-J1] A multiscale failure analysis for layered composites with statistical account of manufacturing defects

Invited

○Ramesh Talreja （Texas A&M University, United States of America）

As composite materials have broadened in their applications from aerospace to automotive and energy industries, their cost-effectiveness has become critical. Since in most cases, a major cost lies in the manufacturing process, the effects of defects on performance has gained renewed attention. Traditional failure analysis has either not considered effects explicitly or has accounted by these in artificial ways. The work to be presented develops a statistical simulation of manufacturing defects such as nonuniform fiber distribution within the matrix by quantifying deviations from uniformity based on fiber mobility during the manufacturing process. Algorithms are implemented to generate representation of the "real" microstructure with quantified anomalies. The representative volume element realizations are subjected to boundary conditions under which the local stress fields are computed. A hierarchical energy based set of failure criteria are used to determine occurrence of the sequence of failure events and their progression. By parametric studies, the effects of defects as well as constituent properties on failure behavior under different loading conditions is clarified.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room10)

[SY-J1] Multiscale Modeling of Fiber Reinforced Materials for Future Aerospace Structures

Invited

○Anthony M Waas （U. Washington, Seattle, WA 98195; also Univ. of Michigan, Aerospace Engineering, Ann Arbor, MI 48109, United States of America）

The current practice of designing composite aerospace structures relies on extensive testing, coupled to a bottom-up, pyramidal building block approach, to ensure structural integrity and damage tolerance. Reducing the number of tests can lead to a substantial decrease in total design cost of many vehicles. Cost reduction is enabled by developing high fidelity computational models which can provide valuable information regarding the performance of a structure up to and including failure. Composites, because of their heterogeneity, display a rich variety of damage (dissipation) and failure (two piece) mechanisms starting at the atomistic scale and progressing up in length scale. An acute understanding of the physics and mechanics of these mechanisms, at different scales, is essential in order to develop physically sound theories and attendant computational methids for predicting the structural performance of a composite structure. With a view towards addressing future, robotically manufactured polymer matrix composite structures for lightweight vehicle applications, this talk will address a multiscale computational modeling framework that the author has developed over the past deacde to model and predict the structural performance of polymer matrix composites. Nonlinear material response, including damage and failure, is incorporated in conjunction with geometric nonlinearity to predict damage evolution and failure that is observed in the laboratory for a variety of examples. Issues related to mesh objectivity will be addressed and the importance of this aspect in numerical predictions will be highlighted.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room10)

[SY-J1] A-DiSC (Adaptive Discrete-Smeared Crack) Model for Multi-Scale Progressive Damage Analysis of Composite Structures

Invited

○Tong-Earn Tay, Xin Lu, Vincent Beng-Chye Tan （National University of Singapore, Singapore）

Laminated fibre-reinforced composite structures often fail in a complex progressive damage process involving interaction of mulitple failure mechanisms, including matrix cracking, interfacial delamination, local micro-buckling and fibre rupture. Modeling these multi-scale mechanisms in a single simulation with sufficient fidelity to the physics while retaining computational efficiency still presents a formidable challenge. Discrete crack models (DCMs)[1-3] offer excellent fidelity, especially for modeling multiple crack interactions, but are impractical and inefficient for structures larger than coupon sizes. Recently, an adaptive DCM has been proposed to improve computational efficiency[4]. On the other hand, smeared crack models (SCMs)[5,6] are suitable for describing diffuse damage such as micro-cracks but unable to properly account for local coupling effects and final fracture. In this presentation, an adaptive discrete-smeared crack model (A-DiSC) is proposed, whereby the DCM is initially used to model matrix cracks and their interaction with delaminations via cohesive interface elements, but non-critical cracks are later converted to diffused damage using SCM. The transitional region from DCM to SCM is effected through satisfaction of certain criterion based on the principle of energy conservation[3]. The proposed A-DiSC model is applied to the tensile failure analysis of open-hole composite laminates.

(Mon. Oct 29, 2018 1:30 PM - 3:15 PM Room10)

[SY-J1] Analysis for the Plane Problem of Layered Magnetoelectric Composite with Collinear Interfacial Cracks

○Wenxiang Tian[1], Zheng Zhong[1,2] （1.School of Aerospace Engineering and Applied Mechanics,Tongji Univ, China, 2.School of Science, Harbin Institute of Technology, China）

A fracture problem of collinear interfacial cracks in layered magnetoelectric composites is studied. The magnetic permittivity of the piezoelectric material and the dielectric constant of the piezomagnetic material are considered. The poling axis of the piezoelectric and piezomagnetic material are all assumed to be perpendicular to the interfacial cracks and an in-plane magnetic potential difference or voltage is applied along the poling axis, which results in in-plane deformation of the composite. Thus, a plane fracture problem is studied in the present paper. A system of singular integral equation of the second kind with Cauchy kernel is obtained by means of Fourier transform and further solved by using Jacobi polynomials. The primary interfacial fracture mechanics parameters, such as the stress intensity factors, the electric displacement intensity factors, the magnetic inductions intensity factors and the energy release rates are then obtained. Analysis reveals that the material combination and the thickness ratio of piezomagnetic/ piezoelectric layer has significant influences on the stress, the electric displacement and the magnetic inductions on the interface versus the thickness of the active response layer. In terms of the defined dimensionless parameters Z_{sigma}, Z_B, Z_D, which represent the interface material mismatch under in-plane deformation, three different cases can be categorized for each parameter, *i.e.* $Z_{sigma}>1$,$Z_{sigma}<1$ and $Z_{sigma}=1$; $Z_B>1$, $Z_B<1$ and $Z_B=1$; $Z_D>1$, $Z_D<1$ and $Z_D=1$; where the stress curves, magnetic inducions curves and electric displacement curves display different monotony, respectively. Based on the three dimensionless parameters, we can define another four dimensionless parameters C_{KI},C_{KII},C_{KD},C_{KB}, which represent the cracked interface material mismatch under in-

plane deformation, different cases can be categorized for different parameters, where the corresponding intensity factor curves display different monotony.

[SY-J2] Symposium J-2

Chairs: Anthony M Waas(University of Washington, United States of America), Junqian Zhang(Shanghai University, China)
Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room10

[SY-J2] Simulation-based Design of Bioinspired Impact-resistant Nanocellulose Films with Bouligand Microstructure
○Sinan Keten （Northwestern University, United States of America）

[SY-J2] **Amelogenesis: Nature's 3D printing system for multi-scale laminates**
○brian n cox （arachne consulting, United States of America）

[SY-J2] **Role of geometrical features on mechanical properties in bio-inspired staggered composites**
Aman Mahar, ○Siladitya Pal （Indian Institute of Technology Roorkee, India）

[SY-J2] Dynamic homogenization for acoustic metamaterials
○Celia Reina, Chenchen Liu （University of Pennsylvania, United States of America）

[SY-J2] **Cracking behavior of ferrite-pearlite pipeline steel with hierarchical and concurrent multiscale modeling schemes**
○Taolong Xu[1,2], Wei Wang[1], Xiaojiao Deng[1], Anlin Yao[1], Jinghong Fan[3,2] （1.Southwest Petroleum University of China, China, 2.International Institute of Material Multiscale Modeling, United States of America, 3.Alfred University, United States of America）

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room10)

[SY-J2] Simulation-based Design of Bioinspired Impact-resistant Nanocellulose Films with Bouligand Microstructure

Invited

○Sinan Keten （Northwestern University, United States of America）

The Bouligand structure, which features a helicoidal layup of in-plane uniaxial arranged fibers, has been widely observed in biomaterials with superior impact-resistant properties. However, the underlying mechanisms for the damage tolerance remain poorly understood, posing great challenges for the design and development of bio-inspired materials with optimized microstructures. Interestingly, many bio-sourced nanomaterials such as cellulose nanocrystals (CNCs) achieve helicoidal ordering through self-assembly. As a step towards mimicking impact tolerant biomaterials, here we present systematically coarse-grained molecular dynamics simulations of nanoscale projectiles impacting CNC films with Bouligand structure as a model system. We report the specific ballistic limit velocity and energy absorption as metrics to quantify impact performance of CNC films. We discover that Bouligand structures with low pitch angles (10-30 degrees) show optimal ballistic resistant performance, and significantly outperform quasi-isotropic baseline structures. Intriguingly, decreasing interfacial interactions helps enhance the performance under impact through allowing dissipative inter-fibril and interlayer sliding events to occur more readily without severe fibril fragments. We show that improved interfacial sliding, enhanced wave propagation, larger in-plane crack opening and through-thickness crack twisting contribute to the improved energy dissipation during projectile penetration for CNC Bouligand films with optimal pitch angles. This study reveals structural and chemical factors that govern the optimal design of Bouligand structures made from 1D nanomaterials for protective applications. Concluding remarks will include comparative analyses on other thin film materials, including layered graphitic and metallic nanostructures through scaling and theoretical arguments, as well as potential strategies for mechanical property improvement through better nanocellulose interface design.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room10)

[SY-J2] Amelogenesis: Nature's 3D printing system for multi-scale laminates

Invited

○brian n cox （arachne consulting, United States of America）

Ameloblasts are pencil-shaped cells with writing (secretory) tips at one end, which mass together in 2D sheets, standing on their writing ends. As they write (secrete protein scaffolds), they slide past one another and/or swap places, so that the secretions of the whole cell population form complex patterns in 3D space as the secreted material accumulates (amelogenesis is additive manufacturing). The secreted protein is the spatial template for the chemical reactions that result in mineralized dental enamel. By forming patterned microstructures, the cells impart exceptional fracture properties to the enamel.

How does each ameloblast know where and how fast to move at any instant during the writing process, so that it will contribute correctly to the desired pattern? There is no analogue of an external computer issuing instructions to all cells (the human engineering approach to 3D printing). Instead, we postulate that cells acquire the timing and positional information they need by sensing their evolving local strain environment: as the population moves, global shape changes map onto local strains around individual cells, and vice versa. Analyzing the mapping from local to global is a complex 3D problem in nonlinear wavelike cell motions. Its

solution leads to deduction of cell "response functions" (rules that state cell actions for a given strain state) that will lead, when assigned to all cells, to correct patterns.

Having discovered the right response functions, we can account for much of the movement of pattern-forming ameloblasts in, e.g., the mouse incisor, including: the complex 3D trajectory of each cell during amelogenesis as layered structures are formed; switching on and off of secretion; the matching of the rate of enamel manufacture to the rate of eruption of the mouse incisor; and the appearance and spatial wavelength of "cohorts" of ameloblasts, which are an instance of spontaneous segmentation of a homogeneous population into a periodic structure.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room10)

[SY-J2] Role of geometrical features on mechanical properties in bio-inspired staggered composites

Aman Mahar, $^{\circ}$Siladitya Pal (Indian Institute of Technology Roorkee, India)

Nacre (mother of pearl), bone, and teeth boast a prominent amalgamation of mechanical facets such as strength, toughness and stiffness. Merger of these properties in engineering materials is still a challenge. Nacre, which is an inner shell layer of many sea-shells, primarily made of 95% of brittle mineral (calcium carbonate), however; it exhibits superior mechanical properties as compared to their major constituents. Micro-structure of nacreous layer reveals the staggered 'brick-bridge-mortar' architecture in which polygonal shaped mineral tablets are stacked and organic layer and mineral bridges act as a glue and interconnection between platelets, respectively. Mimicking of the architecture of these biological materials has captured the attention of research community for development of high performance composites. However, an in-depth knowledge of structure-properties-function relationship is still lacking. Therefore, the goal of the present study is to provide a detailed understanding on the role of geometric parameters towards the origin of extraordinary mechanical properties.

In the present study, we will develop a predictive modeling framework to understand the influence of staggered architectured composite on emergent mechanical behaviors under quasi-static loading condition. Therefore, a finite element framework will be adopted and implemented in parallel computing enviroment. The state-of-art cohesive zone models will be incorporated to account the failure of inter-layers and mineral bridges, separately. Using the model, we will provide systematic parametric study of geometrical features such as overlap ratio, aspect ratio, bridge density and bridge distribution on emergent strength, stiffness and toughness. Finally, detail design map will be constructed that can assist to develop novel architectured composites with tailored mechanical properties.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room10)

[SY-J2] Dynamic homogenization for acoustic metamaterials
$^{\circ}$Celia Reina, Chenchen Liu (University of Pennsylvania, United States of America)

A variational coarse-graining framework for heterogeneous media in the spirit of FE^2 methods is proposed, which allows for a seamless transition from the traditional static scenario to dynamic loading conditions,

while being applicable to general material behavior. The method automatically delivers the coarse-grained macroscopic equations of motion together with a computational multiscale solver. Newmark method is employed for the time discretization, and excellent accuracy, stability, and computational time saving have been certified through the comparison with the standard single scale finite element solver. In addition, the capability of the multiscale solver to capture wave scattering has been demonstrated by the simulations in locally resonant sonic materials.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room10)

[SY-J2] Cracking behavior of ferrite-pearlite pipeline steel with hierarchical and concurrent multiscale modeling schemes

○Taolong Xu[1,2], Wei Wang[1], Xiaojiao Deng[1], Anlin Yao[1], Jinghong Fan[3,2]　(1.Southwest Petroleum University of China, China, 2.International Institute of Material Multiscale Modeling, United States of America, 3.Alfred University, United States of America)

Attempts of two schemes with atomistic-based multiscale simulations for lamellar ferrite-pearlite pipeline steel are evoked in this work. They are hierarchical multiscale method by atomistic-based Cohesive Zone Model (CZM) and concurrent multiscale method by extended Generalized Particle Dynamics Method (XGP), where XGP proposed recently by author and coauthors (Fan, Eng. Fract. Mech., 2017) is an extension of the GP method (Fan, Multiscale Model. Simul., 2009) in which finite element (FE) nodes are connected with the outermost particles, thus encouraging accurate crack-tip parameters are obtained due to reduce artificial effects on the atom-node boundary. The former one bridging crack propagation at the atomistic and mesoscopic scale by local energy release rate G_c extracted from ferrite-cementite grain boundary, where G_c characterized by exponential and trilinear traction-separation law (TSL) complied into VUMAT in finite element software, using the unique cohesive element length (Xu, Eng. Fract. Mech., 2016), tension specimen FE models are designed to reveal the accuracy of the intrinsic correlation between the atomistic and mesoscopic scale under a stress intensity factor, and will be verified by the fracture test result, which proves the practicability of concurrent multiscale method to solve the cracking behavior of engineering material. The latter one investigates the lamellar ferrite-cementite micro-structure with extra size compared to conventional multiscale method such as the quasicontinuum (QC) method, for crack-tip behavior, the GP method provides the possible way to qualify the layer thickness characterize of ferrite, as well as the model size effect via XGP multiscale analysis under one-order larger than GP model, XGP method develops a sufficiently large model bases on proven accuracy may open a new avenue to study the cracking behavior in lamellar structure, also explore a new types of multiscale methods which can improve the accuracy in bridging atomistic and continuum scales. However, each simulation scheme, Bagaryatskii orientation relationship between ferrite and cementite within pearlite is developed by Voronoi geometric method, and then the crystal boundary of lowest energy state is obtained by using conjugate gradient method and annealing under NPT ensemble.

Poster Session | A. Advances in Materials Theory for Multiscale Modeling

[PO-A1] Poster Session 1

Symposium A

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-01] The Coadsorption Effect of Cl- and H_2O on the Various Defect Al_2O_3 Film Surface

○Chuan-Hui Zhang, Bao Chen, Peng Shi （University of Science and Technology Beijing, China）

[P1-02] Incorporation of double cross-slip in continuum dislocation dynamics

○Xingjian Zhou, Yichao Zhu （Faculty of vehicle Engineering and Mechanics, Dalian University of Technology, China）

[P1-03] **Effect of Defect on Structural and Optical Properties in Methyl-Ammonium Lead Iodide(MAPI) Perovskite via First Principles Calculations**

○Abdullah Al ASAD, Keiichi MITANI, Atsushi ISHIKAWA, Kenji TSURUTA （Dept. of Electrical and Electronic Engineering, Okayama University, Japan）

[P1-04] Isogeometric modeling and large-scale computation for stress field around lattice defects

○Shunsuke Kobayashi[1], Ryuichi Tarumi[2], Atsushi Suzuki[3], Masao Ogino[4], Yoji Shibutani[1] （1.Graduate School of Engineering, Osaka Univ., Japan, 2.Graduate School of Engineering Science, Osaka Univ., Japan, 3.Cybermedia Center, Osaka Univ., Japan, 4.Information Technology Center, Nagoya Univ., Japan）

[P1-05] **A local/nonlocal plasticity model for upscaling microstructural effects**

○John Mitchell （Sandia National Laboratories, United States of America）

[P1-06] **First-principles investigation of atomic hydrogen adsorption and diffusion on/into Mo-doped Nb (100) surface**

○Zhong-min Wang, Yang Wu, Qingrong Yao, Yan Zhong, Chaohao Hu, Huaiying Zhou （Guilin University of Electronic Technology, China）

[P1-07] **First-principles Study on Electronic Properties of Hybrid MABX_3 perovskites (MA= $CH_3NH_3^+$; B= Pb, Sn, Ge; X= I, Br, Cl)**

○Narasak Pandech[1,2], Thanundon Kongnok[1], Sirichok Jungthawan[1], Sukit Limpijumnong[1], Walter R.L Lambrecht[2] （1.School of Physics and NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials, Suranaree University of Technology, NakhonRatchasima 30000, Thailand, Thailand, 2.Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106-7079, USA., United States of America）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-01] The Coadsorption Effect of Cl- and H_2O on the Various Defect Al $_2O_3$ Film Surface

○Chuan-Hui Zhang, Bao Chen, Peng Shi （University of Science and Technology Beijing, China）

First-principles calculations have been performed on the perfect surface, point-defect surface, step-defect surface, layer-defect surface of Al_2O_3 film with water molecules and chloride ions. The coadsorption mechanism has effect on the reaction and erosion of the surface. The adsorption energies (E_{ads}), stable adsorbed sites, binding of film, charge transfer, reactants and products, activation energies and transition states are calculated and discussed. The results evidence that for the perfect Al_2O_3 surface, the critical monolayer of Cl- is 3/7, the E_{ads} decrease in three steps, each E_{ads} step only relate to the adsorbed site and the morphology. For point-defect surface, substitution point defects are more sensitive than vacancy point defects for reaction and erosion. The species of products depend on the energy barrier and orientation of water. For step-defect surface, Al1 step-defect and Al3 step-defect surfaces prefer to obtain $Al-H_2O$ compounds, while O2 step-defect surface prefers to form Al-Cl products. There is no obvious linear relationship between the number of products and the number of steps. For layer-defect surface, when low concentrations of Cl ions reach the surface, they prefer to erode the Al layer-defect surface with producing Al-Cl compounds, while they prefer to interact with H_2O upon the O layer-defect surface.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-02] Incorporation of double cross-slip in continuum dislocation dynamics

○Xingjian Zhou, Yichao Zhu （Faculty of vehicle Engineering and Mechanics, Dalian University of Technology, China）

It is widely agreed that the cross-slip mechanism of screw dislocations plays a key role as crystalline materials deform plastically. In discrete dislocation dynamics (DDD) models, the onset of cross-slip is widely formulated as a random event. However, a proper formulation of cross-slip in models of continuum dislocation dynamics (CDD), where dislocation microstructures are described as a density distribution, is still missing. In this presentation, we present a CDD framework incorporating cross-slip mechanism. The discrete-to-continuum (D2C) transition is carried out by translating the probability of a discrete event into a collective frequency. This work is conducted under the framework of dislocation density potential function (DDPFs), where the mean-field stress can be evaluated with related ease. Numerical examples will be shown to demonstrate the role of cross-slip in the determination of material's stress-strain relation.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-03] Effect of Defect on Structural and Optical Properties in Methyl-Ammonium Lead Iodide(MAPI) Perovskite via First Principles Calculations

○Abdullah Al ASAD, Keiichi MITANI, Atsushi ISHIKAWA, Kenji TSURUTA （Dept. of Electrical and Electronic Engineering, Okayama University, Japan）

Hybrid organic/inorganic perovskites(HOIPs) have drawn significant research interests due to the incomparable rapid rise in energy conversion efficiency seen in photovoltaic devices based on $CH_3NH_3PbI_3$. Current research attempts in this field have concentrated on searching for similar perovskites with better properties, especially stability under a humid condition and/or irradiation [1]. In this work, employing first-principles calculations based on the density functional theory, we have investigated effects of vacancy on the optimized structures, bandgap, total and partial density of state, effective on-site and bond charge, by comparing with relevant experimental and/or theoretical data [2]. These analyses reveal that a Pb vacancy induces an asymmetric distortion of the lattice, which leads to a local volume expansion at low temperature [3]. The degenerate states at the conduction band minimum(CMB) are split each other due to the defect and it promotes broadening of the light absorption spectra. Possible effects of interstitial impurity, such as a water molecule, will also discussed in the presentation.

[1] A. K. Chauhan and P. Kumar, J. Phys. D: Appl. Phys. 50 (2017) 325105.
[2] Y. Wang et al., Phys. Chem. Chem. Phys. 16 (2014)1424.
[3] A. Walsh et al., Angewandte Chemie 2 (2015) 1791.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-04] Isogeometric modeling and large-scale computation for stress field around lattice defects

○Shunsuke Kobayashi[1], Ryuichi Tarumi[2], Atsushi Suzuki[3], Masao Ogino[4], Yoji Shibutani[1] （1.Graduate School of Engineering, Osaka Univ., Japan, 2.Graduate School of Engineering Science, Osaka Univ., Japan, 3.Cybermedia Center, Osaka Univ., Japan, 4.Information Technology Center, Nagoya Univ., Japan）

It is well known that classical elasticity yields singular stress field around the core of lattice defects such as point defects and dislocations. Regularization of the stress singularity is therefore primarily important to understand mechanical behavior of defects from a continuum viewpoint. First strain gradient elasticity (FSGE) generalizes the classical elasticity by introducing the characteristic length *l* in the constitutive equation. Recent theoretical investigations revealed that FSGE removes the stress singularity at the core of dislocations and disclinations. Hence, the *non-local* elasticity theory is suitable for multiscale modeling of defects in solid. In the present study, we aim to develop (i) isogeometric models for lattice defects and (ii) their numerical implementation for large-scale computation within the framework of FSGE. At first, we derive the weak form stress equilibrium equation for Cauchy-type FSGE. The integrodifferential Euler-Lagrange equation is then solved numerically using isogeometric analysis (IGA), *i.e.*, Galerkin method with the non-uniform rational B-spline (NURBS) basis functions. Consequently, the boundary value problem is cast into a system of linear algebraic equations whose degree of freedom exceeds 20 million. The large-scale computation was conducted on a supercomputer OCTOPUS which is installed in the cyber media center of Osaka Univ. Point defects were modeled using the first-order approximation for the force dipole and implemented into the weak form equation through the body force. The resulting stress fields showed singularity free distribution and they converged to classical solution with increasing in distance from the core. Dislocation model was constructed referring to the extended finite element method (XFEM). This model successfully reproduces the kink deformation from the pairs of equally arrayed edge dislocations.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-05] A local/nonlocal plasticity model for upscaling microstructural effects

○John Mitchell （Sandia National Laboratories, United States of America）

Despite its importance, why is mesoscale plasticity advancing so slowly? The fundamental equations of equilibrium used for mesoscale modeling have not changed in centuries. In this talk, I will present an innovative idea for combining nonlocal/local models to upscale effects of microstructures on plastic deformations. A local von Mises plasticity model is evolved using a nonlocal and peridynamics [1] inspired yield condition [2]. The application area is the analysis ofadditively manufactured metal parts.

Additive manufacturing produces heterogeneous and poorly understood material microstructures. Practical macroscale models that reflect the nature of AM microstructures do not currently exist: length scale effects, grain shape morphologies, grain orientations, intragrain defects, grain boundary heterogeneities, aggregrate textures. For the purpose of engineering design and qualification, it is essential that we develop and advance models for AM built parts.

[1] S.A. Silling, Reformulation of elasticity theory for discontinuities and long-range forces, Journal of the Mechanics and Physics of Solids, 48(1), (2000), 175-209.

[2] J.A. Mitchell, A nonlocal, ordinary, state-based plasticity model for peridynamics, Sandia National Laboratories, tech report SAND2011-3166, May, 2011.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-06] First-principles investigation of atomic hydrogen adsorption and diffusion on/into Mo-doped Nb (100) surface

○Zhong-min Wang, Yang Wu, Qingrong Yao, Yan Zhong, Chaohao Hu, Huaiying Zhou （Guilin University of Electronic Technology, China）

Based on sequential study of the surface model, surface-model slab, H-adsorption sites, and H-diffusion coefficient (D), we investigate the most likely process of atomic hydrogen adsorption and diffusion on/into Mo-doped Nb (100) surface/subsurface (in the $Nb_{12}Mo_4$ case) via first-principles. Our results reveal that the (100) surface is the most stable Mo-doped Nb surface with the smallest surface energy (2.75 J/m^2). Hole sites (HSs) in the Mo-doped Nb (100) surface are H-adsorption-favorable mainly due to their large adsorption energy (4.27 eV), and the H-diffusion path should preferentially be HS→TIS (tetrahedral interstitial site) over HS→OIS (octahedral interstitial site) because of the correspondingly lower H-diffusion energy barrier. With respect to a pure Nb (100) surface, the Mo-doped Nb (100) surface has a smaller energy barrier along the HS→TIS pathway (0.31 eV) and larger H-diffusion coefficient (5.65 × 10^{-10} m^2s^{-1}).

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-07] First-principles Study on Electronic Properties of Hybrid MA*BX*$_3$ perovskites (MA= CH$_3$NH$_3{}^+$; *B*= Pb, Sn, Ge; *X*= I, Br, Cl)

○Narasak Pandech[1,2], Thanundon Kongnok[1], Sirichok Jungthawan[1], Sukit Limpijumnong[1], Walter R.L Lambrecht[2] (1.School of Physics and NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials, Suranaree University of Technology, NakhonRatchasima 30000, Thailand, Thailand, 2.Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106-7079, USA., United States of America)

Recently, hybrid MA*BX*$_3$perovskites (MA= CH$_3$NH$_3{}^+$; *B*= Pb, Sn, Ge; *X*= I, Br, Cl) have revolutionized emerging photovoltaic technologies with the development of highly efficient solar cells, and have attracted significant fundamental research interest. Despite the extremely fast progress in device fabrication, the materials electronic properties, which determine the photovoltaic performance, are not yet fully understood. Here, we performed calculations of these materials, using a van der Waals-corrected density functional theory (DFT) method using the Perdew-Burke-Ernzerhof (PBE) and Heyd-Scuseria-Ernzerhof (HSE) hybrid functionals. Subsequently, we use the GW-approximation to calculate the bands as quasiparticle excitations including also the spin-orbit coupling. The orientation and position of the MA-cation is found to significantly affect the electronic properties around the band edges of the Pb and Sn based compounds. Because Ge based halides already prefer a rhombohedrally distorted perovskite structure with off-centered Ge even for a simple inorganic cation (e.g. Cs), the three-fold symmetry of the MA ion is compatible with a preferred orientation of the molecules along the rhombohedral axis. The interplay between its dipole and the Ge off-centering leads to interesting ferro-electric behavior.

Poster Session | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[PO-C1] Poster Session 1
Symposium C
Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-08] Pressure effects on dislocation core structures in Mg_2SiO_4 olivine: insights from atomic-scale modeling

○Philippe Carrez, Srinivasan Mahendran, Patrick Cordier （Lille University, Lab. UMET UMR-CNRS 8207, France）

[P1-09] Structural and magnetic properties of long-period stacking ordered (LPSO) structure of iron; A first-principles study

○Takao Tsumuraya[1], Ikumu Watanabe[2], Takahiro Sawaguchi[2] （1.Magnesium Research Center/POIE, Kumamoto Univ., Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan）

[P1-11] Dislocation transmission behaviors of bi-crystal BCC Tantalum with high and low angle symmetric tilt grain boundaries: Multiscale simulation study

○Moon Sunil, Kang Keonwook （Dept. of Mechanical Engineering, Yonsei Univ., Korea）

[P1-12] Ab Initio Dislocation Core Calculations using a Cluster Model

○Jonas Frafjord[1,3], Bjørn Holmedal[4], Jesper Friisj[2,3], Randi Holmestad[1,3], Ingeborg-Helene Svenum[2], Inga Gudem Ringdalen[2] （1.Dept. of Physics, Norwegian University of Science and Technology, Norway, 2.SINTEF Industry, Trondheim, Norway, 3.Centre for Advanced Structural Analysis, SIMLab, Norway, 4.Dept. of Materials Science and Engineering, Norwegian University of Science and Technology, Norway）

[P1-13] Anelastic recovery of a steel wire under pure shear strain with various magnetic treatments

○Shigeo Kotake, Takuro Murata （Dept. of Mechanical Engineering, Mie Univ., Japan）

[P1-14] Possible explanation of sudden stress drop at upper yield point in iron by magnetostriction and unpinning dislocations with law of approach in residual magnetization

○Shigeo Kotake （Dept. of Mechanical Engineering, Mie Univ., Japan）

[P1-15] Investigation of dislocation core structure in Aluminum by using a generalized Peierls-Nabarro model

○Hideki MORI （College of Industrial Technology, Japan）

[P1-16] Crystal orientation evolution analysis during deformation using molecular dynamics

○Keisuke Kinoshita （Nippon Steel &Sumitomo Metal Corporation, Japan）

[P1-17] Nanoindentation of Nanoparticles -A Molecular Dynamics and Discrete Dislocation Dynamics Simulations Study

Roy Shyamal[1], Riccardo Gatti[2], Benoit Devincre[2], ○Dan Mordehai[1] （1.Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel, Israel, 2.LEM, UMR 104, CNRS-ONERA, 29 Av. de la Division Leclerc, 4 Chatillon, France, France）

[P1-18] Machine learning interatomic potentials for molecular dynamics simulations of dislocations

○Eyal Oren, Guy Makov （Dept. of Materials Engineering, Ben-Gurion University of the Negev, Israel）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-08] Pressure effects on dislocation core structures in Mg_2SiO_4 olivine: insights from atomic-scale modeling

○Philippe Carrez, Srinivasan Mahendran, Patrick Cordier （Lille University, Lab. UMET UMR-CNRS 8207, France）

Olivine $(Mg,Fe)_2SiO_4$, a silicate with orthorhombic structure, is one of the most common minerals. As an abundant phase of the upper Earth mantle, its plastic properties strongly constrained the thermal convection of Earth mantle in its upper part. Plastic deformation of olivine involves two types of dislocation corresponding to the shortest Burgers vector [001] and [100]. At low temperature and high stress, [001] slip is supposed to be the most predominant slip system whereas at high temperature and low stress, [100] dislocations dominate. Over the last decades, a number of different slip systems have been thus identified in various domain of temperature, strain rate or pressure.

In this study, we revisit plasticity of this silicate by computing at the atomic scale the intrinsic properties of dislocation in Mg_2SiO_4 single crystal. All the calculations rely on a parametrized potential combining coulombic interactions and a core-shell interaction model for oxygen atoms. We performed a systematic investigation of [100] dislocations metastable configurations and possible dissociations.

Our calculations show that at low pressure, the atomic arrangement within the dislocation core is compatible with the [100](010) slip system observed experimentally. Also we show that the occurrence of several metastable core configurations allows to various cross slip events for which the cross slip energy barrier have been computed. Finally, we will show that the various core configurations are strongly sensitive to pressure leading to some change in the relative metastable states of the dislocation core and ultimately inhibiting some known slip plane at higher pressure.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-09] Structural and magnetic properties of long-period stacking ordered (LPSO) structure of iron; A first-principles study

○Takao Tsumuraya[1], Ikumu Watanabe[2], Takahiro Sawaguchi[2] （1.Magnesium Research Center/POIE, Kumamoto Univ., Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan）

Fe-Mn-Si based alloys is known to exhibit a shape-memory effect associated with deformation-induced martensitic transformation from face-centered cubic (fcc) γ-austenite to hexagonal closed packed (hcp) ε-martensitic phase. The Fe-Mn-Si-based alloys with modified chemical compositions appeared to have outstanding properties of low-cycle fatigue lives, and a Fe-15Mn-10Cr-8Ni-4Si (mass%) alloy developed is practically used in a seismic damping component of architectural constructions. Recently, under cyclic push-pull loading of Fe-Mn-Si-based alloys, a new phase different from ε-phase was found by transmission electron microscopy. The new phase shows electron diffraction spots at the 1/3 position of the {10-11} spots of the ε-phase, which suggests the existence of a long-period stacking ordered (LPSO) structure. In 1960s, a similar phase was reported after several times of thermal cycles of γ-ε phase phase transitions in Fe-Mn-C alloys. However, actual stacking sequence of the LPSO phase and relative stability with γ and ε-phases still remain unclear. To understand these issues, we proposed several structural models of LPSO structure of pure Fe, such as 4H, $6H_1$ and $6H_2$, and discuss structural and magnetic stabilities among the candidate of LPSO structures with first-principles calculation methods. [1] L. I. Lysak, and B. I. Nikolin, Fiz Met. Mettaloved **20**,

547 (1965), *ibid.* **23**, 93 (1967).

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-11] Dislocation transmission behaviors of bi-crystal BCC Tantalum with high and low angle symmetric tilt grain boundaries: Multiscale simulation study

○Moon Sunil, Kang Keonwook （Dept. of Mechanical Engineering, Yonsei Univ., Korea）

In this research, we conducted multiscale (molecular dynamics and dislocation dynamics) simulations to study dislocation transmission behaviors of bi-crystal BCC Tantalum (Ta) with high and low angle symmetric tilt grain boundaries. To investigate dislocation transmission behaviors, we introduced a dislocation loop to describe the Frank-Read source, one of the dislocation multiplications in molecular dynamics simulation. We put dislocation loop on the slip plane where maximum resolved shear stress occurs. In molecular dynamics simulation, we observed interactions between dislocation and grain boundary such as dislocation transmission and absorption. Furthermore, we performed dislocation dynamics simulation to observed similar dislocation transmission behaviors. Finally, we analyzed mechanical property changes (e.g. stress-strain response) as dislocation interacts with grain boundary.

Acknowledgement

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-12] Ab Initio Dislocation Core Calculations using a Cluster Model

○Jonas Frafjord[1,3], Bjørn Holmedal[4], Jesper Friisj[2,3], Randi Holmestad[1,3], Ingeborg-Helene Svenum[2], Inga Gudem Ringdalen[2] （1.Dept. of Physics, Norwegian University of Science and Technology, Norway, 2.SINTEF Industry, Trondheim, Norway, 3.Centre for Advanced Structural Analysis, SIMLab, Norway, 4.Dept. of Materials Science and Engineering, Norwegian University of Science and Technology, Norway）

Solute strengthening is an important mechanism contributing to the strength of metallic alloys. In order to create an accurate framework for strength calculations, this mechanism must be fully understood. In that regard, studies have shown that it is crucial to include the core region of a dislocation in models [1-3], as the core interacts strongly with solute atoms through short-range interactions, and affects the dislocation mobility. The core region can be treated from first principles to include electronic effects. One challenge has been to correctly describe the dissociation of a dislocation at atomic level [4,5]. Dissociation of a perfect dislocation results in a more favourable configuration by reduction of the elastic energy. The equilibrium separation of the partial dislocations generated is due to the cost of the intrinsic stacking fault. This separation width is important for the strengthening mechanism of solutes since it affects the solute-dislocation interaction-energy map.

In this work, a cluster model for dislocation core structures is applied. The model takes the shape of a cylinder, where the dislocation line is elongated through the centre [6]. It consists of an outer region surrounded by vacuum, where the atoms are fixed by an elastic displacement field, and a core region that is relaxed. This model is strongly dependent on the assumption that the elastic theory is respected within the fixed region. The advantage of this model is the simplicity, and its transparency towards the assumptions that are taken. The aim is to improve the capability to set up an atomistic model for dislocations in fcc metals using a cluster model with sufficient accuracy. The setup has been tested for Aluminium with a pure edge dislocation. It will be extended further to screw dislocations.

Using this simple model, the static configuration of a dislocation core structure can be compared to experimental observations and results using the flexible boundary condition applied by other groups [1,4].

[1] doi.org/10.1016/j.actamat.2016.09.046
[2] doi.org/10.1016/j.scriptamat.2014.04.018
[3] doi.org/10.1016/j.actamat.2010.06.045
[4] doi.org/10.1016/j.msea.2005.03.039
[5] 10.1103/PhysRevLett.100.045507
[6] doi.org/10.1016/j.actamat.2016.09.049

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-13] Anelastic recovery of a steel wire under pure shear strain with various magnetic treatments

○Shigeo Kotake, Takuro Murata （Dept. of Mechanical Engineering, Mie Univ., Japan）

Elastic property of a metal under pure shear strain is quite different from that under other strain, since the former doesn't have the volume change of the specimen. Without the volume change, elasticity under the pure shear strain is mainly caused from bowing-out deformation of dislocations in slip planes. After external force is removed, the solid will immediately return to its original size. It indicates deformed dislocation lines are straitened instantly in this condition. On the other hand, people has observed slow recovery of the size of the specimen after unloading, which is called anelasticity. When anelastic phenomenon occurs under pure shear strain, it indicates some dislocations slowly recover its bowing-out shape because of the existence of weak pinning sites. Since dislocations are known to interact with magnetic domain walls in ferrous materials, the domain walls can partially act for weak pinning sites for anelasticity.

To prove this mechanism, we will observe anelastic recovering of steel compression coil spring, whose strain is mainly pure shear state, under various magnetic treatments. The residual elongation cannot be explained from simple relaxation phenomenon of macroscopic spring dynamics. Since the amount of anelastic recover is influenced with magnetic treatment during compression condition, magnetic domain walls can work as weak pinning sites for some dislocations. As temporal change of elongation is logarithmically changed, resultant number of bowing-out dislocations is inversely proportionally decreased with time during recovering.

At last, we will discuss the mechanism of interaction between dislocation and magnetic domain wall. In iron, easy-magnetization axes are <100> and 180-degree magnetic domain walls are located along {011} plane. Slip planes of bcc iron are {110} plane, and dislocation lines are perpendicular to {110}. Since [01-1]

dislocation line, which is perpendicular to a magnetic domain wall, has no interactions to the wall, most dislocation lines across the 180-degree wall in this manner. We will discuss the origin of weak pinning sites of dislocation from the distribution of Bloch wall and Bloch line in the domain wall. And we will show the possibility to understand the interaction from magnetic force caused by swirling flow of electron along dislocation line.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-14] Possible explanation of sudden stress drop at upper yield point in iron by magnetostriction and unpinning dislocations with law of approach in residual magnetization

○Shigeo Kotake （Dept. of Mechanical Engineering, Mie Univ., Japan）

Unique mechanical properties of iron is one of important resources of engineering in modern technology. Since elastic deformation is dominant below the yield stress in iron, people can design a machine under strength of materials. Although sudden drop of stress at the upper yield point is one of prominent phenomena in iron, its mechanism has been a point of controversy in the study of mechanical properties.

On the other hand, Pitman (1990) reported sudden changes in residual magnetization of iron, which shifts towards an anhysteresis curve after applying mechanical stress. Jiles (1995) and Jiles and Li (2004) studied the magnetomechanical effect and discovered the existence of the "law of approach" in residual magnetization, in which the hysteresis converts to an anhysteresis curve under applied stress.

In this study we will try to explain the sudden drop of stress at the upper yield point from magnetostriction and unpinning dislocation with the sudden change of residual magnetization under the law of approach. Because of the positive magnetostriction coefficient of iron, specimen will show sudden drop of stress from the sudden decrease of residual magnetization, in case the initial magnetization is perpendicular to the direction of the applied force. Since the decreased magnetization has been kept, the sudden drop of stress has not been observed just after the first tensile test. Recovery of the phenomenon can be explained from remagnetization of the specimen during the heat treatment of annealing. It will be remaining study to explain the effect from temperature or strain rate to the upper yield stress.

Moreover, it has been noticed there are pinning effects between dislocation lines and magnetic domain walls. The law of approach has been explained from unpinning effect of the dislocations from the magnetic domain walls. Therefore, at the upper yield point, unpinned dislocations can move freely until contact another pinning site to enhance the decrease of stress. And we will show the possibility to understand the pinning interaction from magnetic potential between magnetic domain wall and dislocation line, where swirling electron flows.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-15] Investigation of dislocation core structure in Aluminum by using a generalized Peierls-Nabarro model

○Hideki MORI （College of Industrial Technology, Japan）

We investigate the dislocation core structure in Aluminum (Al) by using generalized Peierls-Nabarro (PN) model.
Same as classical PN model, a generalized PN model expresses the total energy of dislocation core as a sum of local misfit energy and non-local elastic energy.
To integrate micromechanics in classical PN model, the generalized PN model can flexibly and efficiently evaluate the non-local elastic energy [1].
Especially, in isotropic case, the generalized PN model can evaluate the non-local elastic energy with high accuracy [1,2].
In this work, we calculate the generalized stacking fault energy surface by density functional theory (DFT) calculation and empirical atomic potential and evaluate dislocation core structure in Al.
Then we discuss the accuracy of generalized PN model by comparing to result of empirical atomic potential. We also demonstrate that the generalized PN model is a useful tool to investigate the mesoscopic dislocation behavior.

[1] H.Wei,Y.Xiang and P.Ming: Commun. Comput. Phys. 4 (2008) 275-293
[2] V.V.Bulatov and W.Cai: Computer simulations of dislocations (Oxford,2006)

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-16] Crystal orientation evolution analysis during deformation using molecular dynamics

○Keisuke Kinoshita （Nippon Steel &Sumitomo Metal Corporation, Japan）

Usually, metallic materials are anisotropic material, for example, in a tensile testing of single crystal, stress and strain relationship depends on tensile direction. Although, when grains in polycrystalline metals have fully random crystal orientation, respectively, anisotropy of the metals is reduced. However, in the actual metallic materials, the grains don’t have fully random crystal orientation and the grains have been limited to specific crystal orientations that depends on crystal structures and/or plastic deformation processes, etc. In other words, the polycrystalline metals have the texture. Mechanical properties of the polycrystalline metals that have texture is depended on the texture. Therefore, controlling the texture is one of important problems for improving the mechanical properties of metals. The mechanism of the texture formation during deformation is rotation of each grain, macroscopically. An elementary step of the rotation of the grains is dislocation movement, microscopically. The dislocation movements depend on the crystal structures and the stress state, etc. In result, the texture depends on the crystal structures, etc. Although, the dislocation movement is the elementary step of the texture formation, the texture formation should be reproducible by molecular dynamics. But the simulation result reports are not many.
In this study, we will show molecular dynamics simulation results for the crystal rotation of body-centered cubic iron during deformation at 300 K. We will show two results. First, an algorithm that is determined equivalent crystal orientation from atomic configures is described and inspected. Second, crystal rotation evolution during tensile deformation on molecular dynamics simulation using the algorithm will be shown. As a result, we will show two results, 1) the crystal rotation of the simulation is corresponded to the theoretical result, and 2) when multi slip systems are activated, crystal orientation is stable, but when single slip system is activated, crystal orientation is changed.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-17] Nanoindentation of Nanoparticles -A Molecular Dynamics and Discrete Dislocation Dynamics Simulations Study

Roy Shyamal[1], Riccardo Gatti[2], Benoit Devincre[2], ○Dan Mordehai[1] （1.Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel, Israel, 2.LEM, UMR 104, CNRS-ONERA, 29 Av. de la Division Leclerc, 4 Chatillon, France, France）

When decreasing the size of metallic specimens into the sub-micrometer scale, they can drastically change their mechanical properties. While plasticity at this scale is commonly studied using compression tests, nanoindentation can reveal the importance of free surfaces on the depletion of dislocations during the deformation. In this talk, we present a computational study on how the size and shape of defect-free nanoparticles affect the mechanical response to nanoindentation. Using Molecular Dynamics (MD) simulations and Discrete Dislocation Dynamic (DDD) simulations, we simulate nanoindentation of Au faceted nanoparticles in a height range of 9-150 nm. The DDD simulations are coupled with a finite element analysis, in order to reproduce the stress field generated during nanoindentation. Since the nanoparticles are initially pristine (dislocation free), a nucleation criterion for dislocations is introduced in the DDD simulations. When indenting along a <111> direction, the simulations show that shear dislocation loops are nucleated beneath the indent on all {111} slip planes. Those shear dislocation loops interact and form v- and u-shaped dislocations or prismatic loops that glide towards the lower part of the nanoparticles, facilitating their escape from beneath the indent. Two other mechanisms are shown to control the escape of dislocations laterally from the upper part of the nanoparticle. In one, segments of shear dislocation loops, that are nucleated on the {111} slip plane parallel to the upper surface of the nanoparticle, cross-slip and escape from the upper surface, forming two half prismatic loops that glides parallel to the upper facet. In another mechanism, dislocations on two different slip planes interact and form a glissile dislocation segment that glides lateraly and escapes the nanoparticles. The effect of size on the various dislocation mechanisms is discussed.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-18] Machine learning interatomic potentials for molecular dynamics simulations of dislocations

○Eyal Oren, Guy Makov （Dept. of Materials Engineering, Ben-Gurion University of the Negev, Israel）

The mechanical response of crystalline materials is largely controlled by the mobility of dislocations. It is possible to study the mobility of individual dislocations using molecular dynamics simulations, e.g. [1], but the validity of these studies depends on the quality of the interatomic potentials employed. In the present contribution we employ machine learning techniques for the construction of interatomic potentials using ab-initio data as input, validate the interatomic potential accuracy against experimental and ab-initio observables and apply to the study of dislocations.

[1] E. Oren, E. Yahel, G. Makov, Dislocation kinematics: a molecular dynamics study in Cu, Model. Simul. Mater. Sci. Eng. 25 (2017) 25002.

Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E1] Poster Session 1

Symposium E

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-21] Large-scale molecular dynamics simulations: coupling with dislocation dynamics
○Pavel A. Pokatashkin, Denis K. Ilnitsky, Alexei V. Yanilkin （Dukhov Research Institute of Automatics (VNIIA), Russia)

[P1-22] **Hydrogen embrittlement controlled by reaction of dislocation with grain boundary in alpha-iron polycrystals**
○Liang Wan[1,2], Wen Tong Geng[2,3], Akio Ishii[2], Jun-Ping Du[2,4], Nobuyuki Ishikawa[5], Hajime Kimizuka[2], Shigenobu Ogata[2,4] （1.Wuhan University, China, 2.Osaka University, Japan, 3.University of Science and Technology Beijing, China, 4.Kyoto University, Japan, 5.JFE Steel Corporation, Japan）

[P1-23] Study of solute effect on the yield strength of Fe-based dilute alloy using atomistically informed kinetic Monte Carlo method
○Shuhei Shinzato[1], Masato Wakeda[2], Shigenobu Ogata[1] （1.Dept. of Mechanical Science and Bioengineering, Osaka Univ., Japan, 2.National Institute for Materials Science, Japan）

[P1-24] **Molecular Dynamics Simulations of Low-cycle Fatigue Behavior in Single Layer Molybdenum Disulfide**
Yu-Chieh Lo[1], ○Yu-Cheng Su[1], Ming-Chen Chung[2], Alice Hu[3] （1.National Chiao Tung University, Taiwan, 2.National Cheng Kung University, Taiwan, 3.City University of Hong Kong, Hong Kong）

[P1-25] Fracture behavior of multi-walled carbon nanotube under biaxial loading condition
○Masaomi Nishimura[1], Naoki Kazami[2], Daiki Kato[2] （1.Dept. of Mechanical Systems Engineering, Shinshu Univ., Japan, 2.Graduate School of Science and Technology, Shinshu Univ., Japan）

[P1-26] **On the role of amorphous shells on mechanical properties of fcc Ni nanoparticles under compression**
○Alexandra Goryaeva[1,2], Claudio Fusco[2], Matthieu Bugnet[2], Jonathan Amodeo[2] （1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France, 2.INSA-Lyon, Université de Lyon, MATEIS, 69621 Villeurbanne, France）

[P1-27] Molecular dynamics analysis of hydrogen diffusion behavior in alpha-Fe bi-crystal under stress gradient
○Ken-ichi Saitoh[1], Haruka Koga[2], Tomohiro Sato[1], Masanori Takuma[1], Yoshimasa Takahashi[1] （1.Kansai Univ., Japan, 2.Kobe Steel, Ltd., Japan）

[P1-28] Understanding Interactions of Dislocations with Interfaces in Nickle-based Superalloys: Insights from Molecular Dynamics Simulations
○Jian Huang[1], Yunjiang Wang[2] （1.Shanghai Institute of Ceramics Chinese Academy of Sciences, China, 2.Institute of Mechanics, Chinese Academy of Sciences, China）

[P1-29] The influence of nano-sized Ti_3Al particles on the mechanical properties of α-titanium alloys
○Yan He[1,2,3], Wang Hao[1], Dongsheng Xu[1], Yang Rui[1] （1.IMR, CAS, China, 2.Coll. of Physics Science and Technology, SYNU, China, 3.Univ. of chinese Academy of Sciences, China）

[P1-30] The atomic study of tensile property for nickel nanowires with helium bubble

○Hengfeng Gong, Rui Li, Tong Liu （CGN, China）

[P1-31] Componets of fracture response of alkali-activated slag mortars with steel fibers

○Hana Simonova, Petr Frantik, Zbynek Kersner, Pavel Schmid, Pavel Rovnanik （Brno University of Technology, Faculty of Civil Engineering, Czech Republic）

[P1-32] Molecular Dynamics Simulation of Crack Growth Behavior of Single Crystal γ -TiAl Alloy Under Different Nb Substitution Mode

○Yuxi Feng[1,2], Zhiyuan Rui[1,2], Hui Cao[1,2], Ruicheng Feng[1,2], Xiaocui Fan[1,2], Xing Yang[1,2]

（1.Mechanical and Electronical Engineering College, Lanzhou University of Technology, China, 2.Key Laboratory of Digital Manufacturing Technology and Application, the Ministry of Education, Lanzhou University of Technology, China）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-21] Large-scale molecular dynamics simulations: coupling with dislocation dynamics

○Pavel A. Pokatashkin, Denis K. Ilnitsky, Alexei V. Yanilkin （Dukhov Research Institute of Automatics (VNIIA), Russia）

Various dislocation-related mechanisms: phonon drag, forest-harderning, thermal activated processes (climb, cross-slip) contribute to material properties e.g. strength. Until recently, studying of deformation via molecular dynamics (MD) considered simulations of only extremely high strain-rates. However contribution of various mechanisms might change significantly while proceeding to lower strain rates. Therefore the accuracy of dislocation dynamics (DD) models used for large strain rate range is an open question due to extrapolation.

Recent advances in computational powers increased both spatial and temporal scales available for atomistic modeling. Therefore it is possible to make coulping between MD and DD for strain rates ~10^7 s^{-1} and higher. We consider such materials as: iron, molybdenum, and uranium.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-22] Hydrogen embrittlement controlled by reaction of dislocation with grain boundary in alpha-iron polycrystals

○Liang Wan[1,2], Wen Tong Geng[2,3], Akio Ishii[2], Jun-Ping Du[2,4], Nobuyuki Ishikawa[5], Hajime Kimizuka[2], Shigenobu Ogata[2,4] （1.Wuhan University, China, 2.Osaka University, Japan, 3.University of Science and Technology Beijing, China, 4.Kyoto University, Japan, 5.JFE Steel Corporation, Japan）

Hydrogen atoms absorbed by metals in the hydrogen-containing environments can lead to the premature fracture of the metal components used in load-bearing conditions. Since metals used in practice are mostly polycrystalline, grain boundaries (GBs) can play an important role in hydrogen embrittlement of metals. Here we show that the reaction of GB with lattice dislocations is a key component in hydrogen embrittlement mechanism for polycrystalline metals. We use atomistic modeling methods to investigate the mechanical response of GBs in alpha-iron with various hydrogen concentrations. Analysis indicates that dislocations impingement and emission on the GB cause the GB to locally transform into an activated state with a more disordered atomistic structure, and introduce a local stress concentration. The activation of the GB segregated with hydrogen atoms can greatly facilitate decohesion of the GB. We show that the hydrogen embrittlement model proposed here can give better explanation of many experimental observations.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-23] Study of solute effect on the yield strength of Fe-based dilute alloy using atomistically informed kinetic Monte Carlo method

○Shuhei Shinzato[1], Masato Wakeda[2], Shigenobu Ogata[1] （1.Dept. of Mechanical Science and Bioengineering, Osaka Univ., Japan, 2.National Institute for Materials Science, Japan）

Solid solution hardening/softening is one of the ways to control mechanical properties of alloys. The trend of change in mechanical properties of solid solution alloys due to solute addition is generally non-linear against a solute element, concentration, strain rate, and temperature. In order to develop the advanced alloy, prediction of mechanical strength is important to reduce the cost and development time.

It is well known that the solute atoms in crystalline metals affect mechanical strength by interacting other lattice defects such as dislocation. Although many researchers have studied the interaction between dislocation and solute atoms to understand solid solution hardening/softening, detail of solute effect on dislocation motion is not fully clarified yet.

In this work, we investigate the solute effect on the yield strength of body-centered cubic (BCC) alloy by analyzing dislocation motion using kinetic Monte Carlo (kMC) model based on atomistic understanding. We focus on dilute BCC Fe-based alloy including substitutional solute Si atom.

First, we analyze the solute effect on screw dislocation motion, which mainly dominates plastic deformation of BCC metals, based on atomistic modeling. In order to estimate the solute effect on screw dislocation motion, we performed nudged elastic band calculation to obtain activation energy of dislocation motion via kink mechanism which includes a kink-pair nucleation and kink migration processes.

Then, obtained activation enthalpy of each process and solute effect on them is introduced to kMC model to calculate activation rate of dislocation motion. By performing kMC simulation, we estimate dislocation velocity in different concentration, temperature, and stress conditions, and evaluate the solute effect on dislocation velocity.

Finally, we predict yield strength from estimated dislocation velocity and discuss the effect of solute atoms.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-24] Molecular Dynamics Simulations of Low-cycle Fatigue Behavior in Single Layer Molybdenum Disulfide

Yu-Chieh Lo[1], OYu-Cheng Su[1], Ming-Chen Chung[2], Alice Hu[3] (1.National Chiao Tung University, Taiwan, 2.National Cheng Kung University, Taiwan, 3.City University of Hong Kong, Hong Kong)

Graphene-like two-dimensional transition metal dichalcogenides (TMDs) have attracted much interest in the last decade because of it astonishing properties. Molybdenum disulfide (MoS2) is one of TMDs. It has direct band gap of 1.8 eV in monolayer but its bandgap can change with the number of layers. Such properties make it industrial important. In order to ensure the reliability of nano-devices made by MoS2, much attention has been focused on their mechanical properties including elastic modulus, stiffness and breaking strength. However, only limited studies have been done on cyclic deformation and fracture behavior. As a result, we report on molecular dynamics simulations of low-cycle fatigue behavior in single layer molybdenum disulfide. We choose the Reactive Empirical Bond Order (REBO) potential to describe the interatomic interactions. The REBO potential is used to estimate the failure strain and the tensile strength. The simulations and subsequent analysis suggest that the tensile stress will make the vacancies penetrate the whole plane, and induce the fracture for incremental brittle crack growth to occur during near-threshold fatigue. We want to clarify whether the plastic-strain-controlled fatigue tests would show the Coffin-Manson relation in fatigue life. Such power-law form originates from plastic-strain-dependent microscopic damage accumulation. Lastly, the effect of a crack on low-cycle fatigue of monolayer MoS2 in terms of failure mode and fatigue life is also discussed.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-25] Fracture behavior of multi-walled carbon nanotube under biaxial loading condition

○Masaomi Nishimura[1], Naoki Kazami[2], Daiki Kato[2]   (1.Dept. of Mechanical Systems Engineering, Shinshu Univ., Japan, 2.Graduate School of Science and Technology, Shinshu Univ., Japan)

One-dimensional carbon materials such as Carbon Fibers (CFs) and Carbon nanotubes (CNTs) are applied in a wide range of areas. For example, carbon fiber reinforced plastics are put to practical use for bodyworks of cars and airplanes. Though carbon materials in composites are subjected to complex deformation by multiaxial loading, the fracture mechanism of them is not clarified under multiaxial stress conditions.
 In this study, we have performed deformation simulations on multi-walled CNTs under biaxial loadings in order to clarify the fracture criterion of one-dimensional carbon materials from nanometer scale viewpoints. CNTs in simulation cell are compressed in a radial direction, and extended in a longitudinal direction by molecular dynamics simulation using the adaptive intermolecular reactive empirical bond order (AIREBO) potential. Fracture of CNTs originates from a bond breaking by the tensile loading for longitudinal direction, under small compressive stresses for the radial direction. On the other hand, high compressive stresses for the radial direction trigger a collapse of six-membered ring structures before the bond breaking by the longitudinal tension. The collapse occurs in the neighborhood of the innermost layer in highly compressed CNTs.
 In addition, we have also performed biaxial deformations of composite models which are made by filling amorphous polyethylene structure in the space between MWCNTs. As a result, fracture behavior varies with stress conditions, as in the case of models without polyethylene. A collapse of six-membered ring structures under high compressive stresses occurs not from the innermost layer but from the outermost layer by the interaction between polyethylene and CNTs.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-26] On the role of amorphous shells on mechanical properties of fcc Ni nanoparticles under compression

○Alexandra Goryaeva[1,2], Claudio Fusco[2], Matthieu Bugnet[2], Jonathan Amodeo[2]   (1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France, 2.INSA-Lyon, Université de Lyon, MATEIS, 69621 Villeurbanne, France)

Nano-objects, such as nanoparticles, nanowires, nanopillars *etc.*, are characterized by the large surface to volume ratio that, to a certain degree, defines their exceptional physical properties, significantly different from those in their bulk counterparts. In particular, nanocrystals are known for their promising mechanical properties: a size-dependent elastic regime, large values of yield strength and ductility, that are mainly linked to the dislocation nucleation from surface.

In this context, the various surface states of a sample are expected to lead to significant differences in terms of mechanical behavior. So far, *in situ* nano-compression experiments in the TEM occasionally report the presence of amorphous overlay at the top of nano-objects [1], while theoretical atomic scale studies are mainly focused on perfect crystalline systems [2, 3, 4].

Here we present a Molecular Dynamics (MD) study that aims to investigate the influence of amorphous shells

on mechanical response of Ni nanospheres upon compression. In order to avoid complex effects of chemistry on the onset of plasticity, we focus on pure Ni compound, without adding alloying elements to the amorphous overlay. Based on multiple EAM potentials and various sample elaboration tests, a unique methodology that provides a reasonably slow "crystallization" rate of the amorphous Ni on fcc substrate is proposed. Then, mechanical properties of the designed 20 nm nanospheres with different shell thickness are investigated under uniaxial compression. The mechanical response of the composite systems is compared with that of purely crystalline and amorphous particles, with a particular focus on dislocation-based deformation processes.

References

[1] W. Han *et al.*, Advanced Materials **27**, 3385 (2015)

[2] J.-J. Bian &G.-F. Wang, J Comput Theor Nanosci **10**, 2299 (2013)

[3] D. Mordehai *et al.*, Acta Materialia **59**, 5202 (2011)

[4] S. Bel Haj Salah *et al.*, Comput Mater Sci **129**, 273 (2017)

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-27] Molecular dynamics analysis of hydrogen diffusion behavior in alpha-Fe bi-crystal under stress gradient

○Ken-ichi Saitoh[1], Haruka Koga[2], Tomohiro Sato[1], Masanori Takuma[1], Yoshimasa Takahashi[1] （1.Kansai Univ., Japan, 2.Kobe Steel, Ltd., Japan）

Delayed fracture in high-strength steel wires produced by drawing is an important issue. The major cause of the delayed fracture is supposed hydrogen embrittlement (HE), and some researches so far show that HE phenomena is very sensitive to the amount of plastic deformation in drawing process. The hydrogen(H)-atom diffusion is affected largely by ambient thermal and mechanical conditions, such as, stress, pressure and temperature. Besides, effect of stress gradient (SD) on atomic diffusion is supposed to be crucial, but is still unclear. Most of metallic materials which have been provided plastic deformation, like drawn pearlitic steel wires, have a enormous residual stresses particularly in surface and interface region, which shows strong SD. In this study, we investigate the behavior of H-atoms diffusing in pure iron (α-Fe) in the condition accompanied by SD. Since the behavior is observable just in atomic-scale, molecular dynamics (MD) simulation using EAM potentials for Fe and H atomic system is conducted. There are two types of SD condition: one is the gradient for overall specimen, which can be reproduced by bending deformation of specimen. Another is an atomic-scale gradient in the interface region, e.g. one provided by grain boundary (GB) structure. Thus, we build a bi-crystal model including GB structure, and it is applied bending deformation. For a moderate flexure, the bending stress distributes in a linear fashion along the lateral cross-section of the specimen. Diffusion coefficient of H-atoms in bulk region increases with increase of the SD value. Besides, it is clearly observed that the direction of diffusion depends on the distribution of SD. It is found that H-atom diffusion increases with the decrease of cohesive energy evaluated around the H-atom. From these MD results, we realize that the increase of H-atom diffusion shows exactly exponential relation to

SD values. So, we can successfully obtain an expression between diffusion coefficient and SD value. We also understand that, by setting temperature effects aside, the increase of SD will lead to substantial change of entropy effect for diffusion.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-28] Understanding Interactions of Dislocations with Interfaces in Nickle-based Superalloys: Insights from Molecular Dynamics Simulations

○Jian Huang[1], Yunjiang Wang[2]　(1.Shanghai Institute of Ceramics Chinese Academy of Sciences, China, 2.Institute of Mechanics, Chinese Academy of Sciences, China)

Nickel-base superalloys, as the favorite material for the turbine blade of the engines, have attracted a lot of attention due to their excellent creep properties and good microstructure stability. The evolution of dislocations during creep procedure and core structures of dislocations play an important role in the strengthening mechanism of nickel-base superalloys. Especially, the dislocation reactions and their interaction with γ/γ' interfaces of nickel-base superalloys contribute to a stable stage of creep. Here, based on developed mechanistic framework, we study the interactions of dislocations with interfaces to better understand the origin of ductility of nickel-base superalloys. Using atomistic reaction pathway calculations based nudged elastic band (NEB) method, we elucidate the slip transfer reaction mediated by interfaces of nickel-base superalloys. The findings offer new idea on the possible means to optimize the ductility and strength through interfacial engineering for nickel-base superalloys.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-29] The influence of nano-sized Ti_3Al particles on the mechanical properties of α-titanium alloys

○Yan He[1,2,3], Wang Hao[1], Dongsheng Xu[1], Yang Rui[1]　(1.IMR, CAS, China, 2.Coll. of Physics Science and Technology, SYNU, China, 3.Univ. of chinese Academy of Sciences, China)

In α-titanium alloys, Ti_3Al (α_2 phase) precipitates under a perceivable aluminum content. The size and distribution of α_2 particles has significant influence on the mechanical property of α-Ti alloys. Experimentally, it is found that nanometric α_2 particles drastically decrease the toughness of α-Ti alloys after certain thermal treatment. However, the strength and the ductility do not vary linearly with the size of α_2 particles and the atomic details of hardening and fracture remain unclarified. Therefore, we employed molecular dynamic simulation with the embedded-atom potential to systematically study the deformation process of α-Ti with different size and distribution of α_2 particles. The result shows that 1) the α/α_2 interface is coherent; 2) in an α grain with an α_2 particle and incoming dislocations, the existence of an α_2 particle blocks the dislocations and the strength increases with the size of the α_2 particle; and subsequently cracks nucleate at the impacting site on the gain boundary with the crack stress decreasing with the size of the α_2 particle; 3) the resulting strength and toughness vary with the size of the α_2 particle in a parabola manner. The present simulation result quantitatively agrees with experiments and helps identifying the critical α_2 particle size for the design of structural titanium alloys.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-30] The atomic study of tensile property for nickel nanowires with helium bubble

○Hengfeng Gong, Rui Li, Tong Liu （CGN, China）

Tensile deformation behavior of nickel nanowires with helium bubble has been investigated using molecular dynamics (MD) simulation. MD simulations were performed at 1K to 300K employing a strain rate of $2\times10^9 \text{s}^{-1}$ and $2\times10^{10}\text{s}^{-1}$ for the nanowires with cross section width(S)ranging from $8a_0$ to $12a_0$(a_0=3.5157Å). The diameters were set from 1.2 nm to 1.6nm for helium bubbles, and the ratio of helium-to-vacancy inside bubble for 1:1, 2:1, 4:1 and 1:0. With the strain rate increasing, the elastic modulus and yield stress are also increased. However, they present the declined trend at the high temperature. As the helium bubble size increases or the cross section of nanowires decreases, the elastic modulus and yield stress increases, while the yield strain become smaller. In addition, the mechanism of yielding is discussed in details based on the snapshots of defects evolution. As the radio of helium-vacancy increases, the elastic modulus and yield stress also decrease. The helium bubble could accelerate the fracture to some extent. This study on the plastic properties of metal nanowires will be helpful to further understanding of the mechanical properties of nanomaterials.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-31] Componets of fracture response of alkali-activated slag mortars with steel fibers

○Hana Simonova, Petr Frantik, Zbynek Kersner, Pavel Schmid, Pavel Rovnanik （Brno University of Technology, Faculty of Civil Engineering, Czech Republic）

Knowledge of mechanical fracture parameters of composites based on brittle matrix is essential for the quantification of their resistance against crack initiation and propagation as well as for the definition of material models used to simulate the quasi-brittle behaviour of the structures or their parts made from this type of composites. The variability of results experimentally obtained from fracture tests of composites with different kind of fibres is much higher in comparison with composite without fibres due to the natural heterogeneity of composite containing fibres. Therefore, the main objective of this paper is to quantify the contribution of the matrix of alkali-activated slag mortars with steel fibres on their fracture response.
First alkali-activated slag material was a reference without fibres; the other composites contain steel fibres in amount 5, 10, 15 and 20 % of weight of slag, respectively. The mechanical fracture parameters were determined using evaluation of fracture tests carried out on 40 × 40 × 160 mm beam specimens with an initial central edge notch. The load vs. displacement (deflection in the middle of span length) and load vs. crack mouth opening displacement diagrams were recorded during the fracture tests. Each diagram was processed in order to obtain the component that corresponds to the structural response of the matrix of the composite consisting from alkali-activated slag and steel fibres reinforcing that matrix. The values of fracture parameters were determined using work-of-fracture method and double-K fracture model.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-32] Molecular Dynamics Simulation of Crack Growth Behavior of Single Crystal γ-TiAl Alloy Under Different Nb Substitution Mode

○Yuxi Feng[1,2], Zhiyuan Rui[1,2], Hui Cao[1,2], Ruicheng Feng[1,2], Xiaocui Fan[1,2], Xing Yang[1,2] （1.Mechanical and Electronical Engineering College, Lanzhou University of Technology, China, 2.Key Laboratory of Digital Manufacturing Technology and Application, the Ministry of Education, Lanzhou University of Technology, China）

Because of the low plasticity at room temperature, high rate of crack propagation of TiAl alloy, its application in the aerospace has been severely restricted. The addition of Nb contributes to solving this problem.The Ti-Al-Nb ternary system has become the main trend of development of TiAl alloys, and the influence of alloying elements Nb on the properties of TiAl alloys has become the focus of extensive attention and research in the field of materials engineering.In this paper,the effect of different substitution modes of Nb on the crack propagation of γ-TiAl alloy was studied from the microscopic scale by molecular dynamics method.The effect of cracks on the performance of γ-TiAl alloys without Nb, Nb substitutional Al systems, and Nb substitutional Ti systems was analyzed.The results show that the interaction between Nb and the neighboring matrix atoms is stronger than the interaction between Ti-Al atoms before the substitution, and the doped Nb is enhanced compared to the γ-TiAl alloy without Nb. The bonding and bonding strengths between the atoms in the matrix and the atoms in the TiAl alloy increase the bond strength of the unit cell, increase the bonding force and cohesion between the surrounding atoms, and make the atoms in the crack tip region bond tightly, making it difficult to break bonds and become crack propagation. An obstacle is the passivation of the crack tip, the slower rate of crack propagation, and the change in the crack propagation path, which increases the tensile and fracture toughness of the alloy.The substitutional Ti system has a higher yield strength than the substitutional Al system, Nb occupies a sublattice of Ti, and the short-range interaction between dislocations and Nb atoms results in solid solution strengthening, which enhances the strength of the alloy.The lattice distortion of the substitutional Al system is more serious than that of the substitutional Ti system, and the dislocation density is higher and the fracture toughness is higher. The difference in this phenomenon is more pronounced at a high Nb concentration of 6%.

[PO-F1] Poster Session 1

Symposium F

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-33] UNDERSTANDING OF DELAYED HYDRIDE CRACKING FAILURE MECHANISM IN E110 ZIRCONIUM BASED FUEL CLADDINGS BY EBSD AND IN-SITU MECHANICAL TESTING

○Hygreeva Kiran NAMBURI[1], Zbynek Spirit[1], Patricie Halodova[1], Ondrej Libera[1], Jakub krejci[2] （1.Research Centre REZ, Czech Republic, 2.UJP Praha, Czech Republic）

[P1-34] Transition-metal alloying of γ '-Ni$_3$Al: Effects on the ideal uniaxial compressive strength from first-principles calculations

○Minru Wen[2,1], Chongyu Wang[2] （1.Guangdong University of Technology, China, 2.Tsinghua University , China）

[P1-35] **The Influence of Deposition Pattern on Stress and Mechanical Properties in Wire Arc Additive Manufacturing**

○Changmeng Liu, Qianru Wu, Jiping Lu, Shuyuan Ma （Beijing Institute of Technology, China）

[P1-36] On the Significance of the Higher-Order Neighbors for Abnormal Grain Growth and Recrystallization Nucleation

○Markus Kuehbach （Max-Planck-Institut fur Eisenforschung GmbH, Germany）

[P1-37] **Hydrogen trapping in carbon supersaturated a-iron and its decohesion effect in martensitic steel**

○Wen-Tong Geng[1,2], Vei Wang[1,3], Jin-Xu Li[2], Nobuyuki Ishikawa[4], Hajime Kimizuka[1], Kaneaki Tsuzaki[5,6], Shigenobu Ogata[1,6] （1.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 2.University of Science and Technology Beijing, China, 3.Department of Applied Physics, Xi' an University of Technology, China, 4.Steel Research Laboratory, JFE Steel Corporation, Japan, 5.Department of Mechanical Engineering, Kyushu University, Japan）

[P1-38] **Size Scale Effect on Energy Absorption Property of Aluminum Foam**

○zengyou liang, fudi liang, dezhi deng, chunzhuang miao, mingguang wang （North University of China, China）

[P1-39] Development of charge-transfer type interatomic potential for SiC oxidation

○So Takamoto[1], Takahiro Yamasaki[2], Takahisa Ohno[2], Chioko Kaneta[3], Asuka Hatano[1], Satoshi Izumi[1] （1.The Univ. of Tokyo, Japan, 2.NIMS, Japan, 3.Fujitsu Lab., Japan）

[P1-40] Alpha-phase in engineering aluminum alloys: a multiscale modeling approach to its mechanical behavior

○Duancheng Ma （Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria）

[P1-41] Multi-phase-field lattice Boltzmann modeling and simulation of equiaxed structure

○Ryotaro Sato[1], Tomohiro Takaki[1], Shinji Sakane[1], Munekazu Ohno[2], Yasushi Shibuta[3] （1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.Tokyo University, Japan）

[P1-42] Simulation of Extrusion Process of TiAl alloy prepared by Triple VAR

○Fan Gao, Zhenxi Li （AECC BEIJING INSTITUTE OF AERONAUTICAL MATERIALS, China）

[P1-43] Experimental-Computational Analysis of Primary Static Recrystallizazion in DC04 Steel

○Martin Diehl, Markus Kühbach, Dierk Raabe （Max-Planck-Institut fuer Eisenforschung GmbH,

Germany）

[P1-44] Combining 4D experiments and phase-field modeling to determine reduced grain boundary mobilities

○Jin Zhang[1,2], Peter W Voorhees[1], Henning F Poulsen[2] （1.Northwestern University, United States of America, 2.Technical University of Denmark, Denmark）

[P1-45] Fiber-intersectant microstructure of fish scale and biomimetic research

○Bin Chen[1], Jinghong Fan[2], Miao Li[1], Wei Ye[1] （1.College of Aerospace Engineering, Chongqing University, China, 2.Division of Mechanical Engineering, Alfred University, United States of America）

[P1-46] Microstructures of turtle shell and biomimetic fabrication

○Bin Chen[1], Jinghong Fan[2], Wei Ye[1], Miao Li[1] （1.College of Aerospace Engineering, Chongqing University, China, 2.Division of Mechanical Engineering, Alfred University, United States of America）

[P1-47] Phase-field Simulation of Solidification Process in Welding Pool of Fe-C Binary Alloy

○lan zhan, Xiangge Qin （Jiamusi Univ., China）

[P1-48] Phase field simulation of the phase separation in the TiC-ZrC-WC system

○Zelin Luo[1], Hong Ma[1], Sai Tang[1], Yingbiao Peng[2], Yong Du[1], Zikui Liu[3], Qianhui Min[1], Yafei Pan[4] （1.State Key Lab of Powder Metallurgy, Central South University, China, 2.College of Metallurgy and Materials Engineering, Hunan University of Technology, China, 3.Department of Materials Science and Engineering, Pennsylvania State University, United States of America, 4.School of materials science and engineering, Hefei University of Technology, China）

[P1-49] Switching of coordinate transformations of a repetitive bar-and-joint framework under uniaxial compression

○Hiro Tanaka[1], Kazutoshi Hamada[1], Yoji Shibutani[1,2] （1.Dept. of Mechanical Engineering, Osaka Univ., Japan, 2.Nanotechnology Program, Vietnam Japan Univ., Viet Nam）

[P1-50] Understanding the effect of Residual Stresses in 3D Printed Metals

○Alankar Alankar, BVSS Bharadwaja, Ritam Chatterjee （IIT Bombay, India）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-33] UNDERSTANDING OF DELAYED HYDRIDE CRACKING FAILURE MECHANISM IN E110 ZIRCONIUM BASED FUEL CLADDINGS BY EBSD AND IN-SITU MECHANICAL TESTING

○Hygreeva Kiran NAMBURI[1], Zbynek Spirit[1], Patricie Halodova[1], Ondrej Libera[1], Jakub krejci[2]　（1.Research Centre REZ, Czech Republic, 2.UJP Praha, Czech Republic）

Zirconium based alloys are commonly used as material for fuel claddings in the light water reactors. Claddings act as first metallic barriers against loss of fission products during the nuclear power plant operation, intermittent storage or final dry storage. During the reactor operation, metallic claddings are prone to water side corrosion and subsequent hydrogen pick-up (in 10's to 100's of ppm) due to higher operating temperatures in reactor. Under specific favorable conditions (stress, temperature and hydrogen concentration level) claddings fail by a time dependent mechanism called Delayed Hydride Cracking (DHC). This results in critical issue for the safe performance of the power plants and storage used claddings.

In this work we present results from the DHC study on zirconium based E110 metallic fuel claddings. Test specimen is oxidized in an autoclave to have desired hydrogen content. DHC experiments are performed in scanning electron microscope chamber by using in-situ tensile testing device at high temperatures.

The paper emphases on microstructural studies, evaluation of threshold stress intensity, crack propagation rate, understanding fialure mechanism and role of crack tip hydrides fracture during the DHC failure in E110 fuel claddings.

Keywords: Zirconium alloys, nuclear fuel claddings, microstructure, crack tip hydride fracture, delayed hydride cracking failure.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-34] Transition-metal alloying of γ '-Ni$_3$Al: Effects on the ideal uniaxial compressive strength from first-principles calculations

○Minru Wen[2,1], Chongyu Wang[2]　（1.Guangdong University of Technology, China, 2.Tsinghua University , China）

The addition of transition metal (TM) elements into the γ' precipitate phase of a Ni-based single-crystal superalloy can significantly affect its mechanical properties, including the intrinsic mechanical property of compressive strength. Using first-principles density functional calculations, the effects of $3d$ (Sc-Zn), $4d$ (Y-Cd) and $5d$ (Hf-Au) TM alloying elements on the ideal uniaxial compressive strength of γ'-Ni$_3$Al were investigated. The stress-strain relationships of pure Ni$_3$Al under [100], [110] and [111] compressive loads and the site occupancy behavior of TM elements in Ni$_3$Al were prior studied using a total-energy method based on density functional theory. Our results showed that the capacity of TM elements for strengthening the ideal compressive strength was associated with the d-electron number. The alloying elements with half-filled d-bands (i.e., Cr, Mo, W, Tc and Re) manifested the greatest efficacy for improving the ideal strength of Ni$_3$Al under a deformation along the weakest compressive direction. Furthermore, the charge redistribution of Ni$_3$Al doped with $5d$ elements were also analyzed to understand the strengthening mechanisms of TM elements

in the γ'-Ni$_3$Al phase.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-35] The Influence of Deposition Pattern on Stress and Mechanical Properties in Wire Arc Additive Manufacturing

○Changmeng Liu, Qianru Wu, Jiping Lu, Shuyuan Ma （Beijing Institute of Technology, China）

Wire arc additive manufacturing (WAAM) has exhibited great advantages of high deposition rate, large fly-to-buy ratio and low cost in aerospace applications. However, the deformation caused by internal stress is still a technical challenge in additive manufacturing, especially during the manufacturing process of the large-scale components. In this work, based on numerical modelling method and physical experiments, by investigating the stress and deformation distribution of Ti6Al4V components deposited by five typical patterns, the preferred deposition pattern will be selected to fabricate components with minimum deformation and uniform stress distribution. The morphology, microstructure and mechanical properties of the components with different deposition patterns were studied as well. The results illustrate that short S-shape pattern is identified as the optimal one which has uniform stress distribution and minimum deformation. The stress distribution of the components with spiral pattern and subarea pattern varies a lot and the reasons have been discussed based on the thermomechanical behavior in WAAM.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-36] On the Significance of the Higher-Order Neighbors for Abnormal Grain Growth and Recrystallization Nucleation

○Markus Kuehbach （Max-Planck-Institut fur Eisenforschung GmbH, Germany）

Successful nucleation of abnormal grain growth and primary static recrystallization constitutes a rare event which affects in many cases only each thousandth (sub-) grain if at all. Consequently, the making of more quantitatively substantiated number density predictions can be improved by studying million-scale initial grain populations. Thanks to representative volume element (RVE) method development and software parallelization, simulating the evolution of such large grain populations has recently become possible.

This work details how 2d and 3d resolved RVE computer simulations with such millions of (sub-) grains within each single domain allow quantifying the process of preferential grain evolution during abnormal grain growth and nucleation to primary static recrystallization to hitherto unachieved statistical significance. By assessing not only the nearest but additionally higher-order neighbors of each grain more precise and accurate predictions at which sites nucleation will likely initiate are possible. Albeit, the study proofs also that to definitely identify which grains succeed --- and as such also the number density --- requires assessing their entire topological event sequence surplus quantifying the distribution of their individual capillary- and stored elastic energy-induced grain boundary face migration speeds.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-37] Hydrogen trapping in carbon supersaturated a-iron and its decohesion effect in martensitic steel

○Wen-Tong Geng[1,2], Vei Wang[1,3], Jin-Xu Li[2], Nobuyuki Ishikawa[4], Hajime Kimizuka[1], Kaneaki Tsuzaki[5,6], Shigenobu Ogata[1,6]　(1.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 2.University of Science and Technology Beijing, China, 3.Department of Applied Physics, Xi'an University of Technology, China, 4.Steel Research Laboratory, JFE Steel Corporation, Japan, 5.Department of Mechanical Engineering, Kyushu University, Japan）

It is generally accepted that the martensite in steels is more susceptible to hydrogen embrittlement than the ferrite. The atomic-scale mechanism underlying this phenomenon, nevertheless, is not fully understood yet. Our first-principles calculations demonstrate hydrogen is more stable in carbon supersaturated martensite than in a-iron, due to the carbon-induced tetragonality in martensite lattice. The trapped hydrogen leads to remarkable decohesion between (110) planes both inside the martensite and along the martensite/ferrite interface, with the former being more significant than the latter. This decohesion can explain recent precise observations that in martensite/ferrite dual-phase steels the hydrogen-promoted crack was initiated in the martensite region and that in lath martensite steel it propagated not on lath boundaries but showed quasi-cleavage feature along (110) planes at very high hydrogen concentration.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-38] Size Scale Effect on Energy Absorption Property of Aluminum Foam

○zengyou liang, fudi liang, dezhi deng, chunzhuang miao, mingguang wang　(North University of China, China）

Abstract: Foam metal is extensively used in the fields of petrochemical engineering, aerospace and automobile manufacturing for its excellent properties. As a typical representative of foam metal,Aluminum foam is an excellent material in energy absorption,that it can produce larger plastic deformation under the lower flow stress.Relative to the cell dimension,the size of specimen is an important factor which affects the performance of its energy absorption. Based on the technological process of the infiltration casting method, a microscopic structure model of aluminum foam is established by Monte Carlo method and Gravity Accumulation method ,with the assistance of PFC3D software so as to study the influence of size scale effect on energy absorption property of aluminum foam. A finite element model of aluminum foam is generated according to MATLAB software. Combining with SPH algorithm, numerical simulation to the compression behavior of the different specimen size of aluminum foam is performed. From numerical simulation,we can draw the conclusion that the greater the ratio of specimen dimension to cell dimension is,the better energy absorption property it performs. The results can provide assistance on design buffer suction device with foam mental.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-39] Development of charge-transfer type interatomic potential for SiC oxidation

○So Takamoto[1], Takahiro Yamasaki[2], Takahisa Ohno[2], Chioko Kaneta[3], Asuka Hatano[1], Satoshi Izumi[1]
（1.The Univ. of Tokyo, Japan, 2.NIMS, Japan, 3.Fujitsu Lab., Japan）

Silicon carbide (SiC) is an attractive semiconductor material for applications in power electronic devices and the fabrication of a high-quality SiC/SiO$_2$ interface is desired. It is well known that there is a great difference in oxidation rate between the Si-face and C-face, and that the quality of oxide layer on the Si-face is better than that on the C-face. However, the atomistic mechanism of the thermal oxidation of SiC remains to be solved. In this work, we developed a new Si-C-O interatomic potential to reproduce the kinetics of the thermal oxidation of SiC. More than 1000000 properties obtained by DFT calculations were used for the fitting process. Using this interatomic potential, large-scale SiC oxidation simulations were performed. In order to focus on the reaction of O$_2$ molecules, the oxidation process is realized by inserting O$_2$ molecules into SiO$_2$ region. The results showed that the activation energy of the Si-face is much larger than that of the C-face. Also, the numbers of intermediate oxide states of Si atoms are in good agreement with the experimental result. In the case of the Si-face, a flat and aligned interface structure including Si^{1+} was created. We estimated activation energies of the change of intermediate oxide states and proposed that the stability of the flat interface structure is the origin of the high activation energy of the oxidation of the Si-face. In contrast, in the case of the C-face, it is found that the Si atom at the interface are pulled up by the O atoms. This process generates the disordered interface and decreases the activation energy of the oxidation.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-40] Alpha-phase in engineering aluminum alloys: a multiscale modeling approach to its mechanical behavior

○Duancheng Ma （Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria）

Alpha-phase, i.e., Al(Fe,Mn)Si, is very common in engineering aluminium alloys. During ingot casting, coarse beta-phase forms. In the subsequent homogenization heat treatment, the beta-phase transforms into coarse alpha-phase. In the following forming and solution annealing processes, the coarse alpha-phase remains in the matrix and never dissolve. Since the size of the coarse alpha-phase is large (a few micrometers), they hardly contribute to the strengthening effect. There are many examples, however, showing that it is one of the potential damage nucleation sites. Despite being common in engineering aluminium alloys and being the damage nucleation sites, little is known about the mechanical properties of the alpha-phase. In this study, we use a multiscale modeling approach, i.e. from electronic to continuum scale, to investigate its mechanical behavior in aluminium.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-41] Multi-phase-field lattice Boltzmann modeling and simulation of equiaxed structure

○Ryotaro Sato[1], Tomohiro Takaki[1], Shinji Sakane[1], Munekazu Ohno[2], Yasushi Shibuta[3] （1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.Tokyo University, Japan）

Equiaxed structure formed during a solidification process of metals and alloys determines the mechanical property of materials. Therefore, it is crucial to accurately predict and control the formation process of the equiaxed structure. However, the formation process of equiaxed structure is a complicated multiphysics problem including a motion of multiple grains.

In this study, we construct a multi-phase-field-lattice Boltzmann model which can express the growth, motion, collision, and coalescence of multiple dendrites and following grain growth. In this model, the growth and motion of multiple dendrites are expressed by a multi-phase-field method and equations of motion, respectively, and the liquid flow is computed by lattice Boltzmann method. The collision and coalescence of multiple dendrites and/or grains are also modeled in a concept of diffuse interface. Moreover, the simulation is accelerated by employing the active parameter tracking and graphics processing unit. By using the developed method, the formation simulations of the equiaxed structure are demonstrated.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-42] Simulation of Extrusion Process of TiAl alloy prepared by Triple VAR

○Fan Gao, Zhenxi Li （AECC BEIJING INSTITUTE OF AERONAUTICAL MATERIALS, China）

TiAl alloy with low density and excellent mechanical properties at the high temperature is one of the most potential materials in aerospace industry, however the extrusion of the ingot with industrial scale is difficult due to the poor ductility. In this study, FEM was employed to describe the extrusion plastic deformation behavior of this alloy which prepared by triple VAR. Under various extrusion conditions, the strain distribution and the extrusion load were studied by numerical analysis. The influence of the die angle and the extrusion ratio were examined. The results showed that the peak extrusion force was enhanced with the increased die angle with a certain slop coefficient. The die angle with 100° was suggested to obtain the uniform deformation. With the raising of extrusion ratio, the effective strain, extrusion load in billet would be increased. Then extrusion experiment of triple VAR TiAl ingot was carried out successfully with extrusion ratio of 10.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-43] Experimental-Computational Analysis of Primary Static Recrystallizazion in DC04 Steel

○Martin Diehl, Markus Kühbach, Dierk Raabe （Max-Planck-Institut fuer Eisenforschung GmbH, Germany）

Low-alloyed steels with body-centered cubic crystal structure (bcc, ferrite) are a material class which is widely used in automotive sheet metal forming applications. When produced with an adequate crystallographic texture, the mechanical behavior of steels for forming applications is characterized by an isotropic in-plane flow behavior in combination with a low yield strength. To obtain these beneficial mechanical properties, an adequate cold rolling strategy in terms of the number of passes, deformation rates,

and total reduction needs to be followed by an annealing procedure with a time-temperature profile that facilitates primary static recrystallization. The most fundamental connection between cold rolling and heat treatment consists in the reduction of the dislocation-related free energy stored during deformation by the formation of new grains with a very small dislocation content. Hence, the local variation in crystallographic orientation and defect population lead to very inhomogeneous grain boundary migration velocities.

We present here results of a coupled experimental-computational approach for studying microstructure evolution in industrially cold rolled DC04 steel under quasi-isothermal conditions. For the experimental characterization, quasi in-situ experiments consisting of interrupted isothermal holding at 600˚C and subsequent Electron Backscatter Diffraction (EBSD) orientation imaging were conducted. The results reveal a strong correlation between local dislocation density, quantified via the Kernel Average Misorientation (KAM), and the local increase of recrystallized volume fraction. To complement the experimental findings and gain further insights into the influence of the sub-surface microstructure, a Cellular Automata (CA) model was utilized. The employed three-dimensional microstructure model was directly built from the experimentally characterized deformation microstructure. Different approaches of scaling the KAM into dislocation density values, i.e. the driving force for recrystallization, are employed. Similarities and deviations between experimental and computational results are discussed with the aim at increasing the understanding the mechanisms of static primary recrystallization.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-44] Combining 4D experiments and phase-field modeling to determine reduced grain boundary mobilities

○Jin Zhang[1,2], Peter W Voorhees[1], Henning F Poulsen[2]　(1.Northwestern University, United States of America, 2.Technical University of Denmark, Denmark)

Reduced grain boundary mobilities play an essential role in accurate multi-scale modeling of grain growth in polycrystalline materials. The reduced mobility is a function of a large five-dimensional parameter space. Traditional bi-crystal experiments only determine one point in this space at a time. In this paper, we present a method to determine the reduced mobilities by comparison between 4D experiments and phase-field simulations. The growth of 1327 grains in a pure iron sample is visualized in 3D using diffraction contrast tomography (DCT) at a synchrotron source. Using the first time-step from the experimental microstructure as input, the evolution of the entire grain structure is simulated using a phase-field model. A fitting approach is applied to find the set of reduced mobilities that yield the best match between the experimental microstructure and the simulated microstructure. An efficient fitting algorithm is constructed based on a sensitivity analysis. The fitting algorithm converges fast, and more than 1000 reduced mobilities can be determined simultaneously.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-45] Fiber-intersectant microstructure of fish scale and biomimetic research

ᴼBin Chen[1], Jinghong Fan[2], Miao Li[1], Wei Ye[1] (1.College of Aerospace Engineering, Chongqing University, China, 2.Division of Mechanical Engineering, Alfred University, United States of America)

The microstructures of the scale of a chub fish are observed with scanning electronic microscope (SEM). It is shown that the scale is a kind of natural biocomposite consisting of parallel hydroxyapatite fiber layers and collage matrix. The hydroxyapatite fiber layers consist of long and thin hydroxyapatitefiber fiber sheets. It is also observed that the fiber sheets in adjacent fiber layers compose a fiber-intersectant microstructure. Based on the observed result, the fiber-intersectant microstructure is employed as the pattern for the design of man-made fiber-reinforced composite. A kind of fiber-reinforced composite with the fiber-intersectant structure is biomimetically fabricated. The fracture toughness of the biomimetical composite is tested and compared with that of the conventional composite with fiber-parallel structure. It is indicated that the fracture toughness of the biomimetical composite is remarkably larger than that of the composite with the fiber-parallel structure.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-46] Microstructures of turtle shell and biomimetic fabrication

ᴼBin Chen[1], Jinghong Fan[2], Wei Ye[1], Miao Li[1] (1.College of Aerospace Engineering, Chongqing University, China, 2.Division of Mechanical Engineering, Alfred University, United States of America)

Scanning electron microscope (SEM) observation shows that the shell of red-ear turtle is a kind of natural sandwich composite consisting of exterior cortex and interior cancellus. It is also observed that the hydroxyapatite fibers in the composite continuously surround the holes of the composite forming a particular fiber-surrounded-hole structure. Based on the result of the observation, a biomimetic composite with the fiber-surrounded-hole structure is fabricated. The ultimate strength of the biomimetic composite is tested and compared with that of the conventional composite with the non-fiber-surrounded-hole structure. It is indicated that the ultimate strength of the biomimetic composite is remarkably larger than that of the conventional composite.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-47] Phase-field Simulation of Solidification Process in Welding Pool of Fe-C Binary Alloy

ᴼIan zhan, Xiangge Qin (Jiamusi Univ., China)

Abstract: In this paper, the phase field method was used to study the growth process of Fe-C binary alloy welding pool dendrite. In the phase field model, the characteristics of small volume, fast cooling rate, large temperature difference and high degree of superheat of the welding pool were considered. And base on the model, the influence of undercooling on the crystal morphology of the alloy was predicted. Firstly, the growth morphology of Fe-C alloy dendrites in welding pool was successfully simulated by using the phase field model. Meanwhile, The effects of C concentration distribution on dendrite growth morphology and dendritic spacing were further investigated. The simulation results are consistent with the melten pool solidification theory.

Keywords: Fe-C alloy;solidification of weld molten pool;phase field method; dendritic morphology

---

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-48] Phase field simulation of the phase separation in the TiC-ZrC-WC system

○Zelin Luo[1], Hong Ma[1], Sai Tang[1], Yingbiao Peng[2], Yong Du[1], Zikui Liu[3], Qianhui Min[1], Yafei Pan[4]　（1.State Key Lab of Powder Metallurgy, Central South University, China, 2.College of Metallurgy and Materials Engineering, Hunan University of Technology, China, 3.Department of Materials Science and Engineering, Pennsylvania State University, United States of America, 4.School of materials science and engineering, Hefei University of Technology, China）

TiC-ZrC-WC system with high hardness is a promising material being widely used in industries like processing and manufacturing. Understanding the microstructural evolution and the mechanism during phase separation process is still a formidable challenge nowadays. Microstructural evolution mechanisms during phase separation process are explained for the first time through the methodology combing our CALPHAD data and two-dimensional Cahn-Hilliard/elastic strain energy model, and we used the parameters in our database of thermodynamics and dynamics. We investigate the effect of elastic strain on lamellar structure, agreeing well with previous results in terms of the variation of the periodicity of the distribution of element composition and the periodicity of regularly lamellar microstructures. It is obvious that phase field method coupled with thermodynamic database is a useful approach to study the microstructure evolution of TiC-ZrC-WC materials and in further speed up the research and development of new materials of TiC-ZrC-WC system.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-49] Switching of coordinate transformations of a repetitive bar-and-joint framework under uniaxial compression

○Hiro Tanaka[1], Kazutoshi Hamada[1], Yoji Shibutani[1,2]　（1.Dept. of Mechanical Engineering, Osaka Univ., Japan, 2.Nanotechnology Program, Vietnam Japan Univ., Viet Nam）

In recent years, a variety of artificial microstructures with multi-functionality have been extensively developed by incorporating specific geometric features. The topic appears in a wide range of fields from geometry to crystallography to engineering, and indeed the mechanical behaviors of many of these structures remain unexplored. Some examples of such behaviors include auxeticity in materials of negative Poisson's ratio, origami-based folding and deployment, and deformability of hierarchically arranged structures. In this context, we proposed the compressive structural system switching two types of kinematic transformations toward diamond- and square-patterns. To clarify the transition mechanism, we modelled a specific repetitive bar-and-joint framework with the two angular variables specifying the rotation and distortion of the linked square components. Numerically exploring the equilibrium paths then reveals a transition state of the structure at a critical value of the internal stiffness. A simplified formulation of the model with weak nonlinear terms yields an exact solution of its transition state. We further investigated the viscoelastic transition feature of the proposed structure to replace the cell-binding springs inside structure with damping components, and

revealed the interesting transformation characteristics, which depend on the compressive load speeds. The main idea is that our abstract representation might provide an original perspective to nonlinear elastic phenomena in solid state matter.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-50] Understanding the effect of Residual Stresses in 3D Printed Metals

○Alankar Alankar, BVSS Bharadwaja, Ritam Chatterjee （IIT Bombay, India）

We present phase field and atomistically informed simualtions of 3D printed CP-Ti. In the simulations, the microstructure can be controlled as a function of heat intensity, source velocity and powder size. Also, these process parameters are shown to have direct effect on the preferred crystallographic texture, porosity fraction and residual stresses in the additively created microstructure. This syntheic microstructure is then used as input for crystal plasticity model. In the crystal plasticity model the effect of voids coupled with crystallographic texture is studied as a function of various boundary conditions.

Poster Session | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[PO-H1] Poster Session 1
Symposium H
Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-51] Multi-scale modeling of DNA-dendrimers in electrolyte solutions
○Natasa Adzic[1], Clemens Jochum[2], Gerhard Kahl[2], Christos Likos[1] （1.Faculty of Physics, University of Vienna, Austria, 2.Institute for Theoretical Physics, Vienna University of Technology, Austria）

[P1-52] Structural and dynamical properties of star block-copolymers in shear flow.
○Diego Felipe Jaramillo - Cano[1], Manuel Camargo[2], Christos N. Likos[1] （1.Faculty of Physics, University of Vienna, Austria, 2.CICBA, Universidad Antonio Nariño - Campus Farallones, Colombia）

[P1-53] Multiscale simulation of polymeric solids for fracture processes
○Takahiro Murashima[1], Shingo Urata[2] （1.Dept. of Physics, Tohoku Univ., Japan, 2.AGC, Japan）

[P1-54] Quantification and validation of the mechanical properties of DNA nicks
○Jae Young Lee, Jae Gyung Lee, Do-Nyun Kim （Dept. of Mechanical and Aerospace Engineering, Seoul National Univ., Korea）

[P1-55] Investigating the mechanical properties of azobenzene-tethered DNA for controlling self-assembling DNA nanostructures
○Jae Gyung Lee, Chanseok Lee, Do-Nyun Kim （Dept. of Mechanical and Aerospace Engineering, Seoul National Univ., Korea）

[P1-56] FTMP-based Modeling and Simulations of Glassy Polymers.
○Soushi Miyamoto, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P1-57] Shock Wave Induced Damage in Tumor Cells: Experiments and Simulations
○Martin Steinhauser （Fraunhofer Ernst-Mach-Institute, EMI, Germany）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-51] Multi-scale modeling of DNA-dendrimers in electrolyte solutions

○Natasa Adzic[1], Clemens Jochum[2], Gerhard Kahl[2], Christos Likos[1]　（1.Faculty of Physics, University of Vienna, Austria, 2.Institute for Theoretical Physics, Vienna University of Technology, Austria）

We have studied a novel class of macromolecules, the so-called DNA-based dendrimers. They have recently been synthesized from the enzymatic ligation of Y-shaped DNA building blocks. In order to describe such dendrimers of various generations we have performed MD simulations employing two independent models: a bead-spring model and the oxDNA model. The former one models each base-pair of double-stranded DNA as a single charged monomer and the interactions and interaction parameters in the model have been carefully chosen to mimic the structural properties of a single DNA chain. The system was immersed in water, which was modeled as a uniform dielectric and counterions were introduced in the system to preserve electroneutrality. Furthermore, we added salt, treating it explicitly, in order to investigate its influence on conformational characteristics of a single dendrimer molecule. On the other hand, the oxDNA model allowed us to take a closer look into the DNA structure, treating DNA as a string of rigid nucleotides which interact through potentials that depend on the position and orientation of the nucleotides. Equilibrium properties of a single dendrimer-like DNA molecule from the first to the sixth generations obtained from these two models have been investigated and the obtained simulation results have also been compared to the experiments. We have found an excellent agreement between the theoretical and experimental results, which has encouraged us to use the introduced models for theoretical analysis of novel self-assembled structures, such as cluster crystals in the bulk. The study of these charged dendrimer-systems is an important field of research in the area of soft matter due to their potential role in various interdisciplinary applications, ranging from molecular cages and carriers for drug and gene delivery in a living organism to the development of dendrimer-based ultra-thin films in the area of nanotechnology.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-52] Structural and dynamical properties of star block-copolymers in shear flow.

○Diego Felipe Jaramillo - Cano[1], Manuel Camargo[2], Christos N. Likos[1]　（1.Faculty of Physics, University of Vienna, Austria, 2.CICBA, Universidad Antonio Nariño - Campus Farallones, Colombia）

Star block-copolymers (SBCs) have been demonstrated to constitute self-assembling building blocks with specific softness, functionalization, shape, and flexibility. In this work, we studied the structural and dynamical behavior of an isolated SBC under a shear flow by means of particle-based multiscale simulations (MD+MPCD) covering a wide range of system parameters, which include the functionality (number of arms of the star), the amphiphilicity degree, and the solvent quality. We systematically analyzed the conformational properties of low-functionality SBC, as well as the formation of attractive patches on their corona as a function of the shear rate. Three mechanisms of patch reorganization under shear were identified, which determine the dependence of the patch numbers and orientations on the shear rate, namely, free arms joining existing patches, a fusion of medium-sized patches into bigger ones, and fission of large patches into two smaller ones at high shear rates [1]. As well as, the dynamics of the SBC was investigated by means of the so-called Eckart's frame, which allows separating pure rotational and vibrational motions [2,3]. It is shown that SBCs display a richer structural and dynamical behavior than athermal star polymers in a shear flow [4] and therefore they are also interesting candidates to tune the viscoelastic properties of complex fluids.

Because the conformation and dynamics of single SBCs are expected to be preserved in low-density bulk phases, the presented results are the first step in understanding and predicting the rheological properties of semidilute suspensions of this kind of polymers.

[1] Jaramillo-Cano et al. J. Phys. Chem. B (2018) In press
[2] Sablic et al. Soft Matter 13: 6988 (2017)
[3] Jaramillo-Cano et al. (2018) In preparation
[4] Ripoll et al. Phys. Rev. Lett. 96: 188302 (2006)

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-53] Multiscale simulation of polymeric solids for fracture processes

○Takahiro Murashima[1], Shingo Urata[2] (1.Dept. of Physics, Tohoku Univ., Japan, 2.AGC, Japan)

We have developed a new multiscale simulation technique in order to investigate polymeric solids. Macroscopic features of polymeric solids are described by finite element method and microscopic features are described by molecular dynamics simulation. Each of finite elements has its microscopic simulator instead of using a constitutive equation. Polymers are described by the Kremer-Grest model, namely the bead-spring model. This model is simple but it can consider entanglements of polymers, which cause long time hysteresis. We solve macroscopic continuum mechanics and microscopic molecular dynamics concurrently. We have applied our multiscale simulation technique to fracture processes of polymeric solids under uniaxial tension.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-54] Quantification and validation of the mechanical properties of DNA nicks

○Jae Young Lee, Jae Gyung Lee, Do-Nyun Kim (Dept. of Mechanical and Aerospace Engineering, Seoul National Univ., Korea)

Understanding the mechanical properties at a nick site of double-stranded DNA is important to precisely design self-assembling DNA nanostructures because they inevitably contain many nicks that are structural discontinuities of DNA backbones. It is, however, difficult to characterize the mechanical properties of DNA nicks experimentally due to its resolution limit while those for normal DNA double helix without nicks have been relatively well measured. Here, we quantitatively studied the sequence-dependent characteristics of DNA nicks at the base-pair scale using the molecular dynamics (MD) simulation. We found that a primary structural role of DNA nicks is the relaxation of torsional constraint by sugar-phosphate backbones and that neighboring base-pair sequences affect the degree of mechanical rigidity changes by a nick. To validate these findings, we designed DNA nanostructures sensitive to torsion where the torsional rigidity at nick sites was regulated by using various sequences of DNA nicks and measured their overall twist angle using the atomic force microscope (AFM). We expect our study for nicks offers a versatile way of fine tuning the shape and properties of DNA nanostructures.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-55] Investigating the mechanical properties of azobenzene-tethered DNA for controlling self-assembling DNA nanostructures

○Jae Gyung Lee, Chanseok Lee, Do-Nyun Kim （Dept. of Mechanical and Aerospace Engineering, Seoul National Univ., Korea）

Advances in structural DNA nanotechnology have enabled the construction of a nanostructure with various shapes using self-assembling characteristics of DNA strands. Recently, there is an increasingly higher demand for building a dynamic, morphing structure in response to environmental signals so that DNA nanostructures can be used as a functional structure as well.

Azobenzene is one of the representative molecules that change its conformation under the change of light source. It switches from the trans isomer to the cis isomer when absorbing ultraviolet lights, while it is reversibly isomerized under visible lights. Multiple azobenzene molecules can be combined with DNA by intercalated between base-pair steps through threonine linkers and non-planar cis-azobenzenes destabilize the stacking interaction of DNA bases unlike planar trans-azobenzenes. Hence, azobenzene-tethered DNA (AzoDNA) can serve as a structural motif that triggers the conformational change of DNA nanostructures with lights. Nevertheless, its mechanical properties and transition dynamics are rarely known. Here, we investigate the mechanical properties of AzoDNA at its trans and cis states by performing molecular dynamics simulation. To validate, we construct a DNA nanostructure whose bending angles are controlled by the rigidity of AzoDNA at the hinge part.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-56] FTMP-based Modeling and Simulations of Glassy Polymers.

○Soushi Miyamoto, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

Multiscale modeling of glassy solids, such as polymers and metallic glasses, will require mathematically rational as well as effective treatments of the glassy states (free volume) responsible for carrying the viscoplastic flow. For amorphous polymers, it is rephrased as "modeling network degrees of freedom (NW-DOFs)" in connection with the orientating polymer chains. The "glassy states" can then be expressed in this context as those with curled and/or entangled chains with no net orientation, whereas the "strength" is attributed to their fully-extended counterparts with the alignments in the load-bearing direction, referred to as orientation hardening. To express the NW-DOFs, we introduce Finslerian geometry for an extended description of FTMP, together with the polymer-slip system-based kinematics proposed by Shizawa, et al. as the framework that allows direct treatments of the orientation change of the consisting polymer chains in a

similar manner to the conventional crystal plasticity. The current extension enables one to deal explicitly with the associated microscopic degrees of freedom of underlying kinds, e.g., cross-linking and unzipping. Targeted material here is PMMA for modeling the early-stage viscoplastic and the attendant softening responses as typical mechanical properties of engineering polymers. By allocating the vecotrial field in the extended Finslerian formalism to the representative direction of the polymer chains, together with the associated fabric tensor field, the study attempts to express the NW-DOFs. Assuming that the NW-DOFs are given as a function of the incompatibility, on the basis of the "flow-evolutionary" perspectives in FTMP, the evolving "free volume" can be effectively expressed, with which both the targeted properties are successfully reproduced. The free volume change, on the other hand, is shown to qualitatively agree with that reported in the literature.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-57] Shock Wave Induced Damage in Tumor Cells: Experiments and Simulations

○Martin Steinhauser （Fraunhofer Ernst-Mach-Institute, EMI, Germany）

ABSTRACT

Despite the therapeutic success of extracorporeal shock wave therapy in medicine, e.g. for disintegrating concrements, the effects of shock waves on the damage of biological cells and their membranes remain widely unknown. We present experimental results on the destruction of tumor cells using laser-induced shock waves. For the simulation of biological systems such as membranes under highly transient conditions such as external shock wave load, we propose a thermodynamically consistent and energy conserving coupling scheme between the atomistic and the continuum domain. The coupling scheme links the two domains using the DPDE (Dissipative Particle Dynamics at constant Energy) thermostat and is designed to handle strong temperature gradients across the atomistic/continuum domain interface. Using DPDE we investigate the effects of shock-wave impact on the damage of lipid bilayer membranes. A coarse-grained model for the phospholipid bilayer in aqueous environment is employed, which models single lipids as short chains consisting of a hydrophilic head and two hydrophobic tail beads. Water is modeled by mapping four water molecules to one water bead. Using the DPDE method enables us to faithfully simulate the non-equilibrium shock-wave process with a coarse-grained model as the correct heat capacity can be recovered. At equilibrium, we obtain self-stabilizing bilayer structures that exhibit bending stiffness and compression modulus comparable to experimental measurements under physiological conditions. We study in detail the damage behavior of the coarse-grained lipid bilayer upon high-speed shock-wave impact as a function of shock impact velocity and bilayer stability. A single damage parameter based on an orientation dependent correlation function is introduced.

REFERENCES

[1] Martin O. Steinhauser, Computational Multiscale Modeling of Fluids and Solids - Theory and Applications, Springer 2nd ed., Berlin, Heidelberg, New York 2017.

[2] Tanja Schindler, Dietmar Kröner, Martin O. Steinhauser, On the dynamics of molecular self-assembly and the structural analysis of bilayer membranes using coarse-grained molecular dynamics, Biochimica at Biophysica Acta, **1858**, 1955-1963, 2016

[PO-I1] Poster Session 1
Symposium I
Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-58] Phase-field modeling of anisotropic grain growth with incorporation of Sigma 3 CSL grain boundaries.
○Kunok Chang （Kyung Hee Univ., Korea）

[P1-59] Direct mapping from molecular dynamics to phase-field simulations for accurate prediction of grain growth
○Eisuke Miyoshi[1], Tomohiro Takaki[1], Yasushi Shibuta[2], Munekazu Ohno[3] （1.Kyoto Institute of Technology, Japan, 2.The University of Tokyo, Japan, 3.Hokkaido University, Japan）

[P1-60] Density functional theory plus Hubbard U study of the segregation of Pt to the CeO_{2-x} grain boundary
Guoli Zhou, Pan Li, Qingmin Ma, ○Zhixue Tian, Ying Liu （Hebei Normal Univ., China）

[P1-61] **Interfacial charge transfer and enhanced photocatalytic mechanism for Bi_2WO_6/BiOCl heterostructure: A first-principles theoretical study**
○Pan Li （Hebei Normal Univ., China）

[P1-62] Investigation of abnormal grain growth conditions by phase-field method
○Nobuko Mori, Eisuke Miyoshi, Tomohiro Takaki （Kyoto Institute of Technology, Japan）

[P1-63] **Phase Field Crystal Modeling of Mechanism of Strain-Driven for Nucleation and Grain of Deformed-Grain**
○Ying-Jun Gao （Guangxi University, China）

[P1-64] **Diffusion and trapping of hydrogen at grain boundaries scale in fcc polycrystalline nickel: some implications of the atomic volume and the interstitial self-stress**
○xavier Feaugas, jiaqi Li, abdel malek Hallil, abdelali oudriss, arnaud metsue, jamaa bouhattate （university of La Rochelle, France）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-58] Phase-field modeling of anisotropic grain growth with incorporation of Sigma 3 CSL grain boundaries.

○Kunok Chang （Kyung Hee Univ., Korea）

Understanding of grain growth is one of the major on-going challenges of materials science. Since grain growth is complex multi-physics phenomena, it is extremely difficult to describe grain growth phenomenon analytically with the completed theory. Therefore, a number of researchers have tried to investigate grain growth using computational techniques. Among them, the phase-field method has been used one of the efficient and strong tools. So far, 3D grain growth with isotropic grain boundary energy has been intensively studied and their microstructural characteristics have been quantitatively analyzed. On the other hand, since anisotropic 3D grain growth is way more complicated than isotropic phenomena, only a few attemps have been made with simplified assumptions. In this study, we performed anisotropic 3D grain growth with consideration of Sigma 3 CSL grain boundary. To perform the modeling within realistic time window, we implemented OpenMP parallelized technique. We analyzed how degree of anisotropy in grain boundary energy and fraction of CSL boundaries affects growth kinetics and evolution of microstructural characteristics.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-59] Direct mapping from molecular dynamics to phase-field simulations for accurate prediction of grain growth

○Eisuke Miyoshi[1], Tomohiro Takaki[1], Yasushi Shibuta[2], Munekazu Ohno[3] （1.Kyoto Institute of Technology, Japan, 2.The University of Tokyo, Japan, 3.Hokkaido University, Japan）

For numerically predicting grain growth, two different approaches have been used: atomistic simulations typified by molecular dynamics (MD); and continuum-based treatments including the Monte-Carlo, phase-field, and vertex methods. The former can model the spontaneous nucleation process that precedes grain growth. However, due to the large computational cost, it is difficult to simulate grain growth until the late stage using only atomistic methods. On the other hand, continuum-based models allow for relatively efficient computations. In particular, the multi-phase-field (MPF) model [I. Steinbach and F. Pezzolla, Physica D, 134 (1999) 385], which is an extension of the phase-field model to polycrystalline systems, is widely employed in recent years as a prominent tool for simulating grain growth with accuracy and efficiency. Nevertheless, the MPF model cannot directly reproduce the nucleation phenomenon. Considering the strong dependence of grain growth behaviors on the initial structure, there is a pressing need for a means of providing realistic initial structures for MPF simulation.

In this study, we aim to achieve more accurate and efficient prediction of grain growth by exploiting the merits of atomistic and continuum simulations. To this end, we propose a method to convert MD-generated atomic configurations into the MPF interfacial profiles; this enables us to perform MPF grain growth simulations in succession to MD nucleation simulation. Furthermore, using the proposed method, MPF and MD grain growth simulations from the same initial structure are directly compared, via which the difference between each simulation result is quantified. Through the detailed investigation of the causes of the difference, a way to improve the accuracy of the MPF model is discussed.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-60] Density functional theory plus Hubbard U study of the segregation of Pt to the CeO_{2-x} grain boundary

Guoli Zhou, Pan Li, Qingmin Ma, $^{\circ}$Zhixue Tian, Ying Liu （Hebei Normal Univ., China）

Grain boundaries (GBs) can be used as traps for solute atoms and defects, and the interaction between segregants and GBs is crucial for understanding the properties of nanocrystalline materials. In this study, we have systematically investigated the Pt segregation and Pt-oxygen vacancies interaction at the sigma 3 (111) GB in ceria (CeO_2). The Pt atom has a stronger tendency to segregate to the sigma3 (111) GB thanto the (111) and (110) free surfaces, but the tendency is weaker than to (112) and (100). Lattice distortion plays a dominant role in Pt segregation. At the Pt-segregated-GB (Pt@GB), oxygen vacancies prefer to form spontaneously near Pt in the GB region. However, at the pristine GB, oxygen vacancies can only form under O-poor conditions. Thus, Pt segregation to the GB promotes the formation of oxygen vacancies, and their strong interactions enhance the interfacial cohesion. We propose that GBs fabricated close to the surfaces of nanocrystalline ceria can trap Pt from inside the grains or other types of surface, resulting in the suppression of the accumulation of Pt on the surface under redox reactions, especially under O-poor conditions

---

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-61] Interfacial charge transfer and enhanced photocatalytic mechanism for Bi_2WO_6/BiOCl heterostructure: A first-principles theoretical study

$^{\circ}$Pan Li （Hebei Normal Univ., China）

First-principles calculations based on density functional theory are used to explore the interfacial structure and properties of the Bi_2WO_6/BiOCl heterojunction aiming at gaining insights into the photocatalytic mechanism of the Bi_2WO_6/BiOCl heterojunction. Bi_2WO_6/BiOCl interface has a good lattice match, with the interface formation energy is -4.67eV. The calculated band alignment between the Bi_2WO_6 and BiOCl reveals that the valence band offset and conduction band offset between BiOCl and Bi_2WO_6 are 0.37 eV and 1.02 eV, respectively. The calculated Mulliken charge population and electron difference density maps reveal that there is a self-induced internal electric field along the perpendicular direction to the layers in the BiOCl and Bi_2WO_6. Based on the obtained work function and band edge positions of BiOCl and Bi_2WO_6, the formation mechanism of the internal electric field at the interface of Bi_2WO_6/BiOCl heterostructure is studied. The existence of band offsets and the internal electric field can facilitate the separation of the photo-generated electron-hole pairs, resulting in the enhanced photocatalytic activities of the heterostructures.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-62] Investigation of abnormal grain growth conditions by phase-field method

○Nobuko Mori, Eisuke Miyoshi, Tomohiro Takaki　(Kyoto Institute of Technology, Japan)

To improve the properties of materials by controlling their textures and grain sizes, it is essential to accurately predict abnormal grain growth, a phenomenon through which a few grains undergo preferential growth. In addition, the abnormal grain growth is considered to be one of the origins for the nucleation of recrystallized grains and, thus, is of great importance for modelling recrystallization processes.

As a prominent theory of abnormal grain growth, that proposed by Humphreys (here referred to as the cellular microstructural stability (CMS) theory) is well known. In this theory, a complicated polycrystalline microstructure, where grain size, boundary energy, and boundary mobility are not uniform, is simplified as a cellular microstructure model. The model consists of two ingredients: a specific grain and its surrounding matrix with uniform grain size and boundary properties. This modelling makes it possible to describe the abnormal grain growth behavior of the specific grain using only three parameters, i.e., its relative size, boundary energy, and boundary mobility normalized by those of the matrix. However, the validity of this theory has not been confirmed yet neither in experiment and simulation.

In this study, we aim to evaluate the applicable range of the CMS theory via systematic two-dimensional numerical simulations. As the numerical model, the multi-phase-field model [2] is employed, enabling accurate treatment of curvature-driven grain boundary migration in polycrystalline systems. Grain growth simulations are performed while varying the size, boundary energy, and boundary mobility of a specific grain in the matrix. By comparing the simulated results with the prediction of the CMS theory, we reveal the validity and applicable range of the theory.

[1] F. J. Humphreys, Acta Mater., 45, (1997), 4231.
[2] I. Steinbach, F. Pezzolla, Physica D, 134, (1999), 385.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-63] Phase Field Crystal Modeling of Mechanism of Strain-Driven for Nucleation and Grain of Deformed-Grain

○Ying-Jun Gao　(Guangxi University, China)

The phase-field-crystal (PFC) method is used to investigate dynamic strain-induced a splitting of grain boundary (GB) to generate a deformed grain with high strain energy and to drive it to grow in two dimensions. The simulated results show that the essence of the splitting process of the original GB is that new deformed grain is nucleated, and results in formation of high-density ensembles of mobile lattice dislocation that is capable of plastic flow localization (deformed banding). The GB migration is the process of the new deformed grain with higher strain energy consuming the original grain to extend. The deformed grain stores the strain energy through climbing of the dislocation, as well as changing the orientation of the original grain. The deformed grain growth (DGG) is the acceleration process of the speed, and its area extension is proportional to the time square. The rule of the time square of the DGG can also be deduced by establishing the dynamic equation of the strain-driven for the dislocation and the deformed grain extension.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-64] Diffusion and trapping of hydrogen at grain boundaries scale in fcc polycrystalline nickel: some implications of the atomic volume and the interstitial self-stress

○xavier Feaugas, jiaqi Li, abdel malek Hallil, abdelali oudriss, arnaud metsue, jamaa bouhattate （university of La Rochelle, France）

The mobility of hydrogen in metals is a key parameter for understanding the basic mechanisms of hydrogen embrittlement (HE). This problem is directly related to the mechanisms of diffusion and trapping of hydrogen within a specific metallurgical state. These mechanisms depend on the various microstructural heterogeneities and in particular the grain boundaries (GBs), triple junction (TJs) and several defects (dislocations, vacancies ⋯). Although a number of theories have been proposed to describe the role of GBs for hydrogen diffusion and segregation, none of them is able to give an exact answer. In present work we report our recent works, which support the investigation of diffusion and trapping of hydrogen in two elementary systems: nickel single crystals and bi-crystals to highlight the impact of GB on hydrogen mobility in polycrystalline fcc metals. We developed a methodology combining experimental tools (electrochemical permeation / TDS, HRTEM, EBSD) and numerical methods (FEM-COMSOL / EAM-LAMMPS). We propose to screen several bi-crystals of pure nickel with different grain boundaries (*Σ11-50˚30<110>{311}, Σ11-129˚ 30<110>{332}, Σ3-70˚30<110>{111}* and *Σ5-37˚<100>{310})*.

The results allow us to associate the short-circuit diffusion and trapping phenomena to the grain boundaries and defect characters (excess volume, defects density and distribution ⋯). In each situation, we highlight the importance of the self-stress on the processes of diffusion and segregation. The segregation energy of hydrogen depends on the nature of the site (the local free volume and the elastic energy associated with the incorporation of solute). The diffusion of hydrogen is directly influenced by the nature of the grain boundary (the free volume and the distribution of the segregation sites). Our results, at the atomic scale, show a correlation between the solubility and the free volume of the grain boundary. The grain boundaries with a higher free volume have more favorable diffusion paths for hydrogen than in the crystal lattice and at the same time more segregation sites.

[PO-J1] Poster Session 1

Symposium J

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-65] Multiscale Model for Interlayer Defects in Heterogeneous Bilayer Material

○Shuyang Dai[1], David Joseph Srolovitz[2], Yang Xiang[3]　(1.Wuhan University, China, 2.University of Pennsylvania, United States of America, 3.Hong Kong University of Science and Technology, Hong Kong）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-65] Multiscale Model for Interlayer Defects in Heterogeneous Bilayer Material

○Shuyang Dai[1], David Joseph Srolovitz[2], Yang Xiang[3] （1.Wuhan University, China, 2.University of Pennsylvania, United States of America, 3.Hong Kong University of Science and Technology, Hong Kong）

We present a multiscale model to describe the interlayer defects in bilayer materials. The model incorporates both the anisotropy elasticity of each layer and the first-principle calculation informed interaction between two layers, i.e., the 3-dimensional generalized stacking-fault energy. The force balance between these two contributions determines the structure. We apply this approach to determine the structure and energetics of twisted bilayer material. In twisted bilayer graphene, two distinct, modified Moiré structures are observed. We also study the buckling twisted heterogeneous bilayer material such as bilayer graphene/hexagonal boron nitride. We investigate the structure and corresponding dislocation network due to various misfits and twist angles between two layers. The relaxation of the Moiré structure reduces the symmetry and increases the period of the bilayer material. Our model agrees well with the atomistic results. An analytical description is developed based on the obtained structural features.

[PO-L1] Poster Session 1
Symposium L
Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-66] Molecular dynamics study on temperature and loading rate dependence of nano-indentation pop-in load
○Yuji Sato[1], Shuhei Shinzato[1], Takahito Ohmura[2], Shigenobu Ogata[1,3] （1.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan, 3.Center for Elements Strategy Initiative for Structural Materials (ESISM), Kyoto University, Japan）

[P1-67] Geometry of curved surface and energetics of in graphene with defects
○Ako Kihara[1], Xiao-Wen Lei[1], Akihiro Nakatani[2] （1.Dept. of Mechanical Engineering, Univ.of Fukui, Japan, 2.Dept. of Adaptive Machine Systems, Osaka Univ., Japan）

[P1-68] Collective motion of dislocation associated with local plasticity initiation and subsequent behavior in bcc metals
○Takahito Ohmura （National Institute for Materials Science, Japan）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-66] Molecular dynamics study on temperature and loading rate dependence of nano-indentation pop-in load

$^{\bigcirc}$Yuji Sato[1], Shuhei Shinzato[1], Takahito Ohmura[2], Shigenobu Ogata[1,3]　(1.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan, 3.Center for Elements Strategy Initiative for Structural Materials (ESISM), Kyoto University, Japan）

Nano-indentation test is commonly used to investigate mechanical properties of materials in nano-scale. In nano-indentation test, a displacement burst behavior of indenter, "pop-in", can be usually observed. Pop-in is considered to be attributable to dislocation nucleation phenomena, thus pop-in can be associated with incipient plasticity in materials. It is well-known that the pop-in occurs when a shear stress along a slip system beneath the indenter reaches near theoretical shear strength. However, the temperature and loading rate dependency of pop-in load is still unclear. In this study, using atomistic simulation with EAM interatomic potentials, we computed stress dependent activation energy of homogeneous dislocation nucleation event in BCC Fe and Ta under actual complex stress condition beneath a spherical indenter. Based on the computed activation energy and stochastic modeling method, temperature and loading-rate dependent probability distribution of the critical indentation load was successfully predicted. Eventually, we compared the atomistic predictions with experiments, and confirmed validity of our atomistic modeling.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-67] Geometry of curved surface and energetics of in graphene with defects

$^{\bigcirc}$Ako Kihara[1], Xiao-Wen Lei[1], Akihiro Nakatani[2]　(1.Dept. of Mechanical Engineering, Univ.of Fukui, Japan, 2.Dept. of Adaptive Machine Systems, Osaka Univ., Japan）

Two-dimensional (2D) materials have attracted attentions as unique functional materials.
Among them, graphene is well-known as a fundamental structure of 2D materials of nano-carbon.
In 2D materials, lattice defects, such as dislocations and disclinations, cause out-of-plane deformation.
For example, carbon nano-cone or nano-horn is formed geometrically by the wedge disclination of graphene sheet (GS).

In this study, we focus on the fundamental mechanism which can explain how the shape of 2D materials with defects is determined.
Typical four structure models of GS with defects are studied, i.e. positive perfect wedge disclination, negative perfect wedge disclination, positive partial wedge disclination, and negative partial wedge disclination.
The partial wedge disclinations are implemented by the array of edge dislocations in which the local structure consists of pentagon-heptagon atomic bonds.
Then the equilibrium configuration is calculated by using large-scale atomic/molecular massively parallel simulator (LAMMPS).

The obtained surfaces are examined by fitting to analytical test functions.
All results of out-of-plane displacement z are organized by a universal form of $z=rf(\theta)$, in a cylindrical coordinate (r, θ, z), in which $f(\theta)$ is an appropriate function of θ.

This result means that the all models of GS are represented as conical surfaces in a broad sense.

From a local viewpoint, according to the distribution of atomic site potential energy, it is observed that the energy values at atoms in pentagon ring are relatively high, but the energy values at atoms in heptagon ring are relatively low.

From a global viewpoint, the energy values decrease with increasing distance r from the core of disclination.

After a detail examination, we found the site potential energy is proportional to the square of curvature.

The fundamental knowledge obtained would be applicable to desgin/control the shape of 2D materials.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-68] Collective motion of dislocation associated with local plasticity initiation and subsequent behavior in bcc metals

○Takahito Ohmura （National Institute for Materials Science, Japan）

Nanoindentation-induced mechanical behavior was investigated for bcc metals. Pop-in event that corresponds presumably to local plasticity initiation was detected on load-displacement curves with major parameters of critical load P_c and corresponding excursion depth *deltah*. In a plot of P_c vs delta*h*, the P_c increases monotonically with the *deltah*, and the slope depends on alloy systems. On the other hand, brittle-to-ductile transition temperature (BDTT) also depends on the alloy systems, and the alloy with higher BDTT shows higher slope in the P_c vs delta*h* plot. Dislocation structures underneath the indenter were observed through TEM before and after a pop-in event. No dislocations were observed before initiation while considerable dislocations were generated right after the event. These results suggest that dislocation nucleation and multiplication occur drastically upon plasticity initiation based on collective dislocation motion. Since the BDTT is closely consistent with pop-in event, crack propagation might be related with plasticity initiation. Statistical analysis of the events suggests physical models of the phenomena. In the case of the first pop-in event, the probability of the event to the P_c is Gaussian distribution, which indicates that a thermally activated process dominates the event. For the second or later cases, the probability to the magnitude of the event shows power law function like Gutenberg-Richter model, which suggests a dislocation avalanche.

Poster Session | M. Time- and History-Dependent Material Properties

[PO-M1] Poster Session 1

Symposium M

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-69] FORMATION OF PHYSICAL GELS BY ARRESTED SPINODAL DECOMPOSITION IN CHARGED COLLOIDS

○Jose Manuel Olais-Govea[1], Alonso Gomez-Canales[1], Leticia Lopez-Flores[2], Martin Chavez-Paez[2], Magdaleno Medina-Noyola[2]　(1.Instituto Tecnologico y de Estudios Superiores de Monterrey, Mexico, 2.Universidad Autonoma de San Luis Potosi, Mexico)

[P1-70] How to improve the ductility of CuZr BMGs based on cyclic pre-straining: MD simulations and mechanical testing

○Jonathan Amodeo[1], Oriane Baulin[1], Damien Fabregue[1], David Rodney[2]　(1.MATEIS, Univ. Lyon 1, France, 2.ILM, Univ. Lyon 1, France)

[P1-71] Modeling plastic deformation of amorphous solids from atomic scale mechanisms

○Francesca Boioli[1], Tristan Albaret[2], David Rodney[2]　(1.LEM, CNRS-ONERA, Chatillon, France, France, 2.ILM, University of Lyon 1, France, France)

[P1-72] Thermally Activated Creep and Constant Shear Rate Deformation in Amorphous Materials

○Samy MERABIA[1], Julien LAM[2], François DETCHEVERRY[1]　(1.CNRS and Universite Lyon 1, France, 2.Université de Bruxelles, Belgium)

[P1-73] Numerical analysis of shrinkage process based on the experimental data

○Barbara Kucharczykova[1], Hana Simonova[2], Petr Frantik[2]　(1.Brno University of Technology, Faculty of Civil Engineering, Institute of Building Testing, Czech Republic, 2.Brno University of Technology, Faculty of Civil Engineering, Institute of Structural Mechanics, Czech Republic)

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-69] FORMATION OF PHYSICAL GELS BY ARRESTED SPINODAL DECOMPOSITION IN CHARGED COLLOIDS

○Jose Manuel Olais-Govea[1], Alonso Gomez-Canales[1], Leticia Lopez-Flores[2], Martin Chavez-Paez[2], Magdaleno Medina-Noyola[2]　(1.Instituto Tecnologico y de Estudios Superiores de Monterrey, Mexico, 2.Universidad Autonoma de San Luis Potosi, Mexico)

The general understanding of gelation processes is recognized as a major challenge in soft matter field. Particularly, attractive liquids that suffer a suddenly instantaneous isochoric quench an homogeneous state to thermodynamic instability could form a physical gel. Although, both experimental and simulation advances in understanding gelation phenomenon had led to build a general comprehension about physical gel properties and even had discussed the perform of novel materials as amorphous solids, there is no a clear theoretical approach to explain these class of ubiquitous materials. In recent work, however, the general theory referred to as the non-equilibrium self-consistent generalized Langevin equation (NESCGLE) theory, based on a non-equilibrium extension of Onsager's canonical theory of thermal fluctuations, was adequately adapted to describe memory effects, protocol-dependent preparation and irreversible aging processes associated with the glass and the gel transitions in attractive simple liquids. In particular, this theory was capable of predict a glass-glass transition line and propose a glass-gel line in a monocomponent attractive Yukawa simple fluid (HSAY) by arested spinodal decomposition when that system is instantaneously quenched inside spinodal region. In the present work, we extend this analisys in the context of a very specific model system, namely, let us consider an screened restricted primitive model (YRPM), represented as an electroneutral mixture of charged hard spheres embedded in a dielectric medium of uniform dielectric constant. Additionaly we show pertinent comparisons between our theoretical results and the gel formation in a mixture of equally-sized oppositely charged colloids both experimentally and by means of computer simulations.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-70] How to improve the ductility of CuZr BMGs based on cyclic pre-straining: MD simulations and mechanical testing

○Jonathan Amodeo[1], Oriane Baulin[1], Damien Fabregue[1], David Rodney[2]　(1.MATEIS, Univ. Lyon 1, France, 2.ILM, Univ. Lyon 1, France)

Bulk metallic glasses are currently used as technical materials(*e.g.*magnetic transmitters, golf clubs, brazing materials) for their high elastic and strength properties, significantly larger than their crystalline counterparts. However, their use is generally limited to elastic engineering applications due to their quasi-brittle behaviour caused by the early initiation of localized shear bands upon plastic deformation.

In this study, we used a combination of atomistic simulations and compressive mechanical testing to investigate the role of mechanical pre-cycling on the stress response and elementary deformation processes of a CuZr glass. In the experiments, unprestrained $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$(Vitreloy 105) samples show a plastic strain before failure of about 3% strain and a yield strength of about 1900 MPa. After applying a limited number of cycles with a maximum amplitude of 400 MPa (n=2, 4 or 6), the plastic strain increases up to 15%. It remains however in the same low range for higher pre-cycling amplitudes of 700 and 1200 MPa. MD simulations performed on $Cu_{64.5}Zr_{35.5}$thin films show that (i) unprestrained samples deform due to a local

shear banding process, (ii) pre-cycled samples are characterized by the occurrence of homogeneous deformation zones with a concentration that depends on the cyclic stress amplitude *i.e.*the lower the stress amplitude of the pre-cycles, the higher the proportion of homogeneous deformation. This emphasizes the existence of a critical stress under which the main shearing process of CuZr BMGs changes due to pre-cycling, reducing shear localization and the early occurrence of cracks. These results are confirmed by the statistical analysis of experimental vein patterns on fracture surfaces that show larger cusps ($\phi > 3500$ m^2), attributed to highly localized plastic events, only in the cases of samples pre-cycled at high stress amplitude.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-71] Modeling plastic deformation of amorphous solids from atomic scale mechanisms

$^\circ$Francesca Boioli[1], Tristan Albaret[2], David Rodney[2]　(1.LEM, CNRS-ONERA, Chatillon, France, France, 2.ILM, University of Lyon 1, France, France)

Amorphous solids are characterized by high strength and low ductility. The latter property is a consequence of the localization of the plastic deformation in shear bands, which leads to catastrophic failure. As a consequence, understanding the localization of plastic deformation and the formation of shear bands is of utmost importance. Generally, it has been accepted that local irreversible rearrangements of small clusters of atoms, Shear Transformations (STs), are the elementary processes involved in the deformation of amorphous systems and several mesoscale models based on STs have been proposed. Still the fundamental mechanisms underlying ST occurrence and shear bands formation are not yet clear. In this context, atomistic simulations can provide significant details that would otherwise be unavailable.

In this work we characterize shear transformations (STs) at the atomic scale in a model of amorphous silicon using a mapping on Eshelby inclusions. First, by using Nudged Elastic Band calculations, we measure the energy barrier against ST activation. Analyzing different paths leading to either an isolated ST or an avalanche, we show that the barrier is systematically controlled by the first ST with an activation volume equal to the effective volume of the ST at the activated state, which represents only a fraction of the complete ST volume. The activation volume is also found smaller for avalanches, presumably because of accumulated local damage. Furthermore, we investigate the dynamic process of ST formation, determining the characteristic time involved in the development of STs and the influence of the strain rate on the STs distribution and organization. This work provides essential information to build reliable mesoscale models of plasticity.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-72] Thermally Activated Creep and Constant Shear Rate Deformation in Amorphous Materials

$^\circ$Samy MERABIA[1], Julien LAM[2], François DETCHEVERRY[1]　(1.CNRS and Universite Lyon 1, France, 2.Université de Bruxelles, Belgium)

In this contribution, we shall discuss two issues related to the deformation of amorphous materials.
The first issue concerns transient creep also called Andrade creep, characterized by strain slowly increasing algebraically with time, a regime interrupted by fluidization and eventually steady flow. Here we characterize

creep and fluidization on the basis of a mesoscopic viscoplastic model that includes thermally activated yielding events and a broad distribution of energy barriers, which may be lowered under the effect of a local deformation. We relate the creep exponent observed before fluidization to the width of barrier distribution and to the specific form of stress redistribution following yielding events. We show that Andrade creep is accompanied by local strain hardening driven by stress redistribution and find that the fluidization time depends exponentially
on the applied stress, in qualitative agreement with experiments.
The second issue to be discussed concerns constant shear rate deformation of molecular glasses. Recent experiments on polymer glasses [2] have demonstrated enhanced mobility in the preyield regime accompanied by a narrowing of the distribution of segmental relaxation times. Yet, the mechanisms at play remain partially understood.
In the light of the mesoscopic model [1], we characterized the evolution of the distribution of energy barriers during constant shear rate deformation. Our simulation results account for enhanced mobility and the narrowing of the distribution of relaxation times. Good agreement is obtained with the experimental observations of Bending et al., without any adjustable parameter.
All the simulation results are interpreted in the light of a mean-field analysis, and should help in rationalizing the creep and deformation phenomenology as observed in disordered materials.

References

[1] S. Merabia and F. Detcheverry, Thermally activated creep and fluidization in flowing disordered materials, EPL (2016)

[2] B. Bending, K. Christison, J. Ricci, and M. D. Ediger, Measurement of Segmental Mobility during Constant Strain Rate
Deformation of a Poly(methyl methacrylate) Glass, Macromolecules (2014)

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-73] Numerical analysis of shrinkage process based on the experimental data

○Barbara Kucharczykova[1], Hana Simonova[2], Petr Frantik[2] （1.Brno University of Technology, Faculty of Civil Engineering, Institute of Building Testing, Czech Republic, 2.Brno University of Technology, Faculty of Civil Engineering, Institute of Structural Mechanics, Czech Republic）

The shrinkage process in cement based materials is still an actual problem of civil engineers and manufacturers of cement based composites, such as concrete, mortars, floor compounds etc. There are many standardized and non-standardized testing techniques which are used for estimation/determination of real value of shrinkage process during the whole time of material ageing, unfortunately the results are often inconsistent, especially because of different measurement equipment, dimensions of the test specimens and initial time of the start or evaluation of measurement. There are also incomplete experimental data of early-age volume changes, which can be used for numerical prediction models. The article focuses on the implementation of the experimentally obtained data to the shrinkage model B4 designed by research group of prof. Z. P. Bazant. The results show that especially the early-age part of real-measured shrinkage process does not correspond with the prediction model. In order to improve the correlation between the measured process and the prediction model, it is necessary to adjust the existing correction factors. The published

Poster Session | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[PO-O1] Poster Session 1

Symposium O
Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-74] Designing Lubricant Additives for Titanium Carbide Surface: First-principles and Molecular Dynamics Investigations

○Tasuku Onodera, Jun Nunoshige, Hiroshi Kanemoto （Research &Development Group, Hitachi, Ltd., Japan）

[P1-75] Crystal Growth Molecular Dynamics Simulation of alpha-Al_2O_3 Cutting Tools for Realizing Their Best Tribological Properties

○Shandan BAI[1], Hiroya Nakata[1], Jingxiang Xu[2], Nobuki Ozawa[2], Momoji Kubo[2] （1.KYOCERA Cop., Japan, 2.Tohoku Univ., Japan）

[P1-76] Atomistic modeling of polymer friction

○Robin Sam Vacher （SINTEF-NTNU, Norway）

[P1-77] A two degree-of-freedom extension to the Prandtl Tomlinson-model for friction strengthening in layered materials

○David Andersson[1,2], Astrid de Wijn[2] （1.Department of Physics, Stockholm University, Sweden, 2.Department of Mechanical and Industrial Engineering, Norwegian University of Science and Technology, Norway）

[P1-78] Analysis of Friction Characteristics of Steel Powders using Parallelized Discrete Element Method

○Naoki Yashiro[1,2], Kouya Oohira[2], Natsuko Sugimura[1], Hitoshi Washizu[1] （1.Graduate School of Simulation Studies, University of Hyogo, Japan, 2.Advanced Technology R&D Center, NTN Corporation, Japan）

[P1-80] Dynamics of Polymer Under Shear in Confinement Geometry

○Taiki Kawate[1], Soma Usui[1], Hiroaki Yoshida[2], Hitoshi Washizu[1] （1.Univ. of Hyogo, Japan, 2.Toyota Central R&D Labs, Japan）

[P1-81] Dynamics of a Polymer in Bulk Solution under Shear Flow

○Soma Usui[1], Taiki Kawate[1], Hiroaki Yoshida[2], Hitoshi Washizu[1] （1.Univ. of Hyogo, Japan, 2.Toyota Central R&D Labs., Japan）

[P1-82] Mechanochemistry induced atomic wear in chemical mechanical polishing processes

○Jialin Wen, Tianbao Ma, Xinchun Lu （Dept. of Mechanical Engineering, Tsinghua Univ., China）

[P1-83] Adsorption property of a fatty acid on iron surface with grain boundary

○Yuki Uchiyama, Yoshinori Shiihara, Ivan Lobzenko （Toyota Technological Institute, Japan）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-74] Designing Lubricant Additives for Titanium Carbide Surface: First-principles and Molecular Dynamics Investigations

○Tasuku Onodera, Jun Nunoshige, Hiroshi Kanemoto （Research &Development Group, Hitachi, Ltd., Japan）

In order to highly improving performance of industrial products such as automobile, the innovative technology should be strongly required, especially for the fields of surface and interface technology. Several problems on surface fractures, i.e. fatigue, wear, corrosion and erosion have been arisen in a metallic bearing or gear which typically work under the conditions of high temperature, extreme pressure and shear.

One of the technologies for reducing surface fractures is a hard coating on surface. For example, in the field of tribology, diamond-like carbon (DLC) coatings have been strenuously investigated so far. Covering surface with the film leads to low friction and low wear performances, contributing to extending a product lifetime and to reducing a maintenance work of products. However, under the lubrication by engine oil, DLC coating unexpectedly caused wear. This negative effect may be due to existence of organic molybdenum compounds in engine oil as a friction modifier. A novel additive compound has been developed by modifying adsorption property. This story tells us that tailor-made additives have to be required for own hard coating applied to shear parts.

Titanium-based hard coatings are also forcused for extending lifetime of products. Especially, titanium carbides show extremely high hardness and coincidently have anti-wear, anti-corrosion, and anti-oxidant properties. This material has been applied to cutting tools used at high temperature, extreme pressure and shear. Hence, titanium carbide seems to be a suitable surface coating material for extending lifetime.

In the present study reported here, for the purpose of extending lifetime of industrial products, a chemical composition of lubricant oil was optimized for titanium carbide coatings. An optimum molecular structure of additive compounds and its interaction with titanium carbide were theoretically investigated by using a method of density functional theory (DFT). An adsorption energy on TiC(100) was calculated for several additive compounds. The simulation results showed that the amide-type molecule showed high adsorption energy, suggesting that these additives would exhibit a good lubrication performance.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-75] Crystal Growth Molecular Dynamics Simulation of alpha-Al_2O_3 Cutting Tools for Realizing Their Best Tribological Properties

○Shandan BAI[1], Hiroya Nakata[1], Jingxiang Xu[2], Nobuki Ozawa[2], Momoji Kubo[2] （1.KYOCERA Cop., Japan, 2.Tohoku Univ., Japan）

Aluminum oxide (Al_2O_3) as coating materials has been used for cutting tools. It is widely applied on machining metals, because Al_2O_3 films show the tribological properties of high hardness and heat resistance. The Chemical Vapor Deposition (CVD) coating process for Al_2O_3 film is a very effective way to get its excellent tribological properties. $AlCl_3/CO_2/H_2$ gas system is used for the CVD process to obtain the Al_2O_3 coating. At the beginning step of the CVD process, the surface reactions affect the orientation of Al_2O_3 surface. However, the relationship between the surface reactions and Al_2O_3 orientation is difficult to be clarified by the

experiments. In this study, we investigate the details of surface reactions on the alpha-Al_2O_3 (0001) and (11-20) surfaces using computational simulation methods at the molecular scale. The alpha-Al_2O_3 take place through the hydrolysis reactions of $AlCl_3$ and H_2O. In order to clarify the surface reaction mechanism on alpha-Al_2O_3 (0001) and (11-20), we calculate the $AlCl_3$ molecule adsorption on these surfaces using the first principles calculation. GGA-PBE functional is employed. One $AlCl_3$ molecule is placed on various sites atom of alpha-Al_2O_3 (0001) and (11-20), and the system is optimized. The highest adsorption energies are -107.63 and -60.87 kcal/mol, respectively. The result indicates that $AlCl_3$ molecule easily adsorbed on the alpha-Al_2O_3 (0001) surface. After the optimization of the $AlCl_3$ molecule, the 6-coordinated Al and 4-coordinated Al of the $AlCl_3$ molecule are observed on the alpha-Al_2O_3 (0001) and (11-20) surfaces, respectively. It means that 6-coordinated Al shows the stable adsorption state. Furthermore, molecular dynamics simulation is performed to clarify the surface reaction dynamics on the alpha-Al_2O_3 (0001) and (11-20). The details will be discussed on our presentation.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-76] Atomistic modeling of polymer friction

○Robin Sam Vacher （SINTEF-NTNU, Norway）

Polymers are present in our daily life and we are using their tribological properties even without noticing it, walking with shoes is just one example. However, the theoretical understanding of the friction and wear of polymers is still lacking and therefore, development of novel low friction material of solid polymers can only be achieved by trial and error procedures including expensive testing. In this work, the focus is put on the influence of structural properties of solid polymers on the friction and wear. Molecular dynamic simulation is used to capture the crystallization process of PolyVinyl Alcohol (PVA). The coarse grain potential for PVA (CG-PVA) developed by Meyer and Muller-Plathe ("*Formation of chain-folded structures in supercooled polymer melts*", *J. Chem. Phys. 2001, 115, 7807*) has been used in order to drastically speed up the simulation. Depending on the cooling rate and the number of monomers per chain, the crystalline domains will have different structural properties (eg. crystallinity level). We create samples of polymers with different crystalline structure, and investigate numerically by simulating the effect of rubbing the surface with an AFM tip the relation between friction, wear, and crystallinity.

Keywords : molecular dynamic, polymers, friction and wear

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-77] A two degree-of-freedom extension to the Prandtl Tomlinson-model for friction strengthening in layered materials

○David Andersson[1,2], Astrid de Wijn[2] （1.Department of Physics, Stockholm University, Sweden, 2.Department of Mechanical and Industrial Engineering, Norwegian University of Science and Technology, Norway）

The Prandtl Tomlinson-model model has been exceedingly successful in describing the stick-slip friction response signal observed in atomic systems. However, recently it has been observed in both experiments and MD simulations that layered materials exhibit an initial period of friction strengthening, which is not found

within the Prandtl Tomlinson-model [1][2]. Furthermore, out-of-plane bending has been proposed as a driving mechanism for this friction strengthening regime [2][3]. In this paper we propose an extension to the Prandtl Tomlinson-model to account for friction strengthening. We show that this model successfully exhibits friction strengthening for a wide range of parameters, and that it is consistent with the out-of-plane bending hypothesis as well as previous experiments. Moreover, we make predictions as to the importance of commensurability for friction strengthening in these systems.

[1] Frictional Characteristics of Atomically Thin Sheets, Lee at al, Science 2010, doi: 10.1126/science.1184167
[2] The evolving quality of frictional contact with graphene, Li at al, Nature 2016, doi: 10.1038/nature20135
[3] Flexible graphene strengthens friction, de Wijn, Nature Communication 2016, doi:10.1038/539502a

---

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-78] Analysis of Friction Characteristics of Steel Powders using Parallelized Discrete Element Method

○Naoki Yashiro[1,2], Kouya Oohira[2], Natsuko Sugimura[1], Hitoshi Washizu[1]　(1.Graduate School of Simulation Studies, University of Hyogo, Japan, 2.Advanced Technology R&D Center, NTN Corporation, Japan）

In order to increase the application of sintered metal parts, high dense and less pores parts have to be produced with stable quality. Since sintered metal parts cannot be fully densified during sintering, it is essential to understand the steel powders' characteristics in detail and to densify them in the compaction step. Sufficient powder characteristic data, however, cannot be evaluated by conventional versatile methods, and there are few cases where actual powder characteristics are applied to large scale particle simulation. In this study, we evaluated flowability and friction characteristics of steel powders experimentally in detail, and applied them to parallelized discrete element method (DEM).

 We prepared steel powders with different kinds of solid lubricant and addition process. Their characteristics were evaluated by a method using a powder yield locus (PYL). The evaluation indexes are flowability (uniaxial collapse stress), inter-particle friction (internal friction angle), and friction between particles and mold (wall friction angle).

 The PYL method, which can measure flowabilities under various vertical loads, enabled collection of powder characteristics corresponding to the actual powder behavior in the mold. Furthermore, inter-particle and wall friction coefficients were calculated using the friction angles obtained from these experiments. These coefficients were higher than those which were applied in previous DEM simulation reports.

 We created a parallelized DEM code for powder behavior simulation, using FDPS (Framework for Developing Particle Simulator) developed by Iwasawa et al.[1] in order to develop into large scale parallelization in the future. FDPS is designed to reduce the calculation load at the time of region division and interaction calculation by constructing a tree structure. In this code, we evaluated flowabilities and friction characteristics by changing the model of the contact force between particles, especially the tangential component.

 In the conference presentation, we will show the flowabilities and the friction characteristics of steel powders, which are evaluated by this parallelized DEM code.

[1] Iwasawa *et al.*, *Publ. Astron. Soc. Japan*, 68, 54 (2016)

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-80] Dynamics of Polymer Under Shear in Confinement Geometry

○Taiki Kawate[1], Soma Usui[1], Hiroaki Yoshida[2], Hitoshi Washizu[1] （1.Univ. of Hyogo, Japan, 2.Toyota Central R&D Labs, Japan）

In lubricants, a small amount of polymer named viscosity index improver (VII) is used to control temperature dependence of viscosity. When VII is confined in small space, such as space between piston ring and cylinder bore in combustion engine, the dynamics of the solution changes due to the confinement. Here we simulate the dynamics of polymer under shear flow in confinement geometry. Polymer segment is modeled as sphere Brownian particle. The motion of the particle is tracked by the Langevin equation, whereas the Navier-Stokes equation governing the behavior of the base oil is analyzed by using the lattice Boltzmann method. The two equations are coupled through the friction between the particle and the fluid. The friction force is in proportion to the velocity of a particle relative to the host fluid, which is evaluated locally based on the velocity difference at the position of the point particle. The friction force acting on a particle is estimated by fitting the analytical solution or the flow around a Stokes-let to the flow field obtained numerically. The reaction force acts on the position of the particle, which realizes two-way coupling between the particle and fluid motions. The lattice Boltzmann method is employed for the flow simulation, which is compatible with massive parallel computing, and is easy to apply various types of boundary conditions. In order to describe confined system, periodical boundary is adopted in x, y (flow and transverse) direction, and non-slip boundary is adopted in bottom plate in z direction and moving wall is set in top plate of it. During the simulation, the polymer is pulled to upper layer where the shear field is large. To show the orientation of the molecule, order parameter is calculated. The orientation of the polymers changed to the direction of the external shear force.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-81] Dynamics of a Polymer in Bulk Solution under Shear Flow

○Soma Usui[1], Taiki Kawate[1], Hiroaki Yoshida[2], Hitoshi Washizu[1] （1.Univ. of Hyogo, Japan, 2.Toyota Central R&D Labs., Japan）

This study describes dynamics of viscosity index improver (VII) in bulk lubricants under shear flow. Small amount of polymer named VII is added in basis oil to control viscosity index (VI) which is a parameter to express temperature dependence of viscosity. Controlling VI is one of the commonly used methods to improve the fuel consumption of motor vehicles. Here we simulate the dynamics of polymer under shear flow in Bulk Solution. Polymer segment is modeled as sphere Brownian particle. The motion of the particle is tracked by the Langevin equation, whereas the Navier-Stokes equation governing the behavior of the base oil is analyzed by using the lattice Boltzmann method. The two equations are coupled through the friction between the particle and the fluid. The friction force is in proportion to the velocity of a particle relative to the host fluid, which is evaluated locally based on the velocity difference at the position of the point particle. The friction force acting on a particle is estimated by fitting the analytical solution or the flow around a

Stokes-let to the flow field obtained numerically. The reaction force acts on the position of the particle, which realizes two-way coupling between the particle and fluid motions. The lattice Boltzmann method is employed for the flow simulation, which is compatible with massive parallel computing, and is easy to apply various types of boundary conditions. In order to simulate the system, the computational domain has three-dimensions and Periodic boundary condition. External forces are introduced to form simple shear flow. The dynamics of polymer in shear flow is examined by using two computational methods.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-82] Mechanochemistry induced atomic wear in chemical mechanical polishing processes

○Jialin Wen, Tianbao Ma, Xinchun Lu　(Dept. of Mechanical Engineering, Tsinghua Univ., China)

Chemical mechanical polishing (CMP) is widely applied in the semiconductor industry to achieve ultra-high precision manufacturing of surfaces (such as Si and Cu), however, its mechanisms remain elusive because of interaction between chemical effects (such as the chemical reactions with the existence of H_2O_2 and glycine) and mechanical effects (such as the tribology process). By using molecular dynamics simulations based on the ReaxFF reactive force field, we have explored the CMP mechanisms at the atomic level and have revealed the importance of mechanochemistry induced atomic wear during the CMP processes.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-83] Adsorption property of a fatty acid on iron surface with grain boundary

○Yuki Uchiyama, Yoshinori Shiihara, Ivan Lobzenko　(Toyota Technological Institute, Japan)

Reducing the coefficient of boundary friction on steel surfaces is one of key technologies to improve the efficiency of machines such as automotive engines. It has been shown that the boundary friction on nanostructured steel surfaces in the sliding test using particular lubricant is smaller than the friction of normal steel surfaces [1]. This difference between the nanostructured and a normal surfaces lies in the density of the grain boundary as a surface defect. The surface defect can attract lubricant molecules and enhance lubricating film formation on metal surfaces. This can be one of the mechanism that induces the friction reduction on the nanosructured steel surface. In this work, using first principles calculations, the adsorptivity of a lubricant molecule, a fatty acid, on iron surfaces has been studied.The chemical adsorption of fatty acids is expected to be enhanced at the site near the crystal grain boundary which may have high chemical activity. Adsorption energy calculations were preformed for acetic acids as the simplest fatty acids. Adsorbability of a Fe (110) surface with symmetrical tilt Σ3 (111)grain boundarywas compared to clean Fe(100), (110) and (111) surfaces. As a result, we found that the molecule can adsorb on the particular site on grain boundary more strongly than that on Fe surfaces without grain boundary. [1]

Yoshikazu Todaka, Kenichi Toda, Motohiro Horii, Minoru Umemoto, Tetsu-to-Hagané 101, 10 (2015)

Plenary Talk | Plenary Talk

[PL3] Plenary Talk 3

Plasticity in crystals and glasses: from the atoms up
Chair: William Curtin(EPFL, Switzerland)
Tue. Oct 30, 2018 8:30 AM - 9:20 AM Room1
David Rodney

[PL3] Plenary Talk 3

○David Rodney （Institut Lumière Matière, University of Lyon, France）

(Tue. Oct 30, 2018 8:30 AM - 9:20 AM Room1)

[PL3] Plenary Talk 3

Plasticity in crystals and glasses: from the atoms up

○David Rodney （Institut Lumière Matière, University of Lyon, France）

Plasticity in crystalline metals is probably the most classical multiscale process, around which the Multiscale Materials Modeling community first organized at the end of the 1990s. Plasticity in glasses shares many similarities with their crystalline counterparts. In particular, in both cases, plasticity starts at the atomic scale, involving the motion of dislocation cores in crystals and shear transformation zones in glasses. In both cases also, elementary plastic events interact and organize at the mesoscale through elasticity. There are however specific challenges. In crystals, there is currently a need for quantitative and predictive data, which often require to start with a first principles description of atomic interactions. By way of contrast, in glasses, we are still in need of phenomenological information, which can be addressed with less computationally intensive models. But we are then faced with the high complexity of the configuration space and the energy landscape of disordered materials, making it difficult to characterize and predict simply even the most elementary plastic events. The aim of this talk will be to illustrate the challenges, recent progress and opportunities in the field of multiscale modeling of plasticity and to discuss through selected examples the links between atomic and mesoscopic descriptions of plasticity.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C3] Symposium C-3

Chair: Francois Willaime(DEN-Departement des Materiaux pour le Nucleaire, CEA, Universite Paris-Saclay, France)

Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room1

[SY-C3] Quantifying the effect of hydrogen on dislocation dynamics in microcrystals: A three-dimensional discrete dislocation dynamics study

Yejun Gu, ○Jaafar A. El-Awady　(Johns Hopkins University, United States of America)

[SY-C3] Discrete dislocation plasticity modelling of hydrogen dislocation interactions in micro-cantilevers

○Haiyang Yu[1], Alan Cocks[2], Ed Tarleton[1]　(1.Dept. of Materials, Univ. of Oxford, UK, 2.Dept. of Engineering, Univ. of Oxford, UK)

[SY-C3] Dislocation climb models from atomistic scheme to dislocation dynamics

○Yang Xiang[1], Xiaohua Niu[2]　(1.Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong, 2.Department of Mathematics, Jimei University, China)

[SY-C3] Investigation of the Hall-Petch Effect with DD Simulation

○Maoyuan Jiang[1,2], Benoit Devincre[2], Ghiath Monnet[1]　(1.EDF - R&D, Les Renardieres, France, 2.Laboratoire d'Etude des Microstructures, CNRS/ONERA, France)

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room1)

[SY-C3] Quantifying the effect of hydrogen on dislocation dynamics in microcrystals: A three-dimensional discrete dislocation dynamics study

Invited

Yejun Gu, ○Jaafar A. El-Awady   (Johns Hopkins University, United States of America)

We present a new framework to quantify the effect of hydrogen on dislocation plasticity using large scale three-dimensional (3D) discrete dislocation dynamics (DDD) simulations. In this model, the first order elastic interaction energy associated with the hydrogen-induced volume change is accounted for. The three-dimensional stress tensor induced by hydrogen concentration, which is in equilibrium with respect to the dislocation stress field, is derived using the Eshelby inclusion model, while the hydrogen bulk diffusion is treated as a continuum process. This newly developed framework is utilized to quantify the effect of hydrogen on the different aspects of dislocation-mediated plasticity in Ni single crystal microcrystals. The combined effect of hydrogen concentration, crystal size, and dislocation density is quantified. Finally, the effects of pipe diffusion is also rationalized from comparisons with experimental results.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room1)

[SY-C3] Discrete dislocation plasticity modelling of hydrogen dislocation interactions in micro-cantilevers

○Haiyang Yu[1], Alan Cocks[2], Ed Tarleton[1]   (1.Dept. of Materials, Univ. of Oxford, UK, 2.Dept. of Engineering, Univ. of Oxford, UK)

One of the most widely accepted theories for hydrogen embrittlement is the hydrogen enhanced localized plasticity (HELP) mechanism which claims hydrogen enhances dislocation activity locally. Experimental evidence for this mechanism has been reported across different scales. Simulations however are mainly limited to the atomistic scale, and continuum scale. Direct simulation of hydrogen dislocation interactions in micromechanical tests is rarely simulated, due to the fact that this scale is beyond the computational capacity of most atomistic calculations and beyond the resolution of most continuum approaches. Discrete dislocation plasticity (DDP) is an ideal technique to bridge the gap in multiscale modelling of hydrogen embrittlement. Recently, a framework which incorporates hydrogen effects in a discrete dislocation simulation was derived by Gu and El-Awady [1] enabling direct investigation of hydrogen dislocation interactions at the microscale. We have implemented this formulation in a new code called *EasyDD,* a GPU accelerated version of *DDLab* coupled with FEM, and performed virtual micromechanical tests with mixed boundary conditions. We have simulated the behaviour of hydrogen charged micro-cantilevers and included the hydrogen induced tractions on the free surfaces. Hydrogen is observed to shield dislocation mutual interactions and to enhance dislocation generation, the combination of these effects leads to global softening and local stress concentrations promoting failure; consistent with the HELP mechanism. To the best of our knowledge, this work is the first to reveal hydrogen dislocation interactions at the discrete dislocation scale in finite volumes, acting as an essential bridge in multiscale modelling.

[1] Gu, Y., &El-Awady, J. A. (2018). Journal of the Mechanics and Physics of Solids, 112, 491-507.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room1)

[SY-C3] Dislocation climb models from atomistic scheme to dislocation dynamics

○Yang Xiang[1], Xiaohua Niu[2] （1.Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong, 2.Department of Mathematics, Jimei University, China）

We develop a mesoscopic dislocation dynamics model for vacancy-assisted dislocation climb by upscalings from a stochastic model on the atomistic scale. Our models incorporate microscopic mechanisms of (i) bulk diffusion of vacancies, (ii) vacancy exchange dynamics between bulk and dislocation core, (iii) vacancy pipe diffusion along the dislocation core, and (iv) vacancy attachment-detachment kinetics at jogs leading to the motion of jogs. Our mesoscopic model consists of the vacancy bulk diffusion equation and a dislocation climb velocity formula. The effects of these microscopic mechanisms are incorporated by a Robin boundary condition near the dislocations for the bulk diffusion equation and a new contribution in the dislocation climb velocity due to vacancy pipe diffusion driven by the stress variation along the dislocation. Our climb formulation is able to quantitatively describe the self-climb of prismatic loops at low temperatures when the bulk diffusion is negligible. Simulations performed show evolution, translation, coalescence of prismatic loops by self-climb that agree with the experimental observations.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room1)

[SY-C3] Investigation of the Hall-Petch Effect with DD Simulation

○Maoyuan Jiang[1,2], Benoit Devincre[2], Ghiath Monnet[1] （1.EDF - R&D, Les Renardieres, France, 2.Laboratoire d'Etude des Microstructures, CNRS/ONERA, France）

Dislocation Dynamics (DD) simulation is used to identify the elementary mechanisms controlling the Hall-Petch (HP) effect on the dislocation scale. The influence of grain size is explored by considering simple periodic polycrystalline aggregates made of grains with cube, plate or needle shapes. We show that the HP effect is globally well reproduced with DD simulations. The HP constant is found to be a function of the grain orientations and shapes. A model is proposed to quantify the influence of the grain morphology. The simulated HP effect is justified by the existence of a backstress inside the grains that emerges from strain incompatibility between grains in a deformed polycrystal. As theoretically expected, Geometrically Necessary Dislocations (GND) are found to accumulate at grain boundaries to accommodate the distortion field discontinuities. By virtue of the Nye's tensor, the above property can be directly tested and quantified in DD simulations. For the simplest simulation geometry, the calculated backstress is compared with theoretical predictions. Those results suggest a new strategy for the prediction of the grain size effect in crystal plasticity models.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C4] Symposium C-4

Chair: Dan Mordehai(Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel, Israel)
Tue. Oct 30, 2018 11:15 AM - 12:15 PM Room1

[SY-C4] **Hydrogen consequences on cyclic behaviour of <001> nickel single crystals : a multi-scale approach.**

○xavier Feaugas, Guillaume Hachet, Arnaud Metsue, abdelali Oudriss （université de la rochelle, France）

[SY-C4] **Atomistic and continuum approaches to analyse precipitation hardening in metallic alloys**

Gustavo Esteban-Manzanares[1,2,3], Rodrigo Santos[1,2], Anxin Ma[1], Ioannis Papadimitriou[1], Enrique Martínez[3], Laurent Capolungo[3], Javier Segurado[1,2], ○Javier LLorca[1,2] （1.IMDEA Materials Institute, Spain, 2.Polytechnic University of Madrid, Spain, 3.Los Alamos National Laboratory, United States of America）

[SY-C4] **Dislocation-precipitate interaction in Al-Mg-Si alloys**

○Inga Gudem Ringdalen[1], Sigurd Wenner[1], Jaime Marian[2] （1.Dept. of Materials and Nanotechnology, SINTEF, Norway, 2.Dept. of Material Science and Engineering, UCLA, United States of America）

(Tue. Oct 30, 2018 11:15 AM - 12:15 PM Room1)

[SY-C4] Hydrogen consequences on cyclic behaviour of <001> nickel single crystals : a multi-scale approach.

Invited

○xavier Feaugas, Guillaume Hachet, Arnaud Metsue, abdelali Oudriss （université de la rochelle, France）

A multi-scale study on the influence of hydrogen on cyclically strained <001> oriented nickel single crystals is conducted in order to understand the impact of the solute on the microstructure and the fatigue properties of nickel single crystal. At macroscopic scale, uniaxial cyclic tests are performed to evaluate the impact of pre-charged hydrogen on the work hardening of the material. Then, at microscopic scale, a mechanical database is provided and associated with the dislocation features, which are explored by transmission electronic microscopy (TEM) observations and correlated with the mechanical behaviour of nickel single crystal with hydrogen. In addition, at atomistic scale, molecular dynamics simulations are carried out to quantify the influence of hydrogen on the dipole sizes and the dislocation organisations, which are partially connected to the elastic properties of nickel. Therefore, we have finally performed a comprehensive study on the impact of hydrogen on the elastic properties of nickel single crystal using a theoretical formalism based on Density Functional Theory and uniaxial tensile tests on <001> oriented nickel single crystals with different concentrations of hydrogen.

This multi-scale approach allows to question the main effect of hydrogen on cyclic plasticity mechanisms. The impact of hydrogen on cyclic stress-strain curves highlights a softening behaviour for <001> multi slips orientation in a similar way as previously related for single slip orientation. This result is firstly discussed in term of dislocation organisations, dipole sizes and distribution but also internal stresses states. Hydrogen impacts the density and the distribution of dislocations and consequently, modifies the internal stress state. Moreover, according to TEM observations, hydrogen ingress promotes the formation of vacancy clusters, in agreement with the super-abundant vacancies (SAV) model. The main consequence of this result is a decrease of the elastic properties of the material, which depends mainly on the formation of the defect induced by the incorporation of hydrogen than a direct effect of the solute itself.

(Tue. Oct 30, 2018 11:15 AM - 12:15 PM Room1)

[SY-C4] Atomistic and continuum approaches to analyse precipitation hardening in metallic alloys

Gustavo Esteban-Manzanares[1,2,3], Rodrigo Santos[1,2], Anxin Ma[1], Ioannis Papadimitriou[1], Enrique Martínez[3], Laurent Capolungo[3], Javier Segurado[1,2], ○Javier LLorca[1,2] （1.IMDEA Materials Institute, Spain, 2.Polytechnic University of Madrid, Spain, 3.Los Alamos National Laboratory, United States of America）

Precipitation hardening is one of the most efficient mechanisms to increase the yield strength of metallic alloys but accurate quantitative models for this phenomenon are still lacking. Two different approaches, based on atomistic simulations and discrete dislocation dynamics, are presented to address this problem.

Atomistic simulations, in combination with the transition state theory, were used to determine the interaction between Guinier-Preston zones and dislocations in an Al-Cu alloy and between $Mg_{17}Al_{12}$ precipitates and basal dislocations in an Mg-Al alloy. The rate at which dislocations sheared the precipitates (determined by means of molecular dynamics) was controlled by the activation Gibbs free energy, in agreement with the

postulates of the transition state theory. However, harmonic TST does not hold for this interaction. In addition, the activation enthalpy energy and the activation volume were determined and an estimation of the initial shear flow stress as a function of temperature was carried out from the thermodynamic data provided by the atomistic simulations.

In the case of large precipitates that cannot be sheared by dislocations (such as q' precipitates in Al-Cu alloy), the dislocations overcome the precipitates by the formation of an Orowan loop. The mechanisms of dislocation/precipitate interaction were studied by means of discrete dislocation dynamics using the discrete-continuous method in combination with a fast Fourier transform solver to compute the mechanical fields. Simulations took into account the effect of precipitate shape, orientation and volume fraction as well the elastic mismatch between the matrix and the precipitate, the stress-free transformation strain around the precipitate and the dislocation character as well as dislocation cross-slip. It was found that the influence of the precipitate aspect ratio and orientation were reasonably well captured by the simple Orowan model in the absence of the stress-free transformation strain. Nevertheless, the introduction of the stress-free transformation strain led to dramatic changes in the dislocation/precipitate interaction and in the critical resolved shear stress to overcome the precipitate, particularly in the case of precipitates with small aspect ratio.

(Tue. Oct 30, 2018 11:15 AM - 12:15 PM Room1)

[SY-C4] Dislocation-precipitate interaction in Al-Mg-Si alloys

○Inga Gudem Ringdalen[1], Sigurd Wenner[1], Jaime Marian[2] （1.Dept. of Materials and Nanotechnology, SINTEF, Norway, 2.Dept. of Material Science and Engineering, UCLA, United States of America）

Partial ageing of commercial Al-Mg-Si aluminum results in microstructures characterized by needle-shaped Si/Mg-rich precipitates. These precipitates belong to the non-equilibrium β" phase and are coherent with the fcc Al lattice, despite of which they can cause considerable hardening. We have investigated the interaction between these β" precipitates and dislocations using a unique combination of modeling and experimental feedback. Dislocation-precipitate interactions including precipitate stress fields are simulated using discrete dislocation dynamics. The displacement fields due to the precipitates are captured by expressions that satisfy elastic equilibrium and are fitted to high-resolution electron microscopy measurements. The stress fields are derived from the displacements assuming isotropic elasticity, and used to study the strength of individual precipitates to dislocation glide as a function of precipitate size, orientation, and dislocation character and length. The dislocation dynamics results are then used to parameterize a probabilistic analysis model to study the difference between the bulk material and the precipitate free zones along the grain boundaries of these alloys.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E3] Symposium E-3

Chairs: Benoit Devincre(LEM, CNRS-ONERA, France), Alejandro Strachan(Purdue University, United States of America)

Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room2

[SY-E3] 3D mesoscopic study of the stability of three-dimensional short cracks in FCC metals using the Discrete-Continuous Model

Laurent Korzeczek[1], Riccardo Gatti[1], Arjen Roos[2], ○Benoit Devincre[1] （1.LEM, CNRS-ONERA, France, 2.Safran Tech, France）

[SY-E3] Role of cracks, voids and interfaces in hot spot formation and initiation of energetic materials

Michael Sakano[1], Chunyu Li[1], Nicolo Grilli[2], Brenden Hamilton[1], Camilo Duarte[2], Marisol Koslowski[2], ○Alejandro Strachan[1] （1.School of Materials Engineering, Purdue University, United States of America, 2.School of Mechanical Engineering, Purdue University, United States of America）

[SY-E3] Precipitation hardening effects on extension twinning in magnesium

○Haidong Fan[1], Jaafar El-Awady[2], Dierk Raabe[3] （1.Sichuan University, China, 2.The Johns Hopkins University, United States of America, 3.Max-Planck-Institut für Eisenforschung GmbH, Germany）

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room2)

[SY-E3] 3D mesoscopic study of the stability of three-dimensional short cracks in FCC metals using the Discrete-Continuous Model

Invited

Laurent Korzeczek[1], Riccardo Gatti[1], Arjen Roos[2], ○Benoit Devincre[1] （1.LEM, CNRS-ONERA, France, 2.Safran Tech, France）

The erratic behaviour of short cracks propagation under low cyclic loading in ductile metals is commonly attributed to a complex interplay between stabilisation mechanisms that occur at the mescopic scale. Among these mechanisms, the interaction with the existing dislocation microstructure play a major role. The dislocation microstructure is source of plastic deformation and heat transfer that reduce the specimen stored elastic energy, screen the crack field due to its self generated stress field or change the crack geometry through blunting mechanisms. For the first time, these mechanisms are investigated with 3D-DD simulations using the Discrete- Continuous Model, modelling three different crack orientations under monotonic traction loading promoting mode I crack opening. Surprisingly, screening and blunting effects do not seem to have a key role on mode I crack stabilisation. Rather, the capability of the specimen to deform plastically without strong forest hardening is found to be the leading mechanism. Additional investigations of two different size effects confirm those results and show the minor contribution of a polarised dislocations density and the associated kinematic hardening on crack stabilisation.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room2)

[SY-E3] Role of cracks, voids and interfaces in hot spot formation and initiation of energetic materials

Invited

Michael Sakano[1], Chunyu Li[1], Nicolo Grilli[2], Brenden Hamilton[1], Camilo Duarte[2], Marisol Koslowski[2], ○ Alejandro Strachan[1] （1.School of Materials Engineering, Purdue University, United States of America, 2.School of Mechanical Engineering, Purdue University, United States of America）

The chemical initiation of high-energy (HE) materials following mechanical insults requires the excitation of chemical bonds with lengths of a few angstroms and sub-picosecond vibrational periods. This would be a nearly impossible task were it not for: i) the materials' microstructure that localizes the input energy into hotspots, and ii) the equilibration of inter- and intra-molecular degrees of freedom that transfers input energy to the high-frequency bond vibrations responsible for chemistry. Thus, a predictive understanding of the response of HE to strong mechanical insults requires identifying, characterizing and modeling coupled processes at the microstructural level (interfacial friction, cracks, void collapse), crystal level (dislocations and shear bands) and the molecular/electronic level (inter- and intra-molecular energy transfer and chemical reactions).

While our large-scale molecular dynamics (MD) simulations recently provided an atomic picture of the formation of a steady deflagration wave following shock loading of a defective HE crystal, such simulations cannot capture the complex microstructure of the materials of interest nor the size of the hot spots of interest in real applications. Thus, we developed a multiscale model that combines large-scale reactive and non-reactive MD simulations with a continuum model capable of describing dynamical loading, plastic deformation, fracture and friction, together with thermal transport and chemistry. The MD simulations

provide insight and parameters to characterize energy localization as shock waves interact with several pre-existing defects, including cracks and voids as well as interfaces. In addition, reactive MD simulations are used to characterize thermal transport and develop chemical kinetics models. These results inform the continuum model that is used to predict energy localization in microstructurally complex systems of plastic bonded energetic formulations. These simulations enable us to characterize the relative potency of various microstructural features to general hot spots that can result in sustained chemistry. Both the atomistic and continuum simulations are validated against experiments capable of capturing the physics of interest at scales matching those of the simulations.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room2)

[SY-E3] Precipitation hardening effects on extension twinning in magnesium

○Haidong Fan[1], Jaafar El-Awady[2], Dierk Raabe[3]   (1.Sichuan University, China, 2.The Johns Hopkins University, United States of America, 3.Max-Planck-Institut für Eisenforschung GmbH, Germany）

Precipitation is an efficient method to strengthen metallic materials. While precipitation hardening effects on dislocation slip have been studied extensively in the past, the influence of precipitates on twinning mediated plasticity and the development of corresponding hardening models that account for twin-precipitate interactions have received less attention. The interaction of {10-12} extension twin boundaries (TBs) in pure magnesium with precipitates of plate-, sphere- and rod-like shapes is studied using molecular dynamics (MD) simulations. We find that TBs that engulf precipitates are absorbed by the precipitate-matrix interfaces, and the precipitates are neither twinned nor sheared but deform elastically leading to their rotation. TBs can pass small precipitates (length ≈20 nm) and remain intact. In contrast when TBs are interacting with large precipitates (length ≈50 nm), basal dislocations or stacking faults nucleate from the interfaces, causing local plastic relaxation. The stress field around a plate-like precipitate as calculated in the MD simulations suggests that a strong back-stress is imposed on the TBs. We then coarse grain these mechanisms into an analytical mean field model of precipitation hardening on twinning in magnesium alloys, which is based on the energy conservation during the TB-precipitate interaction. The model is in good agreement with the current MD simulations and published experimental observations. The hardening model shows that spherical precipitates have the strongest hardening effect on twinning, basal and prismatic plate-like precipitates have a medium effect while rod-like precipitates exert the weakest influence. We also find that most types of precipitates show a stronger hardening effect on twinning mediated plasticity than on basal dislocation slip. Finally, prismatic plate-like precipitates are predicted to have reasonable hardening effects on both twinning and basal slip. These results can help guiding the development of magnesium alloys with enhanced strength and ductility.

[SY-E4] Symposium E-4

Chairs: Haifeng Song(Institute of Applied Physics and Computational Mathematics, China), Chenghua Sun(Swinburne University of Technology, Australia)
Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room2

[SY-E4] High-performance first-principles calculation software development with applications to the zirconium

○Haifeng Song[1,2], Xingyu Gao[1,2], Jun Fang[1,2], Yafan Zhao[2], Han Wang[2], Deye Lin[2]　（1.Institute of Applied Physics and Computational Mathematics, China, 2.CAEP Software Center for High Performance Numerical Simulation, China）

[SY-E4] Catalyst design for ammonia synthesis of ammonia

○Chenghua Sun　（Swinburne University of Technology, Australia）

[SY-E4] A solid-solution structure model for multi-component alloys

○Xingyu Gao[1,2], Fuyang Tian[3], Yafan Zhao[2], Deye Lin[2], Haifeng Song[1,2]　（1.Institute of Applied Physics and Computational Mathematics, China, 2.CAEP Software Center for High Performance Numerical Simulation, China, 3.University of Science and Technology, China）

[SY-E4] First-princples prediction of plastic deformation modes in alloys

○Song Lu, Levente Vitos　（KTH Royal Institute of Technology, Sweden）

[SY-E4] The local-orbital construction of strongly correlated electrons based on the PAW method

○Yu Liu[1,2], Xingyu Gao[1,2], Jianzhou Zhao[3], Haifeng Song[1,2]　（1.Institute of Applied Physics and Computational Mathematics, China, 2.CAEP Software Center for High Performance Numerical Simulation, China, 3.Southwest University of Science and Technology, China）

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room2)

[SY-E4] High-performance first-principles calculation software development with applications to the zirconium

○Haifeng Song[1,2], Xingyu Gao[1,2], Jun Fang[1,2], Yafan Zhao[2], Han Wang[2], Deye Lin[2]　(1.Institute of Applied Physics and Computational Mathematics, China, 2.CAEP Software Center for High Performance Numerical Simulation, China)

With the development of high-performance computer, first-principles calculation becomes to be a feasible way in many nuclear material research fields. In this talk, we will give two examples to demonstrate it. Firstly, we develop two high-performance oriented methods for wave functions in solving the Kohn-Sham equations: a more parallel scalable FFT and optimal extrapolation order for the initial guess at next time step. Armed with adaptive time stepping, we estimate the threshold displacement energy of zirconium by large-scale first-principles calculations. We utilize CESSP to realize the calculations of about 100 tasks on the Tianhe-2 supercomputer in 3 months, where each task is the first-principles molecular dynamic simulation of 9600 valence electrons and 1 picosecond. Compared to classical molecular dynamic simulations, we arrive at the results closest to most recent experiment. Secondly, we have combined a novel crystal structure search method based on the basin hopping algorithm into our first-principles code. Several improvements were implemented, including a symmetry structure generation algorithm based on the crystal space groups, a structure adjustment method based on a virtual spring-force to adjust unreasonably structures. The method is also highly paralleled to make full use of the computing resources. We have applied the method into the structure searching of Zr hydrides (ZrHx, x= 0.5, 1.0, 1.5, 2.0). All experimentally observed Zr hydrides are reproduced, and several new structures were found. The dynamic and thermodynamic stability of these Zr hydrides will also be discussed.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room2)

[SY-E4] Catalyst design for ammonia synthesis of ammonia

○Chenghua Sun　(Swinburne University of Technology, Australia)

Ammonia (NH3) is a critical chemical widely used in modern agriculture and chemical engineering. Currently, it is based on the Haber-Bosch process at high temperature and high pressure. This computational work is to design novel catalysts to achieve ammonia synthesis at room temperature. Single-atom catalyst and defects of low-dimensional materials will be particularly considered. As revealed by first pricinple calculations, Mo-based various catalysts are promising for this applications.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room2)

[SY-E4] A solid-solution structure model for multi-component alloys

○Xingyu Gao[1,2], Fuyang Tian[3], Yafan Zhao[2], Deye Lin[2], Haifeng Song[1,2]　(1.Institute of Applied Physics and Computational Mathematics, China, 2.CAEP Software Center for High Performance Numerical Simulation, China, 3.University of Science and Technology, China)

First-principles calculations have been widely used to predict and design the properties of metallic alloys. However, it is still a challenge to generate *ab initio* suitable structure for multi-component random alloys in a

finite supercell. In this talk, we propose a novel solid-solution structure model to mimic the similar local atomic environment (SLAE) of the random alloys. In the SLAE model, local solid-solution environment such as the random disorder, partial disorder, and short-range order can be calibrated via the standard deviation of the pair distribution function and three-body correlation function. Taking the typical high-entropy alloy CoCrFeMnNi, medium-entropy alloy CoCrNi, and continued solid-solution binary alloy TaW as test cases, we evalueate the SLAE models by comparing between the *ab initio* predicted phase stability and some available experiments.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room2)

[SY-E4] First-princples prediction of plastic deformation modes in alloys

○Song Lu, Levente Vitos （KTH Royal Institute of Technology, Sweden）

First-principles alloy theory is used to establish the gamma-surface of alloys. Then we put forward a transparent model solely based on first principles simulations for mapping the deformation modes in alloys. The model bridges intrinsic energy barriers and different deformation mechanisms and resolves the complexity of the observed orientation-dependent deformation mechanisms in alloys. Examples of studies are given in austenitic stainless steels and polysynthetic twinned gamma-TiAl alloys.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room2)

[SY-E4] The local-orbital construction of strongly correlated electrons based on the PAW method

○Yu Liu[1,2], Xingyu Gao[1,2], Jianzhou Zhao[3], Haifeng Song[1,2] （1.Institute of Applied Physics and Computational Mathematics, China, 2.CAEP Software Center for High Performance Numerical Simulation, China, 3.Southwest University of Science and Technology, China）

The effects of electron strong correlation, spin-orbit coupling and multi-configuration bring out challenges in the first principle studies of some nuclear materials and rare-earth materials. Density functional theory (DFT), however, cannot properly describe their electronic structures. For this reason, people have developed Hubbard model based post-DFT method (DFT+X) to correct the strong correlation effect. The coupler that connects the DFT and X still requires more intensive research. In this report, we will present the most recent progress on the DFT+X coupler and its realization in the projector augmented wave (PAW) method under the infrastructure of CESSP code. Firstly, there are three major schemes, namely P0, P1 and P2, to construct the local orbitals of the strong correlated electrons. Prof. Haule from Rutgers University demonstrate the advantages of P2 scheme under the linear augmented plane wave (LAPW) method. However, we are going to show that under the PAW method, P2 is more appropriate for systems with d electrons while P1 is more appropriate for systems with f electrons. Secondly, we realize the correction of spin-orbit coupling and crystal field splitting to the local orbitals, which improves the convergence and accuracy of the DFT+X calculations. We further test our code in the typical strong correlated materials $SrVO_3$ and Ce.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F3] Symposium F-3

Chair: Carl Krill(Institute of Micro and Nanomaterials, Ulm University, Germany)
Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room3

[SY-F3] Biomineralization in molluscan shells: From ideal to hierarchical grain growth

○Dana Zoellner, Igor Zlotnikov （B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany）

[SY-F3] Mesoscale modeling of cement: texture, mechanics and durability

○Katerina Ioannidou[1,2,3], Emanuela Del Gado[4], Franz J. Ulm[1], Roland J.-M. Pellenq[1,2,3] （1.Dept. of Civil and Enviromental Engineering, Massachusetts Institute of Technology, United States of America, 2.MultiScale Material Science for Energy and Environment, Massachusetts Institute of Technology-CNRS/MIT/AMU Joint Lab. at MIT, United States of America, 3.MIT Energy Initiative, United States of America, 4.Dept. of Physics and Institute for Soft Matter Synthesis and Metrology, Georgetown Univ., United States of America）

[SY-F3] Actuation in Metal-Polymer Nanocomposites: Chemoelectromechanical Coupling on Interfaces

○Jana Wilmers, Swantje Bargmann （Chair of Solid Mechanics, University of Wuppertal , Germany）

[SY-F3] Mechanics of Cilia Beating - A Relationship Between Metachronal Wavelength and Fluid Flow Rate

○Jon Hall, Nigel Clarke （The University of Sheffield, UK）

[SY-F3] Biomineralization in molluscan shells: From ideal to hierarchical grain growth

Invited

○Dana Zoellner, Igor Zlotnikov （B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany）

The microstructure of grain networks as they can be found in many polycrystalline materials like metals, alloys, and bionic composite structures have an immense impact on their physical properties. Any change in the structure in terms of the size and shape of the grains leads to a change in the properties. Hence, understanding structural changes is of enormous importance for materials development, processing, and application.

In the present work, we investigate the evolution of the prismatic ultrastructures in molluscan shells in form of a comparative study bringing together large numerical and experimental data sets of molluscan shells from different families. To that aim, a framework has been developed for a quantitative study of the process of shell morphogenesis. The method is based on Monte Carlo Potts model simulations of grain boundary motion that, classically, were developed to study coarsening of polycrystalline metals. By employing this approach, we fully reconstruct the growth process of the different molluscan shells: While the prismatic ultrastructure of *Atrina vexillum* is an archetype of ideal grain growth fulfilling the classical growth theories, shells like *Atrina rigida* and *Pinna nobilis* show retarded growth comparable with triple junction controlled grain growth in nanocrystalline metals, and, finally, the mollusc *Pinctada nigra* is characterized by a two-level hierarchical prismatic microstructure, which can be represented in the Potts model by introducing sub-grain boundaries.

The proposed framework is a fundamental approach to study the structural regulation during biomineralization.

[SY-F3] Mesoscale modeling of cement: texture, mechanics and durability

○Katerina Ioannidou[1,2,3], Emanuela Del Gado[4], Franz J. Ulm[1], Roland J.-M. Pellenq[1,2,3] （1.Dept. of Civil and Enviromental Engineering, Massachusetts Institute of Technology, United States of America, 2.MultiScale Material Science for Energy and Environment, Massachusetts Institute of Technology-CNRS/MIT/AMU Joint Lab. at MIT, United States of America, 3.MIT Energy Initiative, United States of America, 4.Dept. of Physics and Institute for Soft Matter Synthesis and Metrology, Georgetown Univ., United States of America）

Cement is a multiscale porous material, widely produced, more than any other synthetic material on Earth. In this talk, I will present a multiscale bottom-up approach for cement and specifically for calcium-silicate hydrate (C-S-H) that is the most abundant phase of cement. During cement hydration C-S-H nano-scale particles precipitate in the pore solution and form a cohesive gel that is the main binding agent in cement and concrete, crucial for the strength and the long-term evolution of the material. Even more than the molecular structure of C-S-H particles, the C-S-H mesoscale texture over hundreds of nanometers plays a crucial role for material properties. We use a statistical physics framework for aggregating nanoparticles and numerical simulations to obtain a first, to our knowledge, quantitative model for such a complex amorphous material. Our approach is based on precipitation of colloidal particles interacting with effective potentials

associated to the chemical environment. The effective potential can be calculated from atomistic models of C-S-H and are corroborated by experiments. This multiscale informed modelling approach generates realistic micron scale textures in terms of pore size distributions and solid volume fractions and allows to calculate mechanical properties. The extensive comparison with experiments ranging from small-angle neutron scattering, EM imaging, adsorption/desorption of N_2, and water to nano-indentation provides new fundamental insights into the microscopic origin of the cement properties measured. Our results provide a quantitative insight into how the heterogeneities developed during the early stages of hydration persist in the structure of C-S-H and impact the mechanical performance of the hardened cement paste. Moreover, this approach allowed to address durability issues on cement such as freeze-thaw and alkali-silica reaction damage leading to the formation of cracks and fractures.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room3)

[SY-F3] Actuation in Metal-Polymer Nanocomposites: Chemoelectromechanical Coupling on Interfaces

○Jana Wilmers, Swantje Bargmann （Chair of Solid Mechanics, University of Wuppertal , Germany）

Nanoporous metals have recently garnered interest as actuator materials because of their unique microstructure. The characteristic interconnected pore network and resulting high interface-to-volume ratio allows them to react sensitively to electric signals. By coating the metal backbone with ionically-activated polymers, increased actuation strains are achieved while still retaining the metal's superior mechanical properties.

In understanding and modelling the chemoelectromechanically coupled behaviour of such nanocomposite actuators, one has to account for charge carrier transport and coupled effects in the polymer as well as effects arising from build-up of charges in and at the metal-electrolyte interface. We present an interface-extended continuum model that couples large deformations with electrostatics and charge carrier transport for the bulk and the interface. The developed framework utilises the concept of interface stresses to model the different coupling mechanisms occurring on the interface, that is, interface charging and electroadsorption, in addition to the coupled behaviour in the bulk material arising from mass transport in the pore space. This allows to study the different phenomena and their interaction with each other, giving insight into the underlying physical mechanisms. Simulations reveal that both, the nanocomposite's structure and the ions' mobilities, strongly affect the actuator's response, providing the means to tailor the actuator's behaviour to specialised applications.

References
[1] Wilmers, McBride, Bargmann, Interface Elasticity Effects in Polymer-Filled Nanoporous Metals, JMPS, 163-177, 2017.
[2] Wilmers, Bargmann, Functionalisation of Metal-Polymer-Nanocomposites: Chemoelectromechanical Coupling and Charge Carrier Transport, EML, accepted, 2018
[3] McBride, Javili, Steinmann, Bargmann, Geometrically nonlinear continuum thermomechanics with surface energies coupled to diffusion, JMPS 59, 2116-2133, 2011
[4] Soyarslan, Bargmann, Pradas, Weissmüller, 3d stochastic bicontinuous microstructures: generation, topology and elasticity, Acta Mater., 326-340, 2018
[5] Bargmann et al., Generation of 3d representative volume elements (RVEs) for heterogeneous materials: a

review, Prog. Mater. Sci., accepted, 2018

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room3)

[SY-F3] Mechanics of Cilia Beating - A Relationship Between Metachronal Wavelength and Fluid Flow Rate

○Jon Hall, Nigel Clarke (The University of Sheffield, UK)

Cilia driven fluid flow is a complex fluid mechanical system that is dependent on several physical parameters, including mucus rheology, cilia density, and beat coordination. We have developed a computational model of an array of beating cilia using a hybrid immersed boundary lattice Boltzmann algorithm in order to study the how the flow behaviour is affected by these key parameters. Our main focus is on quantifying the relationship between metachronal wavelength and the rate of fluid flow which we find exhibits two maxima at particular wavelengths. We attempt to rationalise this observation by considering how the metachronal wavelength relates to the volume of fluid that is accelerated by each cilium during an active stroke, and thus the momentum of the fluid region as a whole. We also observe that the rate of fluid flow decreases significantly when cilia in close proximity are synchronised, and that this behaviour becomes more dominant as cilia density increases.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F4] Symposium F-4

Chair: Dana Zoellner(B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany)
Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room3

[SY-F4] Showdown! Pitting computer simulations against time-resolved experimental measurements of grain growth in 3D

Mingyan Wang[1], Nan Wang[2], Jules Dake[1], Søren Schmidt[3], ○Carl Krill[1] （1.Institute of Micro and Nanomaterials, Ulm University, Germany, 2.Dept. of Physics, McGill University, Canada, 3.Dept. of Physics, Technical University of Denmark, Denmark）

[SY-F4] Coarsening and grain-growth in an SOFC-anode under surface and grain boundary self-diffusion: A Multiphase-field approach

○Paul Hoffrogge[1], Daniel Schneider[1,2], Britta Nestler[1,2], Patricia Haremski[2,3], Matthias Wieler[3], Piero Lupetin[3] （1.Karlsruhe University of Applied Sciences, Germany, 2.Karlsruhe Institute of Technology, Germany, 3.Robert Bosch GmbH, Germany）

[SY-F4] Solidification Simulation in Additive Manufacturing Process of Ti-Alloy by ICME approach

○Yusuke SHIMONO, Mototeru Oba, Sukeharu Nomoto （Itochu Techno-Solutions Corp., Japan）

[SY-F4] Phase Field Model of Microstructural Evolution in Metal Alloy for Designing Mechanical Property

Wooju Lee, ○Dongchoul Kim （Dept. of Mechanical Engineering, Sogang Univ., Korea）

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room3)

[SY-F4] Showdown! Pitting computer simulations against time-resolved experimental measurements of grain growth in 3D

Invited

Mingyan Wang[1], Nan Wang[2], Jules Dake[1], Søren Schmidt[3], ○Carl Krill[1]　（1.Institute of Micro and Nanomaterials, Ulm University, Germany, 2.Dept. of Physics, McGill University, Canada, 3.Dept. of Physics, Technical University of Denmark, Denmark）

Thanks to dramatic improvements in computational speed, it is now feasible to simulate the coarsening of 3D polycrystalline microstructures containing tens of thousands of grains. Indeed, such calculations have become so powerful that the simulation cells rival—and, in some cases, exceed—sample volumes that can be probed experimentally! But do the computational algorithms underlying these simulations properly capture the physics of microstructural evolution as it occurs in real materials? We have followed a two-pronged strategy to address this question, using (i) three-dimensional x-ray diffraction (3DXRD) microscopy to map the 3D network of grain boundaries in a polycrystalline specimen over the course of stepwise isothermal annealing treatments, and (ii) a phase field model to simulate 3D grain growth starting from the same initial configuration as in experiment. A grain-by-grain showdown between tactic (i) and tactic (ii) offers fresh insights into the phenomenon of grain growth—gleaned not only from discrepancies between measured and simulated size trajectories and grain shapes, but also from instances of agreement.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room3)

[SY-F4] Coarsening and grain-growth in an SOFC-anode under surface and grain boundary self-diffusion: A Multiphase-field approach

○Paul Hoffrogge[1], Daniel Schneider[1,2], Britta Nestler[1,2], Patricia Haremski[2,3], Matthias Wieler[3], Piero Lupetin[3]　（1.Karlsruhe University of Applied Sciences, Germany, 2.Karlsruhe Institute of Technology, Germany, 3.Robert Bosch GmbH, Germany）

Solide oxide fuel cells (SOFCs) convert chemical energy stored in form of a gaseous fuel into electrical energy. Due to the typically high energy-conversion efficiencies achieved, SOFCs are a very promising technology to reduce carbon emission. One of the critical parameters to be economically competitive is the lifetime of an SOFC device. In order to improve the SOFCs long-term performance it is essential to obtain a better understanding of the underlying physical processes leading to a decrease in SOFC performance during operation.

The present study focuses on the evolution of a polycrystalline and porous 3D microstructure of an Ni-YSZ (yttria-stabilized zirconia) SOFC-anode during isothermal coarsening. We employ a multiphase-field model which incorporates self-diffusion of nickel by a grand-chemical formulation to simulate grain-boundary and surface diffusion coupled with simultaneous growth of the inherent Ni-grains. We validate the model by 2D thermal-grooving simulations under surface-diffusion and by a quantitative comparison with analytical results. A comprehensive study of several input parameters such as grain-size on the coarsening behavior of the SOFC-anode is performed. The detailed investigation includes an analysis of the microstructure as a function of particle size, tortuosity and triple-phase boundary length.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room3)

[SY-F4] Solidification Simulation in Additive Manufacturing Process of Ti-Alloy by ICME approach

○Yusuke SHIMONO, Mototeru Oba, Sukeharu Nomoto （Itochu Techno-Solutions Corp., Japan）

Multi-phase field method (MPFM) coupled with thermodynamics database of calculation of phase diagrams (CALPHAD) is a powerful tool for simulating solidification microstructure evolutions in engineering casting processes. As MPFM is based on local (quasi-)equilibrium assumption in solidification theory, applying MPFM to solidification of additive manufacturing (AM) processes is considered to be difficult because of extremely large cooling rate and temperature gradient.

On the other hand, some researchers have recently reported experimental observations of the columnar-to-equiaxed transition in the solidification of the AM processes. These observations suggested that the local (quasi-)equilibrium assumption can be applied to the solidification of the AM processes.

In this study, AM processes of Ti-alloys are simulated. By using temperature distributions obtained by thermal analyses in finite element method simulations, solidification microstructures are calculated by MPFM. It is confirmed that the microstructures have the columnar-to-equiaxed transitions. The results are summarized in a solidification map for the AM process conditions.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room3)

[SY-F4] Phase Field Model of Microstructural Evolution in Metal Alloy for Designing Mechanical Property

Wooju Lee, ○Dongchoul Kim （Dept. of Mechanical Engineering, Sogang Univ., Korea）

Precipitation hardening has been widely employed to improve the mechanical properties of metal alloys. During the precipitation hardening, the supersaturated alloying elements in a solid solution phase form secondary precipitate particles. To design the mechanical properties of metal alloy, the relationship between precipitation conditions and morphology of microstructure of secondary phase should be fully understood. The morphology of microstructure in metal alloy is determined by the composition of the alloy and their intermetallic compounds. Here, we investigate the the morphological evolution of microstructures in metal alloy during precipitation. To simulate the temporal evolution of microstructures, a phase field model is employed. By simulations, the effects of anisotropic interfacial energy and lattice mismatch on the morphology of the microstructure are investigated.

Symposium | M. Time- and History-Dependent Material Properties

[SY-M3] Symposium M-3

Chair: Thomas Franosch(University of Innsbruck, Austria)
Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room4

[SY-M3] Heterogeneous thermal properties in a glass from molecular dynamics calculations

○Jean-Louis BARRAT （Univ. Grenoble Alpes, France)

[SY-M3] Structural-dynamical phase transition in the phase space of histories of a polydisperse hard sphere liquid

○Matteo Campo[1,2], Thomas Speck[1] （1.Johannes Gutenberg University Mainz, Germany, Germany, 2.Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany, Germany)

[SY-M3] Time- and History-dependent Structure and Morphology of van-der-Waals Liquids forming Physical Gels and Porous Glasses

○Magdaleno Medina-Noyola, Leticia Lopez-Flores, Jose Manuel Olais-Govea, Benigno Zepeda-Lopez （Instituto de Fisica (Laboratorio Nacional de Ingenieria de la Materia Fuera de Equilibrio), Universidad Autonoma de San Luis Potosi, Mexico)

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room4)

[SY-M3] Heterogeneous thermal properties in a glass from molecular dynamics calculations

Invited
○Jean-Louis BARRAT （Univ. Grenoble Alpes, France）

It is well known that elastic properties of amorphous systems are heterogeneous, leading to peculiarities in vibrational spectra and thermal properties. In this work, we investigate the heterogeneity in thermoelastic properties, and more precisely in the thermal expansion coefficient, in a model metallic glass. We find heterogeneities that are similar - in terms of length scales - to those in elastic constants. It has been suggested that such heterogeneities could be the reason for "cryogenic rejuvenation" processes observed under thermal cycling in several experiments. We investigate this hypothesis by comparing the values of the local yield stresses with the stresses generated by heterogeneities in thermal dilation.

This work was performed in collaboration with Dr Baoshuang Zhang (University Grenoble Alpes and Beijing Computational Science Research Center).

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room4)

[SY-M3] Structural-dynamical phase transition in the phase space of histories of a polydisperse hard sphere liquid

○Matteo Campo[1,2], Thomas Speck[1] （1.Johannes Gutenberg University Mainz, Germany, Germany, 2.Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany, Germany）

The glass transition is a longstanding problem in condensed matter physics. One of the main points of discussion is whether it is possible to characterize the glass transition using structural arguments, together with dynamical ones. In fact, it is known that supercooled liquids do not show major changes in their global (two-point) structure upon cooling while displaying a dramatic change in their dynamical properties. Recent insights have brought attention to the local structure instead. For a wide range of model glassformers, it is possible to identify certain geometric motifs that minimize the local free energy. These motifs are referred to as Locally Favourite Structures (LFS) and are found to be growing in correlation with the slowing-down of the dynamics. Using tools from large deviation theory and statistical mechanics of histories, it was recently possible to identify for some model glassformers a structural-dynamical transition between the supercooled liquid state and a state composed of trajectories rich in LFS with very slow dynamics. We present here a study of this transition for a fundamental atomistic model glassformer, the polydisperse hard sphere liquid. We reveal the first-order nature of the transition by employing finite size scaling on the length of the histories of the system, and a phase diagram is constructed as a function of the density versus the local order, and the density versus the degree of mobility of the system.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room4)

[SY-M3] Time- and History-dependent Structure and Morphology of van-der-Waals Liquids forming Physical Gels and Porous Glasses

○Magdaleno Medina-Noyola, Leticia Lopez-Flores, Jose Manuel Olais-Govea, Benigno Zepeda-Lopez
（Instituto de Fisica (Laboratorio Nacional de Ingenieria de la Materia Fuera de Equilibrio), Universidad Autonoma de San Luis Potosi, Mexico）

In spite of its relevance, no universal principle seems to exist that explains how Boltzmann's postulate $S = k_B \ln W$ operates for non-equilibrium conditions, predicting, for example, the transformation of liquids into non-equilibrium amorphous solids (glasses, gels, etc.) in terms of molecular interactions. Here, however, we present evidences that the missing fundamental principle to understand non-equilibrium states of matter is provided by Onsager's description of irreversible processes and thermal fluctuations, adequately combined with Boltzmann's postulate and extended to genuine non-equilibrium conditions [J. Phys.: Cond. Matter 21: 504103 (2009)]. Formatted as the non-equilibrium self-consistent generalized Langevin equation (NE-SCGLE) theory of irreversible processes in liquids [Phys. Rev. E 82, 061503 (2010)], this approach has been shown to provide a fundamental tool for the understanding of the most essential fingerprints of the transformation of liquids into amorphous solids, such as their aging kinetics or their dependence on the protocol of fabrication [J. Chem Phys. 143, 174505 (2015); Phys. Rev. E 96, 022608 (2017)]. In this work we focus on the NE-SCGLE-predicted scenario of the structural and morphological transformation of van-der-Waals (or "Lennard-Jones--like") simple fluids into hard-sphere glasses at hight densities and temperatures, into physica gels at intermediate densities and low temperatures, into porous glasses at intermediate densities and even lower teperatures, and into cluster-cluster aggregates al very low densities and temperatures. As an illustration, we present the visualization of the non-equilibrium development and arrest of sponge-like structures by arrested spinodal decomposition. The comparison of the theoretical predictions (based on a simple specific model system), with simulation and experimental data measured on similar but more complex materials, suggests the universality of the predicted scenari.

[SY-M4] Symposium M-4

Chair: Leticia Lopez Flores(University of San Luis Potosi, Mexiko)
Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room4

[SY-M4] Mechanical behavior and emerging morphologies in active matter

○Ignacio Pagonabarraga （CECAM, EPFL, Switzerland）

[SY-M4] Time dependent interaction between intruders in granular media

○Hisao Hayakawa [1], Takahiro Tanabe[2] （1.Yukawa Institute for Theoretical Physics, Kyoto Univeristy, Japan, 2.Graduate School of Advanced Mathematical Sciences, Meiji University, Japan）

[SY-M4] Hystory-dependent shear jamming of granular materials under oscillatory shear

○Michio Otsuki[1], Hisao Hayakawa[2] （1.Graduate School of Engineering Science, Osaka Univ., Japan, 2.Yukawa Institute for Theoretical Physics, Kyoto Univ., Japan）

[SY-M4] Structural predictor for nonlinear sheared dynamics in simple glass-forming liquids

○Trond S. Ingebrigtsen, Hajime Tanaka （University of Tokyo, Japan）

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room4)

[SY-M4] Mechanical behavior and emerging morphologies in active matter

Invited

○Ignacio Pagonabarraga （CECAM, EPFL, Switzerland）

Flocks of birds, schools of fishes, or bacterial colonies constitute examples of living systems that coordinate their motion. In all these systems their constituent elements generate motion due to energy consumption and can exchange information or react sensitively to chemical cues in order to move together or to react collectively to external signals. Artificial systems, such as nanorobots, exploit the heterogeneous compositions of their surface to displace as a result of the heterogeneous chemical processes that take place in the presence of appropriate chemical substances.

All these systems are intrinsically out of equilibrium in the absence of any external driving. Their collective properties result as a balance between their direct interactions and the indirect coupling to the medium in which they displace, and a self-consistent dynamical approach is required to analyze their evolution. The mechanical balance that determines the states they develop spontaneously make these systems very versatile and have a natural tendency to for large scale aggregates.

I will consider simple statistical models to address fundamental questions associated to these systems and will analyze the implications the generic self-propulsion has in the emergence of structures in suspensions of model self-propelled particles. I will discuss the potential of schematic models to address fundamental questions, such as the connection of the effective phase diagram and pressure with effective equilibrium concepts. I will analyze the collective behavior of these emerging morphologues and their response to external forcings, as well as how we can understand the resistance to deformation in this type of systems.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room4)

[SY-M4] Time dependent interaction between intruders in granular media

○Hisao Hayakawa [1], Takahiro Tanabe[2] （1.Yukawa Institute for Theoretical Physics, Kyoto Univeristy, Japan, 2.Graduate School of Advanced Mathematical Sciences, Meiji University, Japan）

In this presentation, we will discuss the interactions between two intruders in two dimensional granular environment from DEM (discrete element method) simulation and phenomenological theory. Through the DEM simulation, we found that the interaction is repulsive if there exists a steady flow or the amplitude of an external oscillation is small enough, but the interaction becomes attractive if the amplitude of the oscillation is large. Such an attractive interaction is known as depletion effect or Casimir effect nearly equilibrium environments, but it is interesting that both attractive and repulsive interactions can be observed in out-of-equilibrium systems such as granular media. We also develop a phenomenology based on an analogous equation to Boltzmann-Enskog equation. The phenomelogy can explain the drag force acting on one intruder in granular environment and the repulsive interaction between two intruders under a steady flow, but is still far away to describe the attractive interaction between two intruders in highly oscillated situations.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room4)

[SY-M4] Hystory-dependent shear jamming of granular materials under oscillatory shear

○Michio Otsuki[1], Hisao Hayakawa[2]　(1.Graduate School of Engineering Science, Osaka Univ., Japan, 2.Yukawa Institute for Theoretical Physics, Kyoto Univ., Japan)

Granular materials have rigidity above a critical density [1]. Such rigidity transition, known as the jamming transition, has attracted much attention among researchers in these days. It is well-known that frictionless grains under small strain exhibit a continuous transition of the shear modulus G, while recent studies have revealed that G of frictional grains with harmonic repulsive interaction discontinuously emerges at the critical density [2].
In this talk, we present our recent numerical results on the shear modulus of frictional grains under oscillatory shear. It is confirmed that the shear modulus depends on the amplitude of the initial oscillatory shear before the mesurament. Even at densities below the transition point, where isotropic jamming occurs without shear, the initial oscillatory shear can induce the finite shear modulus. This behavior is consistent with a transition known as shear jamming [3]. We also discuss the evolution of the force chain network under the initial oscillatory shear and the conection with the discontinuous shear thickenning.

[1] M. van Hecke, J. Phys.: Condens. Matter 22, 033101 (2009).
[2] M. Otsuki and H. Hayakawa, Phys. Rev. E 95, 062902 (2017).
[3] D. Bi, J. Zhang, B. Chakraborty, and R. Behringer, Nature (London)
480, 355 (2011).

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room4)

[SY-M4] Structural predictor for nonlinear sheared dynamics in simple glass-forming liquids

○Trond S. Ingebrigtsen, Hajime Tanaka　(University of Tokyo, Japan)

Glass-forming liquids subjected to sufficiently strong shear universally exhibit striking nonlinear behavior; for example, a power-law decrease of the viscosity with increasing shear rate. This phenomenon has attracted considerable attention over the years from both fundamental and applicational viewpoints [1, 2, 3, 4]. However,
the out-of-equilibrium and nonlinear nature of sheared fluids have made theoretical understanding of this phenomenon very challenging and thus slower to progress. We find here [5] that the structural relaxation time as a function of the two-body excess entropy, calculated for the extensional axis of the shear flow, collapses onto
the corresponding equilibrium curve for a wide range of pair potentials ranging from harsh repulsive to soft and finite. This two-body excess entropy collapse provides a powerful approach to predicting the dynamics of nonequilibrium liquids from their equilibrium counterparts. Furthermore, the two-body excess entropy scaling suggests that sheared dynamics is controlled purely by the liquid structure captured in the form of the two-body excess entropy along the extensional direction, shedding light on the perplexing mechanism behind shear thinning.

References

[1] D. J. Evans, H. J. M. Hanley, and S. Hess. Phys Today 37, 26 (1984).

[2] R. Yamamoto, and A. Onuki. Phys. Rev. E 58, 3515 (1998).

[3] V. Lubchenko. Proc. Natl. Acad. Sci. U.S.A. 106, 11506 (2009).

[4] X. Cheng, J. H. McCoy, J. N. Israelachvili, and I. Cohen. Science 333, 1276 (2011).

[5] T. S. Ingebrigtsen, and H. Tanaka. Proc. Natl. Acad. Sci. U.S.A. 115, 87 (2018).

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O3] Symposium O-3

Chairs: Momoji Kubo(Tohoku University, Japan), Michael Moseler(Fraunhofer Institute for Mechanics of Materials IWM, Germany)
Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room5

[SY-O3] Scale Dependence of Friction: How Elasticity Destroys Superlubricity
Joseph Monti[1], Lars Pastewka[2], ○Mark Owen Robbins[1] （1.Dept. of Physics and Astronomy, Johns Hopkins University, United States of America, 2.University of Freiburg, Germany）

[SY-O3] Coarse-Grain Simulations of Polymer Solutions with Hydrodynamics and Long-range Interactions
○Hitoshi Washizu[1,2], Hiroaki Yoshida[3], Soma Usui[1], Taiki Kawate[1] （1.Univ. Hyogo, Japan, 2.Kyoto Univ., Japan, 3.Toyota Central R&D Labs., Inc., Japan）

[SY-O3] **A Multi-Scale Approach for the Design of Novel Lubricants**
○Georgios Bletsos[1], Konstantinos Gkagkas[2], Varvara Asouti[1], Evaggelos Papoutsis-Kiachagias[1], Daniele Savio[3], Kyriakos C Giannakoglou[1] （1.National Technical University of Athens, Greece, 2.Toyota Motor Europe NV/SA, Belgium, 3.Fraunhofer Institute for Mechanics of Materials IWM, Germany）

[SY-O3] Impact of ionic liquid ordering on their triborheological properties
○Konstantinos Gkagkas[1], Andras Vernes[2,3] （1.Advanced Material Research Division, Toyota Motor Europe NV/SA, Belgium, 2.AC2T research GmbH, Austria, 3.Institute of Applied Physics, TU Wien, Austria）

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room5)

[SY-O3] Scale Dependence of Friction: How Elasticity Destroys Superlubricity

Invited

Joseph Monti[1], Lars Pastewka[2], ○Mark Owen Robbins[1]　(1.Dept. of Physics and Astronomy, Johns Hopkins University, United States of America, 2.University of Freiburg, Germany)

Friction in single-asperity contacts is studied as a function of contact radius a, substrate stiffness G, atomic structure, adhesive strength and adsorbed layers. Friction between bare, rigid surfaces can be obtained by a simple sum over atomic forces. When surfaces are aligned and have the same periodicity, the forces add in phase and the friction force F rises linearly with area A. When the two surfaces are misaligned or disordered, so that there is no common periodicity, forces add out of phase and $F \sim A^x$ with x less than or equal to $1/2$. This is known as structural superubricity and implies that friction vanishes in the limit of large contact sizes. Most surfaces do not share a common period but friction is almost always observed at macroscopic scales. We use an efficient Greens function technique to study contacts with dimensions of micrometers while resolving atomistic interactions at the surface. A new formulation that includes dynamic effects explicitly will be described. For small tips and high loads the contact area follows predictions for contact of rigid surfaces, $x=1$ for identical aligned surfaces, $x=1/2$ for random surfaces and $x=1/4$ for incommensurate crystals. Elasticity becomes important when a exceeds the core width b_{core} of interfacial dislocations. For $a>b_{core}$ parts of the contact can advance independently. The friction for identical aligned surfaces drops as a power law and then saturates at the Peierls stress for edge dislocations. The friction on incommensurate and disordered surfaces saturates at nearly the same value. Thus for all geometries $x=1$ in large contacts. While this means that elasticity destroys superlubricity, the friction between bare surfaces drops exponentially with the ratio of substrate stiffness to local interfacial shear stress. In contrast, when adsorbed layers are included between surfaces, all geometries have $x=1$ with a large prefactor.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room5)

[SY-O3] Coarse-Grain Simulations of Polymer Solutions with Hydrodynamics and Long-range Interactions

○Hitoshi Washizu[1,2], Hiroaki Yoshida[3], Soma Usui[1], Taiki Kawate[1]　(1.Univ. Hyogo, Japan, 2.Kyoto Univ., Japan, 3.Toyota Central R&D Labs., Inc., Japan)

Polymer solution is used as lubricant in Tribological purpose. Viscosity index improver is used to normalize temperature dependence of viscosity of the lubrication oil. Here we show our numerical simulation approach to investigate the dynamics of polymer solution. The numerical scheme is for simulating the dynamics of suspensions of Brownian particles, coupling molecular motion treated by Langevin equation and hydro-dynamics treated by lattice Boltzmann method.

In order to simulate bulk properties of polymers under shear, we apply periodic external field so that to make shear field. The external force is applied to the fluid dynamics part. Polymer is dragged to the region where the shear force is strongest, and changes its shape. The structure change is described by the radius of gyration which decreases with time.

In order to describe confined system, non-slip boundary is adopted in bottom line and moving wall is set in top line. During the simulation, the polymer are pull to upper layer where the shear field is large. To show the orientation of the molecule, order parameter is calculated. Due to the effect of external field, the orientation

of the polymers changed to the direction of the shear force.

In above simulation, the chemical properties of the polymers are not discussed. We simulate the equilibrium structure of polymer using point dipole interactions. We use Monte Carlo Brownian Dynamics method for time integration.The radius of gyration of non-polar polymers are same as analytical theory. The structure of the polymers with functional groups is calculated. The interaction between functional groups make tight structure in low temperature and show high viscosity index than non-polar polymers. The polar polymer shows strong initial distribution dependence.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room5)

[SY-O3] A Multi-Scale Approach for the Design of Novel Lubricants

○Georgios Bletsos[1], Konstantinos Gkagkas[2], Varvara Asouti[1], Evaggelos Papoutsis-Kiachagias[1], Daniele Savio[3], Kyriakos C Giannakoglou[1]　(1.National Technical University of Athens, Greece, 2.Toyota Motor Europe NV/SA, Belgium, 3.Fraunhofer Institute for Mechanics of Materials IWM, Germany)

Friction accounts for ˜15% of fuel energy losses in conventional vehicles. A deeper understanding of lubrication mechanisms in engineering systems and how to accurately model them is therefore necessary. Atomistic simulations can provide fundamental insights in the fluid behaviour under extreme contact conditions, at a high computational cost. On the other hand, continuum methods, while capable of efficiently solving macroscopic problems, cannot resolve features and flow patterns at the nanometer scale, due to the breakdown of the continuum assumption [1]. In this work, we employ a multi-scale approach that combines continuum and particle-based descriptions for simulating hydrodynamic lubrication systems, while seeking ideal designs of virtual lubricants that maximise load carrying capacity and minimize friction.

Inspired by computational [2] and experimental [3] studies of ionic liquids as lubricants, we emulate their layering behaviour and near-wall solidification [2] on the continuum domain by introducing an inhomogeneous viscosity field in the Navier-Stokes equations. Using an Evolutionary Algorithm, optimal viscosity profiles leading to the minimisation of specific friction are identified. By doing so, a potential improvement in friction performance up to 65% was found for a converging hydrodynamic slider.

The study is then extended to nano-hydrodynamic lubrication using Coarse Grain Molecular Dynamics simulations, which can help in selecting specific molecule typologies featuring the aforementioned viscosity variations - and thus the potential for significant friction reduction - under severely loaded contact conditions.

1. I. Cosden and J. Lukes, Comput. Phys. Commun. 184 (8) (2013)

2. K. Gkagkas, V. Ponnuchamy, M. Dašić, and I. Stanković, Tribol. Int. 113 (2016)

3. J. Qu, D. Bansal, B. Yu, J. Howe, H. Luo, S. Dai, H. Li, P.J. Blau, B. Bunting, G. Mordukhovich and D. Smolenski, ACS Appl. Mater. Interfaces 4 (2) (2012)

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room5)

[SY-O3] Impact of ionic liquid ordering on their triborheological properties

○Konstantinos Gkagkas[1], Andras Vernes[2,3]　(1.Advanced Material Research Division, Toyota Motor Europe NV/SA, Belgium, 2.AC2T research GmbH, Austria, 3.Institute of Applied Physics, TU Wien, Austria）

The development of novel lubrication concepts is a multi-scale challenge that requires the correlation of nano- and meso-scale features, such as molecule structure and their ordering, with macro-scale properties such as observed friction. Ionic Liquids (ILs) are interesting lubricants that are shown to have a positive impact on friction reduction. A feature that plays an important role in their behaviour is the Coulombic interaction between ions leading to layering in the transverse direction to the sliding and to a near-wall solidification, as seen both experimentally [1] and numerically [2]. At the same time, in-plane crystalline structures are also formed [3, 4, 5].

In this contribution, we quantify the impact of the internal structure on the triborheological properties of ILs. More precisely, both structure factors and bond-orientational order parameters will be calculated on coarse grain MD models of ILs in order to describe the ion ordering and formation of crystalline structures under bulk and confined conditions. Then an attempt will be made to correlate the detected ordering with internal (ion shapes and sizes), external (wall structure, pressure and shearing velocity) and constitutive (e.g., coefficient of friction) system parameters. Through such quantification, we expect an improved understanding of the underlying physico-chemical mechanisms, guiding us towards the design of optimised tribological systems.

1. A. M. Smith, K. R. J. Lovelock, N. N. Gosvami, P. Licence, A. Dolan, T. Welton, and S. Perkin, J. Phys. Chem. Lett. 4, 378 (2013).
2. K. Gkagkas, and V. Ponnuchamy, Model. Simul. Mater. Sci. Eng. 25 (6), 064004 (2017).
3. K. Gkagkas, V. Ponnuchamy, M. Dašić, and I. Stanković, Tribol. Int. 113, 83 (2016).
4. R. Capozza, A. Vanossi, A. Benassi and E. Tosatti, J. Chem. Phys. 142, 064707 (2015).
5. O. Fajardo, F. Bresme, A. Kornyshev, and M. Urbakh, Sci. Reports 5, 7689 (2015).

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O4] Symposium O-4

Chairs: Aiichiro Nakano(Univ. of Southern California, United States of America), Shandan Bai(KYOCERA Corp., Japan)
Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room5

[SY-O4] Molecular simulation to better understand soot-detergent interactions in engine oils
　　○Sophie LOEHLE[1], Elias Gebremedhn[2], Michael Mazarin[1], Stephan Steinman[2], Carine Michel[2]
　　（1.Total M&S, France, 2.ENS Lyon, France）

[SY-O4] A Molecular Dynamics Study on the Wear Mechanisms of Hydrogenated Diamond-like Carbon
　　○Yang Wang[1], Jingxiang Xu[1], Yusuke Ootani[1], Yuji Higuchi[1], Nobuki Ozawa[1], Koshi Adachi[2], Momoji Kubo[1]　（1.Institute for Materials Research, Tohoku University, Japan, 2.Department of Mechanical System Engineering, Graduate School of Engineering, Tohoku University, Japan）

[SY-O4] Effect of Tribochemical Reactions on Diamond-like Carbon and Wear under Water Lubrication: A Molecular Dynamics Simulation Investigation
　　○Jing Zhang[1], Yang Wang[1], Jingxiang Xu[1], Yusuke Ootani[1], Nobuki Ozawa[1], Koshi Adachi[2], Momoji Kubo[1]　（1.Inst. for Materials Research, Tohoku Univ., Japan, 2.Dept. of Mechanical Systems Engineering, Tohoku Univ., Japan）

[SY-O4] Formation Mechanism of Tribofilm of Silicon Carbide under Water Lubrication: Molecular Dynamics Simulations
　　○Fumiya Nakamura, Yang Wang, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Koshi Adachi, Momoji Kubo　（Tohoku Univ., Japan）

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room5)

[SY-O4] Molecular simulation to better understand soot-detergent interactions in engine oils

Invited

○Sophie LOEHLE[1], Elias Gebremedhn[2], Michael Mazarin[1], Stephan Steinman[2], Carine Michel[2] （1.Total M&S, France, 2.ENS Lyon, France）

In the engine, soot is formed as a result of incomplete combustion. Some of the formed soot is absorbed into the lubricating oil film present until a certain level is reached in which it precipitates. This lead not only to the increase of the lubricant's viscosity but also it adsorbs on the metallic surface, thus increasing engine wear. Most automotive enhancement additives contain, among other additives, detergents which help control the agglomeration and deposition of soot particles and other corrosive contaminants. A typical detergent molecule features a head part with constituting polar functional groups and a long hydrocarbon tail group [1]. The common perception is that the detergents do the job as dispersants and/or through formation of protective coating on steel surfaces. However, little is known about the complex physicochemical and structural details of the soot-detergent interfaces, and it seems that such details are too difficult to capture using conventional experimental techniques alone. In this respect, molecular modeling can fill the gap by providing atomistic level understandings on soot-detergent interactions and interfacial structural features.Finding an atomistic representation of the soot is the crucial step in modeling soot-detergent interactions. First, we show how we developed reliable soot model using experimental data [2-4], we employed a deterministic structural elucidation method to automatically generate representative soot structures. Following, we show how we assessed physisorption energies between the soot models and some polar detergent-head groups using the latest semi-empirical PM7 method, and how the result can be used to complement experimental screening techniques.

References:

1- J.D. Burrington, J. K. Pudelski, J. P. Roski, Chapter 18: Challenges in detergents and dispersants - *Practical Advances in Petroleum Processing* **2007**

2- Christine Esangbedo, Andre L. Boehman, Joseph M. Perez, *Tribology International* **2012**, 47, 194

3- A. La Rocca, F. Bonatesta, M. W. Fay, F. Campanella, *Tribology International* 86 (**2015**) 77-84

4- I. Z. Jenei et al., *Nanotechnology* n°8, Vol 29 (**2018**)

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room5)

[SY-O4] A Molecular Dynamics Study on the Wear Mechanisms of Hydrogenated Diamond-like Carbon

○Yang Wang[1], Jingxiang Xu[1], Yusuke Ootani[1], Yuji Higuchi[1], Nobuki Ozawa[1], Koshi Adachi[2], Momoji Kubo[1] （1.Institute for Materials Research, Tohoku University, Japan, 2.Department of Mechanical System Engineering, Graduate School of Engineering, Tohoku University, Japan）

Diamond-like carbon (DLC) is a promising solid lubricant and widely used as a lubricant coating in various industrial applications such as engine, hard-disk, and space instruments. Hydrogenated DLC coatings show the much better low-friction properties and lubricity than the non-hydrogenated DLC coatings. However, wear of the hydrogenated DLC coatings causes the reduction of the durability of DLC coatings and limits their utilization. For the further improvement of the hydrogenated DLC coatings, the deep and

comprehensive understandings of the wear mechanisms of the hydrogenated DLC are very essential; nevertheless, these understandings are still lacking because the experiments are difficult to observe the complicated atomic-scale friction processes and tribochemical reactions at the interface. To handle these difficulties, we employ a molecular dynamics method to investigate the wear mechanisms of the hydrogenated DLC. We perform friction simulations in the vacuum by using the DLC models with a hydrogen concentration of 0%, 20%, 30%, 40%, and 50%. From the simulation results, we observe two wear mechanisms of DLC: 1) chemical wear as the generation of hydrocarbons desorbing from DLC surface and 2) mechanical wear as the transfer of carbon atoms to the counter substrates. The chemical and mechanical wear co-decide the wear behaviors of DLC. Furthermore, with increasing the hydrogen concentration in DLC, chemical wear increases and mechanical wear decreases, causing a parabolic-like hydrogen dependence of the total wear with a minimum value at the hydrogen concentration of 30%. Our simulations successfully give fundamental understandings about the wear mechanisms of the hydrogenated DLC and provide the theoretical instructions to improve the anti-wear properties of DLC coatings.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room5)

[SY-O4] Effect of Tribochemical Reactions on Diamond-like Carbon and Wear under Water Lubrication: A Molecular Dynamics Simulation Investigation

○Jing Zhang[1], Yang Wang[1], Jingxiang Xu[1], Yusuke Ootani[1], Nobuki Ozawa[1], Koshi Adachi[2], Momoji Kubo[1]
（1.Inst. for Materials Research, Tohoku Univ., Japan, 2.Dept. of Mechanical Systems Engineering, Tohoku Univ., Japan）

Diamond-like carbon (DLC) coatings possess excellent frictional properties. However, the wear of DLC coatings is still a problem. To improve the properties of DLC, clarification of the wear mechanisms is required. It is reported that the wear of DLC under the water lubrication is lower than that in the air. To expound the wear mechanisms, clarification of this phenomenon is strongly demanded. However, the detailed mechanism is still unclear due to the complicated tribochemical reactions. Therefore, we studied the wear mechanisms of DLC under both vacuum and water environment by using the molecular dynamics method. The DLC model is made of two hemispherical substrates, to simulate real rough surfaces. The friction simulations were carried out by sliding two substrates. During the friction, under both environments the transfer of carbon atoms to their counter substrates was observed, indicating the adhesive wear of DLC. The number of transferred carbon atoms under vacuum condition was much larger than that under water lubrication, suggesting that the water environment suppresses the wear of DLC. Considering that interfacial C-C bonds which connect two DLC substrates promotes the transfer of carbon atoms, we investigated the number of interfacial C-C bonds. The number of interfacial C-C bonds under water lubrication was less than that in vacuum, indicating that the formation of the interfacial C-C bonds was suppressed by the water. To understand the cause of the suppression effect of water on the interfacial C-C bonds formation, we investigated the chemical reactions during friction process. With friction time going, the increase in the C-H and C-O bonds and the decrease in water molecules were observed, indicating the reaction between water molecules and carbon atoms. We suggest that these chemical reactions increase H and OH terminations on the DLC substrates and suppress the formation of the interfacial C-C bonds, and therefore the adhesive wear is inhibited.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room5)

[SY-O4] Formation Mechanism of Tribofilm of Silicon Carbide under Water Lubrication: Molecular Dynamics Simulations

○Fumiya Nakamura, Yang Wang, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Koshi Adachi, Momoji Kubo
（Tohoku Univ., Japan）

Water lubrication has the characteristic of low environmental burden. It is known that silicon carbide (SiC) shows quite low friction coefficient by the formation of a tribofilm on the surface of SiC during water lubrication. Understanding of its mechanism is essential to improve friction characteristic for practical use and application. However, it is difficult to observe directly such a complicated phenomenon including friction and chemical reaction by experiments. Therefore, in this study, molecular dynamics method which can simulate chemical reaction was conducted to analyze the structure and formation mechanism of tribofilm in the friction process of amorphous SiC under water environment.

 In the simulation, we prepared the model consisting of two amorphous SiC substrates sandwiching water molecules. The substrates have rough surfaces and the two of substrate surfaces can be in contact during the friction. The substrates were given a constant pressure (3 GPa) and slid for 1000 ps at 100 m/s.

 We performed the sliding simulation of SiC under water lubrication. In the initial structure, the surface of the substrates was corrugated. However, the rough surface of the substrates was smoothed while Si atoms from the a-SiC substrate reacted with water molecules and formed bonds with O atoms of H_2O during friction. Firstly, we investigated the change in number of water molecules and Si-O-Si bonds during friction. It was found that the number of water molecules decreased constantly while the number of Si-O-Si bonds increase correspondingly. This result shows that Si reacts with H_2O to form a SiO_2 layer. Next, we investigated the change in the distribution ratio of C and Si before and after friction. The ratio of C was increased around the substrate surfaces and that of Si was increased on the substrates indicating that the bilayer tribofilm of the SiO_2 and C rich SiC was generated on the substrate by the tribo-chemical reaction.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A3] Symposium A-3

Chair: Katsuyo Thornton(University of Michigan, Ann Arbor, United States of America)
Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room6

[SY-A3] Challenges and gaps in length and time scaling of dislocation models
○David L McDowell （Woodruff School of Mechanical Engineering, Georgia Institute of Technology, United States of America）

[SY-A3] From discrete to continuum dislocations and back: a two dimensional study of microstructure and interaction energies.
○Hengxu Song, Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

[SY-A3] Advances in microstructure prediction: a FFT-based Dislocation Dynamics approach
○Francesca Boioli[1], Benoit Devincre[1], Riccardo Gatti[1], Laurant Dupuy[2], Lionel Gélébart[2] （1.LEM, CNRS-ONERA, Chatillon, France, 2.SRMA, CEA Saclay, France）

[SY-A3] Plasticity and microstructure evolutions at the mesoscale: towards and integrated framework.
○Laurent Capolungo, John Graham, Aaron Kohnert, Ricardo Lebensohn, Richard Lesar, Hareesh Tummala （Los Alamos National Laboratory, United States of America）

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room6)

[SY-A3] Challenges and gaps in length and time scaling of dislocation models

Invited

○David L McDowell （Woodruff School of Mechanical Engineering, Georgia Institute of Technology, United States of America）

We consider multiple crystalline plasticity model constructs that address evolution of dislocation structures over a broad range of length and time scales, from atomistic modeling and coarse-graining strategies through discrete dislocation theory to reduced order generalized and local continuum models. The predictive character of each construct is considered, along with the notion of uncertainty of modeling phenomena at various scales and for two-scale transitions, either concurrent or hierarchical in nature. In each case, we list the set of phenomena that each model construct addresses. Challenges to modeling the evolution of the dislocation network are discussed, including the important role of the entropic barrier to collective dislocation bypass of obstacles. Gaps and future challenges are summarized.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room6)

[SY-A3] From discrete to continuum dislocations and back: a two dimensional study of microstructure and interaction energies.

○Hengxu Song, Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

Continuum dislocation dynamics models, which are proposed to conquer the restrictions of high computational cost that discrete dislocation dynamics models generally experience, have made great progress in the past decades. However, it is inevitable that certain dislocation microstructure information is 'lost' during the averaging/coarse graining process ('upscaling'), for example, dislocation short range interactions. This information, however, is crucial for a correct prediction of the structure-property relation in continuum simulations. We will show a new type of multiscale analysis which is based on the energy density of 2D systems, where we identify the 'missing' information during coarse graining for arbitrary averaging resolution. This methodology can be directly generalized to 3D systems of curved dislocations. Furthermore, based on our database, we will be able to benchmark a number of existing 2D continuum formulations for dislocation interaction. Last but not least, we will show that our data base also will be a useful starting point for recovering statistical information of (ensembles of) discrete dislocations from continuum field data during 'downscaling'.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room6)

[SY-A3] Advances in microstructure prediction: a FFT-based Dislocation Dynamics approach

○Francesca Boioli[1], Benoit Devincre[1], Riccardo Gatti[1], Laurant Dupuy[2], Lionel Gélébart[2] （1.LEM, CNRS-ONERA, Chatillon, France, 2.SRMA, CEA Saclay, France）

Discrete Dislocation Dynamics (DD) is a well-established simulation technique aimed at reproducing the collective behavior of dislocations at the mesoscale. Despite the considerable progresses made in last decades, DD simulations are still unable to precisely reproduce the microstructure of large poly-crystals and, especially, of irradiated polycrystalline materials. An important step in the development of predictive simulations of this class of materials is the improvement of the numerical capabilities of DD codes to model dislocation properties in large volumes representative of the materials microstructures.

Here we propose a promising strategy based on the coupling between two advanced simulation tools. First, the Discrete-Continuous Model (DCM) is employed [O. Jamond et al., Int. J. Plast. 80,19(2016)]. This numerical model based on the Eigenstrain theory, couples an extensive DD simulation code (microMegas), to an elastic solver dedicated to boundary value problems resolution. The DCM allows for the rigorous solution of dislocation-surface and -interfaces interactions and has been proven to efficiently model plasticity in nano- and micro-objects. Nevertheless, its application has been limited to samples of few mm in size. Second, to overcome this difficulty, we employ a solver based on Fast Fourier Transform (FFT) calculation [Bertin et al. Modelling Simul. Mater. Sci. Eng. 23,065009 (2015)]. In particular, we employ AMITEX_FFTP, a new distributed parallel elastic solver based on FFT calculation. Using this approach, the stress state definition in the simulated volumes can be increased from a 64x64x64 grid to a 1024x1024x1024 one, hence allowing the simulation of realistic dislocation density in a multi-grains periodic volume over significant plastic strains (5-10%). In summary, we aim at improving mechanical properties predictions by taking into account both the complexity of multi-crystalline materials microstructure and the local properties of dislocations.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room6)

[SY-A3] Plasticity and microstructure evolutions at the mesoscale: towards and integrated framework.

○Laurent Capolungo, John Graham, Aaron Kohnert, Ricardo Lebensohn, Richard Lesar, Hareesh Tummala
（Los Alamos National Laboratory, United States of America）

A Fast Fourier Transform (FFT) based hybrid discrete dislocation dynamics (DDD) and cluster dynamics (CD) tool is introduced to study plasticity and microstructure evolution in polycrystalline media. The overall intent of the work is to introduce a unified modeling platform applicable at the tens of micron scale that allows for the validation and calibration of constitutive models and rate theory models used at higher length scales. In addition, the proposed framework aims at leveraging novel/advanced characterization methods. As such the model will be able to be directly compared against in-situ characterization methods (TEM, X-Ray diffraction). With regards to the modeling framework, in addition to its common treatment of plasticity, DDD in combination with FFT methods allows for the description of dislocations both as discrete and as continuous objects, thereby providing an ideal linkage with higher order constitutive modeling, which will be demonstrated by taking the example of grain boundary/dislocation interactions and in bicrystals and polycrystals. Further, an application of this framework to the case of twin propagation in hcp metals will be shown. Finally, the coupling between DDD and CD provides for a treatment of the role of dislocation microstructures on the evolution of radiation-induced damage as well as for the quantification of plasticity induced by irradiation. This will be illustrated in the case of pure body centered cubic Iron in which a mapping of the dominant deformation processes as a function of temperature, stress and irradiation condition will be presented.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A4] Symposium A-4

Chair: David L McDowell(Woodruff School of Mechanical Engineering, Georgia Institute of Technology, United States of America)

Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room6

[SY-A4] Effective Transport Properties of Polycrystalline Materials

William Beck Andrews[1], Min-Ju Choe[1], Erik Hanson[1], Max Powers[1], Hui-Chia Yu[1,2], ○Katsuyo Thornton[1]   (1.University of Michigan, Ann Arbor , United States of America, 2.Michigan State University , United States of America)

[SY-A4] **A new E-VPSC polycrystal formulation: fundamentals**

○Carlos Tome[1], Youngung Jeong[2]   (1.Los Alamos National Laboratory, United States of America, 2.Department of Materials Science, Changwon National University, Korea)

[SY-A4] **A new E-VPSC polycrystal formulation: applications**

○Youngung Jeong[1], Carlos Tome[2]   (1.Changwon National Univ., Korea, 2.Los Alamos Natinal Lab, United States of America)

[SY-A4] Modeling microstructural material variability with uncertainty quantification and machine learning techniques

○Reese Jones, Coleman Alleman, Brad Boyce, Ari Frankel, Nathan Heckman, Mohammad Khalil （Sandia National Laboratories, United States of America）

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room6)

[SY-A4] Effective Transport Properties of Polycrystalline Materials

Invited

William Beck Andrews[1], Min-Ju Choe[1], Erik Hanson[1], Max Powers[1], Hui-Chia Yu[1,2], ○Katsuyo Thornton[1]
（1.University of Michigan, Ann Arbor , United States of America, 2.Michigan State University , United States of America）

Most solid materials have surfaces, interfaces, and grain boundaries that enhance or hinder transport; as a result, the properties of polycrystalline solids can be vastly different from their intrinsic properties, especially in nanocrystalline materials. Diffusion in polycrystalline materials plays an important role in a wide range of material systems, including those found in batteries and solid oxide fuel cells. Due to the computational expense in explicitly considering the grain boundary network, establishing rational design rules for nanocrystalline materials with desired transport properties remains a challenge. We apply the Smoothed Boundary Method to evaluate the effective diffusivity of polycrystalline materials with a range of grain morphologies. We find that the anisotropy of grain morphologies plays a critical role in the overall transport behavior, which cannot be quantified using the classical mean field theories. The results are used to obtain an expression for mixed-pathway transport that is capable of universally predicting the effective diffusivity in complex polycrystalline solids without the use of computationally intensive simulations. Such an approach enables efficient simulation of transport in larger-scale systems while accurately capturing the effects of grain morphologies.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room6)

[SY-A4] A new E-VPSC polycrystal formulation: fundamentals

○Carlos Tome[1], Youngung Jeong[2]　（1.Los Alamos National Laboratory, United States of America, 2.Department of Materials Science, Changwon National University, Korea）

Effective medium polycrystal models provide a computationally efficient tool for simulations of elastic and visco-plastic deformation of aggregates. In particular, visco-plastic self-consistent (VPSC) schemes have been widely and successfully applied to predictions of texture, stress-strain, and dislocation density evolution during large strain deformation. In addition, VPSC schemes have been implemented in finite element codes as material subroutines to simulate various metal forming operations. However, a limitation of VPSC models is that they only address deviatoric stress and strain and neglect elastic contributions. As a consequence, they cannot be used to predict internal Cauchy stress evolution (as measured with neutron or X-ray diffraction), or to study constitutive behavior during complex loading scenarios (such as Bauschinger or spring-back) where the contribution of elasticity needs to be accounted for.

Several formulations have been proposed in the last 20 years that empirically combine visco-plastic and elastic regimes to formulate elasto-visco-plastic (E-VPSC) effective medium models. A disadvantage of these formulations is that they increase considerably the computation time, which makes them unwieldy for using in forming simulations.

Here we present a new approximate E-VPSC formulation that, by treating elasticity as a perturbation to the VPSC scheme of Lebensohn and Tomé [1], seems to capture the best of both worlds: efficient numerical processing while providing access to the evolution of Cauchy stress in the grains.

In this presentation we describe such E-VPSC formulation, compare it to previous ones, and provide a simple application - based on Voce hardening - to predictions of stress strain and internal stress evolution in steel subjected to tension-compression reversal tests. In a companion paper [2] we present several applications of this new E-VPSC formulation.

[1] R.A. Lebensohn, C.N. Tomé, "A self-consistent anisotropic approach for the simulation of plastic deformation and texture development of polycrystals: application to zirconium alloys", Acta Metallurgica et Materialia 41(9) (1993) 2611-2624

[2] Y. Jeong, C.N. Tomé, "A new E-VPSC formulation: applications", this conference

---

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room6)

[SY-A4] A new E-VPSC polycrystal formulation: applications

○Youngung Jeong[1], Carlos Tome[2] (1.Changwon National Univ., Korea, 2.Los Alamos Natinal Lab, United States of America)

In this presentation we implement an elasto-visco-plastic (E-VPSC) polycrystal formulation described in a companion paper [1]. In this formulation the contribution of elasticity is introduced as an eigen strain rate into the visco-plastic regime of each grain. The VPSC model of Lebensohn and Tomé [2] provides the implementation platform for the new E-VPSC formulation. The new model is validated by conducting several applications as follows:
Simple uniaxial tension test to validate the model and to demonstrate the numerical performance in comparison with the VPSC model [2], a separate E-VPSC model [3], and a rate insensitive EPSC model [4]. Large strain cyclic shear of low-carbon steel using Voce hardening law to demonstrate the Bauschinger effect. The results are compared with the VPSC-RGVB model [5], where the back-stress is linked to evolution of dislocation structures. Relaxation of internal stress in steel subjected to strain holds during tensile testing.

[1] C.N. Tomé, Y. Jeong, "A new E-VPSC formulation: fundamentals", this conference

[2] R.A. Lebensohn, C.N. Tomé, "A self-consistent anisotropic approach for the simulation of plastic deformation and texture development of polycrystals: application to zirconium alloys", Acta Metallurgica et Materialia 41 (1993) 2611-2624

[3] H. Wang, P.D. Wu, C.N. Tomé, Y. Huang, "A finite strain elastic-viscoplastic self-consistent model for polycrystalline materials", Journal of the Mechanics and Physics of Solids 58 (2010) 594-612

[4] P.A. Turner, C.N. Tomé, "A study of residual stresses in Zircaloy-2 with rod texture", Acta metall mater 42 (1994) 4143-53

[5] W. Wen, M. Borodachenkova, C.N. Tomé, G. Vincze, E.F. Rauch, F. Barlat, J.J. Gracio, "Mechanical behavior of low carbon steel subjected to strain path changes: experiments and modeling", Acta Materialia 111 (2016) 305-314

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room6)

[SY-A4] Modeling microstructural material variability with uncertainty quantification and machine learning techniques

○Reese Jones, Coleman Alleman, Brad Boyce, Ari Frankel, Nathan Heckman, Mohammad Khalil （Sandia National Laboratories, United States of America）

Material variability from heterogeneous microstructure, such as grain and pore morphologies, can have significant effects on component behavior and creates uncertainty around performance. Current engineering material models typically do not incorporate microstructural variability explicitly, rather functional forms are chosen based on intuition and parameters are selected to reflect mean behavior. Conversely, mesoscale models that capture the microstructural physics, and inherent variability, are impractical to utilize at the engineering scale. An enhanced design methodology must be developed for materials with significant variability, such as current additively manufactured (AM) metals, to predict the ensemble response.

To address these challenges we have developed a method based on the Embedded Uncertainty formulation, Sargsyan, Najm, Ghanem (2015) to calibrate distributions of material parameters from high-throughput experimental data. With this method, material variability is directly associated with commonly-used material parameters using a chosen nominal model. One of the benefits of this approach is that expert knowledge can be extended to interpret the effect of (hidden) microstructure on variable mechanical response. In a complementary effort, we are developing machine learning techniques to handle the large volume of data from high-throughput methods. The focus of this aspect is on adapting common machine learning models, such as neural networks, to obey the same exact properties and symmetries as traditional constitutive models while representing features in the data in a flexible, bias-less manner, Tensor Basis Neural Network in Ling, Jones, Templeton (2016). Classical constitutive modeling provides guidance in selecting appropriate microstructural descriptors as inputs and functional frameworks for outputs. Examples of application of these techniques to polycrystalline, porous metals, motivated by current AM materials, will be given.

[SY-I3] Symposium I-3

Chair: Peter Voorhees(Northwestern University, United States of America)
Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room7

[SY-I3] Interaction of moving grain boundaries with solutes: bridging time scales between atomistics and continuum

○Yuri Mishin （George Mason University, United States of America）

[SY-I3] **Phenomenological model for prediction of interaction parameters in grain boundary segregation**

○Pavel Lejcek[1], Siegfried Hofmann[2] （1.Institute of Physics, AS CR, Praha, Czech Republic, 2.Max-Planck-Institute for Intelligent Systems, Stuttgart, Germany）

[SY-I3] Influence of Solutes at Grain Boundaries on Phase Transformations and Mechanical Response

○Stephen M Foiles, Nathan Heckman, Christopher Barr, Fadi Abdeljawad, Khalid Hattar, Brad Boyce （Sandia National Laboratories, United States of America）

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room7)

[SY-I3] Interaction of moving grain boundaries with solutes: bridging time scales between atomistics and continuum

Invited

○Yuri Mishin （George Mason University, United States of America）

Solutes can strongly interact with grain boundaries (GBs) and impact their thermodynamic and kinetic properties. Some of the most interesting effects of solute segregation include the segregation-induced GB phase transformations and the solute drag/pinning effect. An even more interesting is the effect of GB motion on GB phase transformations. Studying these effects by molecular dynamics is highly problematic due to the limited time scale of the method. The talk will present two alternative methods for studying phase transformations in moving GBs. One method is based on a semi-analytical discrete GB model in a binary solid solution. The regular solution model predicts first-order phase transformations in GBs, which can be shown by a GB phase coexistence line and GB spinodals of the bulk phase diagram. The model overcomes the time-scale limitation and treats both GB thermodynamics and GB dynamics within a unified framework. It gives direct access to the solute drag force and the GB free energy, which are difficult to compute by atomistic simulations. GB migration can be modeled on different timescales and over a wide range of velocities in both the transient and steady-state regimes. The simulations reveal interesting effects, such as kinetic stabilization of metastable or even unstable GB phases, dynamic GB phase transformations, and the dynamic GB hysteresis. Other interesting effects include the break-way events in which the GB leaves the segregation atmosphere behind and forms a new segregation. This new segregation atmosphere can represent the same of a different GB phase. It is shown how the discrete model reduces to phase-field model in the limit of wide segregation region. The phase-field simulations within this model yield similar results as the discrete model but have certain computational advantages. The results of this study can be broadly interpreted in terms of extremum principles of non-equilibrium thermodynamics, which predict dynamic stabilization of thermodynamically unstable but kinetically favored phases. Extension of the models to 2D and 3D systems and more accurate thermodynamic treatments will be discussed.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room7)

[SY-I3] Phenomenological model for prediction of interaction parameters in grain boundary segregation

○Pavel Lejcek[1], Siegfried Hofmann[2] （1.Institute of Physics, AS CR, Praha, Czech Republic, 2.Max-Planck-Institute for Intelligent Systems, Stuttgart, Germany）

Grain boundary segregation is a phenomenon studied both experimentally and theoretically for decades. The interest in this phenomenon is evoked not only by its close relationship to temper embrittlement but also by its ability to stabilize nanocrystalline structures by solute segregation in the concept of Grain Boundary Engineering.

A full description of the exact temperature and solute concentration dependence of grain boundary segregation requires reliable values of segregation enthalpy and entropy as well as solute interaction coefficients. However, experimental studies of all these values are rather limited, and theoretical studies are usually restricted to segregation energy at zero Kelvin. It is obvious that such a database does not allow a full description of the grain boundary segregation in most systems of interest.

In this contribution we present a semi-empiric method enabling prediction of all required thermodynamic parameters - ideal enthalpy, ideal entropy and real binary interaction (Fowler) coefficient - which, in combination, describe fully the segregation of any segregant at any temperature and at individual grain boundaries. This method is based on the relationship between the segregation enthalpy and the solid solubility limit, and on the enthalpy-entropy compensation effect. The data for numerous solutes in alpha iron are predicted and they are compared to available data in the literature.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room7)

[SY-I3] Influence of Solutes at Grain Boundaries on Phase Transformations and Mechanical Response

Invited

○Stephen M Foiles, Nathan Heckman, Christopher Barr, Fadi Abdeljawad, Khalid Hattar, Brad Boyce （Sandia National Laboratories, United States of America）

Segregation of solute atoms to grain boundaries is a well-known phenomenon which can modify grain boundary structure, energy and mobility among other properties. In this talk, we present computations of the segregation of Au at grain boundaries in Pt and corresponding experimental validation. The existence of a grain boundary phase transformation between high- and low-segregation states will be demonstrated. The impact of this segregation on the mechanical response of both individual grain boundaries and grain boundary networks will be examined. This work shows that for nanocrystalline samples, the stability of the grain structure against thermal or deformation induced grain growth is enhanced, but that ductility is reduced.

[SY-I4] Symposium I-4

Chairs: Shen J Dillon(University of Illinois, USA), Daniel Pino Munoz(Mines ParisTech / PSL Research University, France)
Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room7

[SY-I4] Atomistic modeling of helium segregation to grain boundaries in tungsten and its effect on de-cohesion

○Enrique Martinez Saez[1], Blas Pedro Uberuaga[1], Brian D Wirth[2,3]　(1.Material Science and Technology Division, MST-8,Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America, 2.Department of Nuclear Engineering, University of Tennessee, Knoxville, TN 37996, United States of America, United States of America, 3.Oak Ridge National Laboratory, PO Box 2008, MS-6003, Oak Ridge, TN 37831, United States of America, United States of America)

[SY-I4] Thermodynamic properties of bcc Fe grain boundaries with segregation of 3d-transition-metal solutes

○Zhuo Xu, Shingo Tanaka, Masanori Kohyama　(AIST, Japan)

[SY-I4] A new thermodynamic model for the austenite-ferrite massive transformation in Fe-C-X alloys.

○Alexandre MATHEVON[1], Michel PEREZ[1], Damien FABREGUE[1], Veronique MASSARDIER[1], Philippe ROCABOIS[2], Patrice CHANTRENNE[1]　(1.INSA Lyon, France, 2.FIVES KEODS, France)

[SY-I4] Multiscale simulation of solid phase sintering of nano copper powder

○Xinyu Zhu, Xiangge Qin　(School of Materials Science and Engineering, Jiamusi Univ., China)

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room7)

[SY-I4] Atomistic modeling of helium segregation to grain boundaries in tungsten and its effect on de-cohesion

Invited

○Enrique Martinez Saez[1], Blas Pedro Uberuaga[1], Brian D Wirth[2,3]　(1.Material Science and Technology Division, MST-8,Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America, 2.Department of Nuclear Engineering, University of Tennessee, Knoxville, TN 37996, United States of America, United States of America, 3.Oak Ridge National Laboratory, PO Box 2008, MS-6003, Oak Ridge, TN 37831, United States of America, United States of America）

Due to their low sputtering yield, low intrinsic tritium retention, high melting point, and high thermal conductivity, W and W alloys are promising candidates for the divertor region in a magnetic fusion device. Transmutation reactions under neutron irradiation lead to the formation of He and H particles that potentially degrade material performance and might lead to failure. High He fluxes ultimately lead to the formation and bursting of bubbles that induce swelling, a strong decrease in toughness, and a nanoscale microstructure that potentially degrades the plasma. Understanding the behavior of He in polycrystalline W is thus of significant importance as one avenue for controlling the material properties under operating conditions. In this work we study the interaction of both substitutional and interstitial He atoms with various grain boundaries in pure W and the effect of the He presence on the system response to external loading. We observe that He segregates to all the interfaces tested and decreases the cohesion of the system at the grain boundary. Upon tension normal to the interface, the presence of He significantly decreases the yield stress, which depends considerably on the bubble pressure. Increasing pressure reduces cohesion, as expected. More complex stress states result in more convoluted behavior, with He hindering grain boundary sliding upon simple shear.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room7)

[SY-I4] Thermodynamic properties of bcc Fe grain boundaries with segregation of 3d-transition-metal solutes

○Zhuo Xu, Shingo Tanaka, Masanori Kohyama　(AIST, Japan)

Grain boundaries (GBs) are one of the key factors to manipulate the material properties. The solute segregation and solute drag effects are remarkable for the thermodynamic properties of GBs, where the microscopic atomic and electronic structures affect the macroscopic behaviors of GB evolution. We have developed the local analysis method to get the local-energy and local-stress of each atom [1], which is of assistance to unveil the microscopic mechanism. In the present study, we firstly focused on the $\Sigma 11(332)$ and $\Sigma 3(111)$ <110> symmetrical tilt GBs in bcc Fe with 3d-transition-metal (TM) solutes. We performed ab-initio calculations together with the local analysis, and observed that the segregation behaviors of 3d-TM solutes can be classified into early TMs (Sc, Ti and V), middle TMs (Cr and Mn), and late TMs (Co, Ni and Cu). The early and late TMs prefer to segregate at the looser and tighter sites of GBs, respectively. The local-energy decomposition indicates that the segregation of early TMs is dominated by the stabilization of surrounding Fe atoms at a GB, while that of late TMs is dominated by the repulsion from the bulk as well as the stabilization of a TM-atom itself. Furthermore, corresponding to the segregation energy of each 3d-TM segregated to the looser or tighter site of GBs, by the multiscale modeling, we estimated the solute drag effects on the mobility and interface energy of GBs, and the grain growth rate. Finally, we discuss the cases of

general GBs, and compare the results with experiment.

[1] Y. Shiihara et al., Phys. Rev. B 81, 075441 (2010). S. Bhattacharya et al., J. Mater. Sci. 49, 3980 (2014).

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room7)

[SY-I4] A new thermodynamic model for the austenite-ferrite massive transformation in Fe-C-X alloys.

○Alexandre MATHEVON[1], Michel PEREZ[1], Damien FABREGUE[1], Veronique MASSARDIER[1], Philippe ROCABOIS[2], Patrice CHANTRENNE[1]　（1.INSA Lyon, France, 2.FIVES KEODS, France）

Predictions of the ferrite to austenite or austenite to ferrite transformation kinetics during heating and/or cooling of ternary Fe-C-X alloys is challenging because diffusion coefficients of interstitial and substitutional elements are very different in both phases. The model described in this paper, is based on the prediction of (i) concentration profiles for all elements and (ii) interface velocity, that corresponds to the minimization of the Gibbs energy (*i.e.* phase field approach). The total energy of the system is given *via* a dynamic coupling with Thermocalc database.

The ferrite/austenite interface is assumed to have a finite width. This allows to deal with a unique diffusion profile for all species. Element fluxes are derived from their chemical potential gradient. Another advantage of such an approach is the possibility of introducing a potential depth within the interface, leading to solute atoms segregation, that is believed to control transformation kinetics in ternary systems.

During the transformation, it is observed that the model automatically switches between different equilibrium conditions (from out-of-equilibrium transformation to para-equilibrium, local equilibrium with and without partitioning until ortho-equilibrium). To our knowledge, it constitutes a real improvement in phase transformation modeling. This model has been calibrated on decarburization experimental kinetics reported in the literature in various Fe-C-X systems. This model shows an interface motion slowing down with the addition of a potential depth at the interface in agreement with experimental observations. By extension, the model has been used on isothermal and non-isothermal heating for complex Dual Phase steels and compared with experiments.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room7)

[SY-I4] Multiscale simulation of solid phase sintering of nano copper powder

○Xinyu Zhu, Xiangge Qin　（School of Materials Science and Engineering, Jiamusi Univ., China）

Powder metallurgy is a processing technology that uses metal powder compacts to produce near net shape parts through sintering and is suitable for mass production. Quantitative prediction of microstructure evolution and sintering kinetics during powder sintering is of great significance for understanding the sintering mechanism and optimizing the sintering process.

In this paper, the packing structure model of nano copper particles was established using the discrete

element method as a powder compact. The solid phase sintering of the powder compact was studied by molecular dynamics simulation using embedded atom method. The sintering mechanism and densification kinetics of the nano powders were analyzed and compared with the experimental results. The effects of diffusion mechanism and grain growth on the sintering densification process are discussed in detail.

Keywords: powder sintering, diffusion, grain growth, discrete element, molecular dynamics

Symposium | L. Structure, Statistics and Mechanics in Crystal Dislocation Plasticity

[SY-L3] Symposium L-3

Chairs: Peter M Derlet(Paul Scherrer Institut, Switzerland), Cynthia Reichhardt(Los Alamos National Laboratory, United States of America)
Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room8

[SY-L3] Intermittent micro-plasticity and its relation to dislocation structure - a linear stability analysis.

○Peter M Derlet[1], Gábor Péterffy[2], Péter Dusán Ispánovity[2] （1.Paul Scherrer Institut, Switzerland, 2.Department of Materials Physics, Eötvös University, Hungary）

[SY-L3] Discrete dislocation dynamics simulations of complexity in crystal plasticity: strain burst statistics and machine learning

○Lasse Laurson （Aalto University, Finland）

[SY-L3] **Nanoindentation in the ultra-nano scale: Microstructure-property relationships using statistical approaches**

Hengxu Song[1,2], Ryder Bolin[1], Michael Tzimas[1], ○Stefanos Papanikolaou[1,2] （1.west virginia university, United States of America, 2.johns hopkins university, United States of America）

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room8)

[SY-L3] Intermittent micro-plasticity and its relation to dislocation structure - a linear stability analysis.

Invited
○Peter M Derlet[1], Gábor Péterffy[2], Péter Dusán Ispánovity[2]　（1.Paul Scherrer Institut, Switzerland, 2.Department of Materials Physics, Eötvös University, Hungary）

The relationship between dislocation network stucture and plasticity is studied via a linear stability analysis of the evolving dislocation configuration. This is done for a simplified one dimensional model of interacting dislocation pile-ups, which exhibits a mean-field depinning transition at yield, and for a two dimensional dislocation dynamics model always in a state of criticality that is well described by a jamming transition. We find that the obtained eigen-modes prior to a plastic event play an important role in characterizing the discrete micro-plastic regime of simulation, reflecting the degree of criticality the system is in, the nature of how a plastic event occurs and its eventual evolution into an avalanche.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room8)

[SY-L3] Discrete dislocation dynamics simulations of complexity in crystal plasticity: strain burst statistics and machine learning

Invited
○Lasse Laurson　（Aalto University, Finland）

First, I will present an overview of our recent studies focusing on the statistical properties of strain avalanches in crystal plasticity as observed in discrete dislocation dynamics (DDD) simulations. These encompass various scenarios, including two and three dimensional DDD models, and considering systems with and without an additional quenched pinning field (due to, e.g., precipitates) interacting with the dislocations. I discuss the results from the perspective of two main mechanisms affecting the nature of dislocation dynamics and hence the deformation process: dislocation (de)pinning and dislocation (un)jamming.

Second, I will briefly present our very recent efforts to apply machine learning to predict the properties of the stress-strain curves of individual microscale samples using features of the initial, pre-exisiting dislocation network as input. The resulting predictability of the deformation process is found to evolve with strain in a non-monotonic fashion, something we attribute to the stochastic nature of the deformation avalanches.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room8)

[SY-L3] Nanoindentation in the ultra-nano scale: Microstructure-property relationships using statistical approaches

Hengxu Song[1,2], Ryder Bolin[1], Michael Tzimas[1], ○Stefanos Papanikolaou[1,2]　（1.west virginia university, United States of America, 2.johns hopkins university, United States of America）

Due to the difficulties of tensile/compressive tests at small length scales, nanoindentation is widely used towards unveiling crystalline mechanical properties. However, crystal plasticity limits the understanding of

nanoindentation results at depths below 500nm: the Indentation Size Effect (ISE) in these scales leads to very noisy and unclear data, with the measured hardness/stiffness being difficult to 'translate' into features of the material microstructure. In this work, we demonstrate two statistical approaches to investigate the ultra-nano regime of FCC metals towards unveiling crystalline properties: First, we notice that indentation together with in-plane tension consist of a phase diagram of the sample elasto-plastic property. The elastic-plastic transition during indentation is naturally continuous for large dislocation densities. In the large dislocation density regime, through the development of scaling functions for an appropriately defined plasticity order parameter, we connect statistically the bulk crystal plasticity transition with nanoindentation. Second, for low dislocation densities, we utilize the noise of the load-depth nanoindentation curves and the post-indent nanoindentation images to statistically connect experiments with 3D discrete dislocation dynamics simulations. We develop a machine-learning approach that can be used for nanoindentation and predict experimentally relevant pre-existing dislocation densities in single crystalline FCC grains.

[SY-L4] Symposium L-4
Chair: Lasse Laurson(Aalto University, Finland)
Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room8

[SY-L4] Dynamic phases, pinning, and pattern formation for driven dislocation assemblies

○Cynthia Reichhardt[1], Caizhi Zhou[2], Charles Reichhardt[1], Irene Beyerlein[3] （1.Los Alamos National Laboratory, United States of America, 2.Missouri University of Science and Technology, United States of America, 3.University of California, Santa Barbara, United States of America）

[SY-L4] Effect of solute atoms and Peierls stress on the critical behaviour of discrete dislocations

○Peter Dusan Ispanovity[1], Gabor Peterffy[1], Peter M. Derlet[2] （1.Eotvos Universty, Hungary, 2.Paul Scherrer Institut, Switzerland）

[SY-L4] Temporal and spatial plastic instability of micrometer-scaled materials

○Yinan Cui[1], Giacomo Po[1], Nasr Ghoniem[1] （1. Mechanical and Aerospace Engineering Department, University of California, Los Angeles, United States of America）

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room8)

[SY-L4] Dynamic phases, pinning, and pattern formation for driven dislocation assemblies

Invited

○Cynthia Reichhardt[1], Caizhi Zhou[2], Charles Reichhardt[1], Irene Beyerlein[3]　(1.Los Alamos National Laboratory, United States of America, 2.Missouri University of Science and Technology, United States of America, 3.University of California, Santa Barbara, United States of America)

We examine driven dislocation assemblies and show that they can exhibit a set of dynamical phases remarkably similar to those of driven systems with quenched disorder such as vortices in superconductors, magnetic domain walls, and charge density wave materials. These phases include pinned-jammed, fluctuating, and dynamically ordered states, and each produces distinct dislocation patterns as well as specific features in the noise fluctuations and transport properties. Our work suggests that many of the results established for systems with quenched disorder undergoing plastic depinning transitions can be applied to dislocation systems, providing a new approach for understanding pattern formation and dynamics in these systems.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room8)

[SY-L4] Effect of solute atoms and Peierls stress on the critical behaviour of discrete dislocations

○Peter Dusan Ispanovity[1], Gabor Peterffy[1], Peter M. Derlet[2]　(1.Eotvos Universty, Hungary, 2.Paul Scherrer Institut, Switzerland)

It is well-known from micropillar and acoustic emission experiments that plastic strain accumulates in sudden avalanche-like events. Based on the statistical analysis of these bursts it is now apparent that plastic deformation can be described as a critical phenomenon. A lot of subsequent attention has been paid to understand the fundamental nature of this criticality: whereas the analysis of experiments suggests that scale-free behavior is characteristic only to the onset of yield, discrete dislocation dynamic (DDD) simulations hint at a more involved picture. Namely, the dynamics of the system is of glassy nature, where power-law distributions arise irrespective of the distance to the yielding threshold. These DDD simulations represent pure systems where neither Peierls stress nor any kind of impurities impede dislocation motion. In the talk we will discuss how addition of these realistic ingredients affect the critical behavior in terms of relaxation properties, avalanche statistics, dynamic correlations and system size dependence.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room8)

[SY-L4] Temporal and spatial plastic instability of micrometer-scaled materials

Invited

○Yinan Cui[1], Giacomo Po[1], Nasr Ghoniem[1]　(1. Mechanical and Aerospace Engineering Department, University of California, Los Angeles, United States of America)

Suppressing plastic instability is a critical goal to improve deformability and ductility in a wide variety of engineering applications. At temporal scale, plastic instability is manifested as intermittent burst and dislocation avalanches, leading to uncontrollable deformation. At spatial scale, plastic instability is manifested as the onset of flow localization, leading to sudden failure. While insight in the physical origin of plastic instability accumulates, the need for a quantitative description of temporal and spatial plastic instability remains challenged due to the lack of clear quantitative relation correlating deformation behavior with microstructural features. Here, we will discuss the quantitative description method of temporal and spatial plastic instability, and present a very simple model to predict them based on the idea of stochastic activation of dislocations sources. Combined with systematic discrete dislocation dynamics simulations, we will present that even though power law scaling is widely used to describe the statistical distribution of strain burst magnitude, power law scaling does not tell the whole story at temporal scale. At spatial scale, highly-irradiated materials will be taken as an example. We will unravel the mystery of how and why irradiation-induced defects enhance or inhibit plastic instability, and how and why dislocation channels arise, and what governs their width.

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H1] Symposium H-1

Chair: Turab Lookman(Los Alamos National Laboratory, United States of America)
Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room9

[SY-H1] **Multiscale modeling of electro-responsive gels**
　　　ºMasao Doi　(Beihang University, China)

[SY-H1] Non-monotonic particle size effect on the glass transition in polymer-
　　　particle blends and its application to shape memory polymers
　　　ºElias M. Zirdehi, Fathollah Varnik　(Ruhr-University Bochum, Germany)

[SY-H1] **Thermomechanical behavior of shape-memory polyurethane copolymer : A**
　　　coarse-grained molecular dynamics simulation
　　　ºSUNGWOO PARK, JUNGHWAN MOON, BYUNGJO KIM, MAENGHYO CHO　(Seoul National
　　　University, South Korea, Korea)

[SY-H1] **Investigation of photo-mechanical behavior of azobenzene-based polymer:**
　　　A coarse-grained molecular dynamics study
　　　ºJunghwan Moon[1], Byungjo Kim[1], Joonmyung Choi[2], Maenghyo Cho[1,3]　(1.Divison of Multiscale
　　　Mechanical Design, School of Mechanical and Aerospace Engineering, Seoul National University,
　　　Korea, 2.Mechatronics R&D center, SAMSUNG ELECTRONICS CO., LTD, Korea, 3.Institute of
　　　Advanced Machines and Design, Seoul National University, Korea)

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room9)

[SY-H1] Multiscale modeling of electro-responsive gels

Invited

○Masao Doi （Beihang University, China）

Certain kind of ionic gels show electro-mechanical coupling: the gel deforms when electric field is applied, and, conversely, electric field is created when the gel is deformed. Such phenomena may be used for actuators and sensors. In this talk, I will discuss the physical modeling of the electro-mechanical coupling in ionic gels.

[References] Masao Doi, Fluid transport in gels, Oxford Handbook of Soft Condensed Matter, Oxford

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room9)

[SY-H1] Non-monotonic particle size effect on the glass transition in polymer-particle blends and its application to shape memory polymers

○Elias M. Zirdehi, Fathollah Varnik （Ruhr-University Bochum, Germany）

Both via experiments and molecular dynamics simulations, it is shown that adding small molecules enhances the dynamics of structural relaxation in polymer melts and glasses [1]. While this effect is a monotonic function of concentration [1], it is found to be a non-monotonic function of particle size [2]. A detailed survey of non-Gaussian parameter for small molecules and polymer beads reveals a separation of time scales for cooperative motion between the above two species. This is indicative of a decoupling of the fast dynamics of small molecules from the chains' relaxation dynamics and a resulting weak effect. The dynamics of large particles, on the other hand, is strongly coupled to that of polymer. However, since large particles are only slightly more mobile than the polymer beads, their enhancing effect is also relatively weak. For intermediate particle sizes, the particles are sufficiently fast and the coupling to polymer strong enough to induce a large enhancement of the chains' relaxation kinetics. This non-monotonic effect occurs both for entangled and non-entangled polymers, hinting towards local packing effects as the main origin of the phenomenon [1]. It is shown that the effect can be explored in shape memory polymers to tune the triggering temperature of the shape recovery process in a non-monotonic manner.

 [1] Elias M. Zirdehi, Axel Marquardt, Gunther Eggeler and Fathollah Varnik, Molecular dynamics simulations of entangled polymers: The effect of small molecules on the glass transition temperature, Procedia Computer Science 198C, 265 (2017).

[2] Elias M. Zirdehi and Fathollah Varnik, Non-monotonic particle size effect on the glass transition in polymer-particle blends (submitted).

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room9)

[SY-H1] Thermomechanical behavior of shape-memory polyurethane copolymer : A coarse-grained molecular dynamics simulation

○SUNGWOO PARK, JUNGHWAN MOON, BYUNGJO KIM, MAENGHYO CHO （Seoul National University, South Korea, Korea）

Shape-memory polymers (SMPs) are smart materials that react to external stimuli to restore their original shape. The stimuli can be various things such as light, heat, humidity, and so on. Segmented polyurethane copolymer is a representative thermo-responsive SMP which are synthesized with a polyol and an isocyanate. The hard-segment which is clustered together helps to memorize the original shape by stabilizing the network, and the soft-segment which can achieve polymer crystallization acts as a switching-segment which fixes the temporary shape and induces the shape-memory effect. This dual-segment system is a necessary condition for shape-memory behavior of polyurethane. Full-atom molecular dynamics (MD) simulation can cover the atomistic structures and shape-memory properties, but it has limitations on observing mesoscale phenomena such as polymer crystallization, and micro-phase separation. To overcome this issue, we have developed a coarse-grained (CG) MD model with reduced degrees of freedom by treating multiple atoms as a single bead. Full-atom MD simulation was performed to obtain intra- and inter-bead potential of the CG model via iterative Boltzmann inversion (IBI) method. As a result, we could observe the crystallinity and shape-memory properties of SMPU models with different hard-segment contents. Then, the effect of microstructure on the mechanical deformation and shape memory behavior were investigated. We expect this study provides an insight to design the segmented polyurethane copolymer with enhanced shape recovery performance.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room9)

[SY-H1] Investigation of photo-mechanical behavior of azobenzene-based polymer: A coarse-grained molecular dynamics study

○Junghwan Moon[1], Byungjo Kim[1], Joonmyung Choi[2], Maenghyo Cho[1,3] （1.Divison of Multiscale Mechanical Design, School of Mechanical and Aerospace Engineering, Seoul National University, Korea, 2.Mechatronics R&D center, SAMSUNG ELECTRONICS CO., LTD, Korea, 3.Institute of Advanced Machines and Design, Seoul National University, Korea）

Photo-active deformable structures have drawn great attention because they can exhibit complex 3D deformations without any electronic circuit. Among the photo-responsive polymers (PRPs), liquid crystalline polymers (LCPs) doped with photochromic azobenzene molecules have diverse applications for soft micro-mechanical actuators because of a reversible photo-isomerization under ultraviolet (UV)/visible light illumination. The micro-scale photo-mechanical behavior of the polymer network can be greatly represented using conventional molecular dynamics (MD) simulations. However, MD simulation cannot be applied to examine the meso-scale phenomena occurred in the photo-deformable structure because too much degrees of freedom (DOFs) are required for full-atomistic description. To overcome this limitation, we propose a multi-scale/multi-physics computational framework based on a coarse-grained (CG) molecular dynamics simulation, which combines molecular switching induced by the photo-isomerization, and overall shape change of the polymer network. The structure-based iterative Boltzmann inversion (IBI) method was utilized to systematically represent the photo-chemical reaction-induced change of the polymeric structure, and effectively expand time- and length-scales of the atomistic simulations. As a result, we could observe the transition between three different liquid crystalline phases (smectic A - nematic - isotropic) under light irradiation, which cannot be reproduced using the all-atom MD simulations. Also, we investigated a unique photo-deformation of the smectic LCP network and its effect on the mechanical properties. We expect the proposed multiscale modeling and simulations to be a guideline for mechanically designing the photo-

responsive smart materials.

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H2] Symposium H-2

Chair: Hansohl Cho(Los Alamos National Laboratory, United States of America)
Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room9

[SY-H2] Hydrogels with Dynamic Sacrificial Bonds - From Toughness to Adhesion to Composites -

○Jian Ping Gong[1,2]（1.Faculty of Advanced Life Science, Hokkaido University, Japan, 2.Soft Matter GI-CoRE, Hokkaido University, Japan）

[SY-H2] Elastic properties and effective interactions of *in silico* realistic microgels

○Lorenzo Rovigatti[1,2], Nicoletta Gnan[1,2], Emanuela Zaccarelli[1,2]（1.Institute for Complex Systems, Uos Sapienza - CNR, Italy, 2.Dipartimento di Fisica, Sapienza Università di Roma, Italy）

[SY-H2] Controlling the mechanics of a synthetic hydrogel with motor-like internal contractility

Marcos Fernandez-Castano Romera[1], Rint P Sijbesma[1],
○Cornelis Storm[1]（1.Theory of Polymers and Soft Matter, Technische Universiteit Eindhoven, The Netherlands）

[SY-H2] Study on viscoelastic behavior of natural rubber with multiscale approach

○Byungjo Kim, Junghwan Moon, Maenghyo Cho（Seoul National University, Korea）

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room9)

[SY-H2] Hydrogels with Dynamic Sacrificial Bonds - From Toughness to Adhesion to Composites -

Invited

○Jian Ping Gong[1,2] （1.Faculty of Advanced Life Science, Hokkaido University, Japan, 2.Soft Matter GI-CoRE, Hokkaido University, Japan）

Invention of the tough double network hydrogels (DN gels), consisting of interpenetrated rigid/brittle network and soft/stretchable network, shows that the effective energy dissipation by the breaking of the covalent bond of the brittle network prevents catastrophic crack propagation upon deformation, and thus, gives the extraordinarily high toughness of the material. Such sacrificial bond effect has been successfully applied to develop tough double network hydrogels of diverse chemistry and also to double and triple network elastomer materials. Thus, sacrificial bond concept is proved to be a general approach for developing tough soft materials. As the internal rupture of DN gels is due to the irreversible breaking of the covalent bonds of the brittle network, the conventional DN gels deteriorate gradually after repeated deformation. To address this problem, many recent works have replaced the covalent bonds with non-covalent bonds to allow the sacrificial bonds to be reformed. In this talk, novel hydrogels with reversible sacrificial bonds developed in author's group are reviewed and their excellent mechanical behaviors such as high toughness, self-healing, adhesion to biological tissues, and fast underwater adhesion are demonstrated. Furthermore, this principle is extended to develop tough composites using tough hydrogels as energy dissipative soft matrix.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room9)

[SY-H2] Elastic properties and effective interactions of *in silico* realistic microgels

○Lorenzo Rovigatti[1,2], Nicoletta Gnan[1,2], Emanuela Zaccarelli[1,2] （1.Institute for Complex Systems, Uos Sapienza - CNR, Italy, 2.Dipartimento di Fisica, Sapienza Università di Roma, Italy）

The bulk behaviour of colloidal suspensions depends crucially on the microscopic details of the particle-particle interaction[1]. For polymer-based building blocks, the interactions depend on a large number of parameters such as the particle microstructure, its composition and related physico-chemical properties (solvophobicity, charge density, *etc.*). Among the huge variety of available systems, stimuli-responsive microparticles built out of polymer networks, so-called microgels, have emerged as one of the most interesting class of soft particles, for both a theoretical and applicative standpoint[2].

Here we build upon a recently-developed method[3] to generate and simulate realistic *in silico* microgels. We first look at the single-particle mechanics by calculating the elastic moduli in the small-deformations regime. We then use Umbrella Sampling and a generalised Widom insertion method to accurately estimate the two-body effective interaction.

We show for the first time that the Hertzian theory works well for large separations, and that in this regime the single-particle elastic moduli can predict the amplitude of *V(r)* for a wide range of network topologies. However, for smaller separations the two microgels start to strongly interact and change their shape and *V(r)* deviates from the predicted Hertzian behaviour.

This work establishes a clear link between the microscopic network properties and the resulting microgel-microgel interactions, paving the way for a deeper understanding of the bulk behaviour of microgel

suspensions.

[1] C. N. Likos, Phys. Rep., **348**, 267 (2001)

[2] A. Fernandez-Nieves, H. Wyss, J. Mattsson, D. A. Weitz, *Microgel Suspensions: Fundamentals and Applications*; John Wiley &Sons (2011)

[3] N. Gnan, L. Rovigatti, M. Bergman, E. Zaccarelli, Macromolecules, **50**, 8777 (2017)

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room9)

[SY-H2] Controlling the mechanics of a synthetic hydrogel with motor-like internal contractility

Marcos Fernandez-Castano Romera[1], Rint P Sijbesma[1],
○Cornelis Storm[1]   (1.Theory of Polymers and Soft Matter, Technische Universiteit Eindhoven, The Netherlands）

Stiffening due to internal stress generation is common in living materials and regulates many biomechanical processes. For example, cells stiffen their surrounding matrix by pulling on collagen and fibrin fibers. At the subcellular level, molecular motors prompt fluidisation and stiffening of the cytoskeleton by sliding polar actin filaments in opposite directions. I will present results showing that synthetic materials, likewise, are able to change their stiffness in response to internally generated and externally applied forces. Theoretical and experimental results are presented for a system where chemical crosslinking of thermoresponsive poly(N-isopropylacrylamide) (PNIPAM) into a fibrous matrix of synthetic semi-flexible polymers allows for internal stress generation upon induction of coil-to-globule transition, resulting in a macroscopic stiffening response spanning up to three orders of magnitude. Strikingly, the forces generated by PNIPAM collapse are sufficient to drive a fluid material into a stiff gel within a few minutes. Rigidified networks dramatically stiffen in response to applied stress featuring power law rheology with exponents that match those of reconstituted actomyosin networks pre-stressed by molecular motors. This concept holds potential for the rational design of responsive synthetic materials that are fluid at room temperature and rapidly rigidify at body temperature to form hydrogels mechanically compatible to cells or tissues.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room9)

[SY-H2] Study on viscoelastic behavior of natural rubber with multiscale approach

○Byungjo Kim, Junghwan Moon, Maenghyo Cho （Seoul National University, Korea）

In this study, the viscoelastic behavior of natural rubber is investigated with the aid of a coarse-grained (CG) molecular dynamics (MD) simulation. It is challenging to understand the long-term nature of polymeric materials using a conventional MD simulation due to the inherent limitation in the time and length scale. To overcome the drawback in terms of scalability in time and length, the CG model can offer a way to assess the long-term physical behavior by substantially reducing a degree of freedoms with the implementation of bead particles which are equivalent to the specific group of atoms. To describe the inter- and intra-interactions between the beads consisting of the system, the iterative Boltzmann inversion (IBI) method is employed. As an important viscoelastic behavior of elastomer, the time-dependent shear relaxation modulus is calculated

using the stress autocorrelation function. The dynamic modulus in a frequency domain is further studied with using the Fourier transformation. The influence of vulcanization and chain length of natural rubber is taken into account. Plus, the spherical shape of SiO_2 nanoparticles are considered as filler materials, and the behavior of filler-rubber is also studied for varying filler loading conditions. With the present work, the viscoelastic nature of rubber is understood by employing CG MD simulations which can enhance the scale of computation in terms of length and time. Further, this work can be extended to examine more complex polymeric system regarding the long-term physical nature or thermodynamic property.

Symposium | J. Multiscale Modeling of Heterogeneous Layered Media

[SY-J3] Symposium J-3

Chairs: Ramesh Talreja(Texas A&M University, United States of America), Tong-Earn Tay(National University of Singapore, Singapore)

Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room10

[SY-J3] Fundamentals of Generalized Particle (GP) Multiscale Methods with Applications to Analyses of Alternatively-Arranged Soft and Hard Layers

○Jinghong Fan （Kazuo Inamori School of Engineering, Alfred University, United States of America）

[SY-J3] **The effect of layer thickness ratio on the plastic deformation mechanisms of nonoindented Ti/TiN nanolayered composite: A molecular dynamics study**

○Georges Y Ayoub[1], Wei yang[2], Iman Salehinia[3], Bilal Mansoor[2], Hussein Zbib[4] （1.Dept. of Industrial and manufacturing system Engineering, Univ. of Michigan, United States of America, 2.Dept. of Mechanical Engineering, Texas A&M Univ., United States of America, 3.Dept. of Mechanical Engineering, Northern Illinois Univ., United States of America, 4.School of Mechanical and Materials Engineering, Washington State Univ., United States of America）

[SY-J3] The attenuation of stress wave propagation in multilayer structure

○Fengyuan Yang, Zhanli Liu （Tsinghua University, China）

[SY-J3] **Multiscale molecular-dynamics simulations of structure and mechanics of polymer nanocomposites**

○Alexey Lyulin[1,2] （1.Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands, 2.Center for Computational Energy Research, Department of Applied Physics, Eindhoven University of Technology, Netherlands）

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room10)

[SY-J3] Fundamentals of Generalized Particle (GP) Multiscale Methods with Applications to Analyses of Alternatively-Arranged Soft and Hard Layers

Invited

○Jinghong Fan （Kazuo Inamori School of Engineering, Alfred University, United States of America）

Alternatively-placed soft and hard layers are investigated using multiscale generalized particle methods, namely the GP and/or XGP methods (Fan 2009, Xu, Fan et al. 2016, Fan et al. 2017). In the methods, material models are divided as several domains with generalized particle of different scales. The distinguished characteristics of the GP methods are that each higher scale particle is formed by lumping the lower scale particle or atoms but their structures are all the same as the atomistic one, such as BCC, FCC and HCP. The fundamentals of this type of multiscale analysis are based on the local bottom-up multiscale analysis. Specifically, the position, mass and physical property of the upper-level particle is determined by all lower-level particles (e.g. atoms) within the individual particle's neighbor link cell (NCL), thus the material behavior naturally follows the displacement and motion of these atoms consisted of the material and the numerical algorithm follows the typical molecular dynamics.

Extrinsic and intrinsic size effects has been successfully investigated to confirm the accuracy and efficiency of the proposed multiscale methods. Among several interesting observations of the atomistic/multiscale simulations, results show that defects in the soft, hard layers and their interface due to loading and manufacturing determine, to a large extent, their deformation and failure behavior. It has been found that some observations are different from previous predictions in the literature for a long period. For instance, simulations show that Langford's famous prediction (1977) of dislocations appearance in cementite layer is not fully accurate. In addition, a direct check of the dislocation pile-up theory proposed by Eshelby, Frank and Nabarro (1951) indicate that the simulation-determined interface stress is much lower than their theory-predicted one.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room10)

[SY-J3] The effect of layer thickness ratio on the plastic deformation mechanisms of nonoindented Ti/TiN nanolayered composite: A molecular dynamics study

○Georges Y Ayoub[1], Wei yang[2], Iman Salehinia[3], Bilal Mansoor[2], Hussein Zbib[4] （1.Dept. of Industrial and manufacturing system Engineering, Univ. of Michigan, United States of America, 2.Dept. of Mechanical Engineering, Texas A&M Univ., United States of America, 3.Dept. of Mechanical Engineering, Northern Illinois Univ., United States of America, 4.School of Mechanical and Materials Engineering, Washington State Univ., United States of America）

Molecular dynamics simulations were performed to identify the underlying deformation mechanisms controlling the plastic behavior of nanoindented nanoscale multilayered Ti/TiN. MD simulations were conducted on pure Ti and pure TiN as well as on four different layer-thickness ratios of Ti/TiN multilayers, Ti:TiN=1, 2.5, 4, and 7.5. The Ti layer thickness varied from 2nm to 15nm. The plastic deformation of nanoindented pure Ti was dominated by the formation of dislocation loops resulting from basal partial dislocations, while very few perfect dislocations that tie dislocation loops together were observed. The plastic

deformation of nanoindented pure TiN was controlled by the activation of perfect dislocation propagation along the *111* plane that dissociates into two partials. Depending on the thickness ratio, either dislocation pile-up or single dislocation crossing through the interface was the controlling plastic deformation mechanism of nanoindented Ti/TiN multilayers. For metal layer thicknesses above 5nm, significant dislocation pile-ups were observed at the interface of the quad-layered samples. The Ti/TiN multilayer with a thickness ratio of 1:1 with individual layer thickness of 2nm exhibited the highest strain-hardening rate. At this length scale, the activation of dislocation sources requires very high stresses, and the single dislocation crossing process is the most dominant deformation mechanism. The initiation of plasticity in the TiN layer occurs at a high level of stress since there is no dislocation pile-up at the interface.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room10)

[SY-J3] The attenuation of stress wave propagation in multilayer structure

○Fengyuan Yang, Zhanli Liu （Tsinghua University, China）

In recent years, many biological structures with excellent impact resistance have been studied, such as the stomatopod dactyl club, fish scales, etc. These biological structures have a multi-layered structure and each layer structure has different material properties. These specific bio-layered structures not only have higher hardness and modulus, but also have higher dissipative stress wave performance. In this paper, the influence of the material properties and the arrangement order of the multilayer structure on the propagation of stress waves is studied, in order to obtain a multilayer structure with higher attenuation stress wave energy. The propagation of stress wave in the material of viscoelastic layer changes with the frequency of stress wave. The transmission coefficient of the stress wave in the multilayer structure has frequency effect and size effect.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room10)

[SY-J3] Multiscale molecular-dynamics simulations of structure and mechanics of polymer nanocomposites

○Alexey Lyulin[1,2] （1.Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands, 2.Center for Computational Energy Research, Department of Applied Physics, Eindhoven University of Technology, Netherlands）

Using multiscale modelling approach we performed molecular-dynamics simulations of both coarse-grained and detailed atomistic (polyimide R-BAPB) amorphous polymer melts consisting of non-entangled, non-crosslinked polymer chains. The inorganic filler surfaces were mimicked either by solid walls, or by explicit insertion of the filler particles. The rise in the glass-transition temperature with increase of the filler fraction was accompanied by a monotonic slowing-down of the relaxation of the incoherent scattering function on all simulated length scales. The filler surface roughness could also lead to slower segmental relaxation. Higher dynamic fragility was observed for smaller film thicknesses.
The cyclic shear deformation is performed to characterize macroscopic properties of the systems before and after filler insertion. The reported coarse-grained simulations show a strong decrease of the nanocomposites storage modulus with increasing strain amplitude, which is accompanied by a maximum in the loss modulus (the so-called Payne effect); the onset of the softening is observed in the linear regime of deformation at

strain amplitude of about 0.01. Moreover, the dependence of the storage modulus on the instantaneous strain exhibits both softening and hardening regimes, in agreement with Large Amplitude Oscillatory Shear (LAOS) experiments. The observed hardening is caused by the shear-induced decrease of the non-affine diffusion of the polymer segments due to filler particles acting as effective crosslinks between polymeric chains and, hence, hindering diffusion. Moreover, the formation of glassy immobile layers at the nanoparticle interface strongly increases the storage modulus at low strain amplitudes. The strain softening with increasing strain amplitude is connected to the mobilization of these glassy layers and an *increase in the dynamic heterogeneity* of the polymer matrix.

Symposium | J. Multiscale Modeling of Heterogeneous Layered Media

[SY-J4] Symposium J-4

Chairs: Brian Cox(Arachne Consulting Inc., United States of America), Tomonaga Okabe(Tohoku University, Japan)

Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room10

[SY-J4] Validation of analytical models for ply cracking of general symmetric composite laminates

○TOMONAGA OKABE （Department of Aeroscpace Engineering, Tohoku University, Japan）

[SY-J4] Two-way coupled modeling of lithium diffusion and diffusion induced finite elastoplastic bending of bilayer electrodes in lithium-ion batteries

Jun Yin, ○Junqian Zhang （Shanghai University, China）

[SY-J4] **Micro-Scale Model of Thermomechanics in Solidifying Saturated Porous Media**

○Michal Benes, Alexandr Zak （Czech Technical University in Prague, Czech Republic）

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room10)

[SY-J4] Validation of analytical models for ply cracking of general symmetric composite laminates

Invited

○TOMONAGA OKABE （Department of Aeroscpace Engineering, Tohoku University, Japan）

Validation of analytical models for ply cracking of general symmetric composite laminates

Polymer matrix composites (PMCs) that have high specific strength and specific rigidity have been used in aerospace fields. Laminates made by stacking unidirectional fiber-reinforced lamina, which have predefined mechanical properties, are commonly used. Fiber-reinforced laminates have a specific fracture mode such as transverse cracking, delamination, and breakage of the fiber. Of these fracture modes, transverse cracking occurs in the earliest stage. In laminates with plies in different fiber orientations, transverse cracks can form from defect in a given ply, and grow traversing the thickness of the ply and running parallel to the fibers in that ply. The most direct effect of transverse cracking is reduction of the thermomechanical properties of the laminate, including changes in the effective values of Young's moduli, Poisson's ratios, and thermal expansion coefficients. Substantial transverse cracking may give rise to more deleterious forms of damage, or provide pathways for the entry of moisture and corrosive liquids. Thus, although this damage mode is not critical from a final fracture point of view, it can result in significant degradation in the properties of laminates. Therefore, it is necessary to understand the mechanical behavior of laminate including transverse cracks. The continuum damage mechanics (CDM) is considered to be a valid approach to this issue. This approach utilizes the internal state variable and damage variable to consider the effect of transverse cracks on the reduction of stiffness.

In this study, the three-dimensional local stress field (3-D LSF) model was formulated at first. Secondly, a Tohoku continuum damage mechanics (TCDM) model, which is an energy-based model of ply cracking of general composite laminates, was presented using the 3-D LSF model and the CDM approach. Especially, the damage variable d_2 in the direction normal to the fiber was derived for the ply including transverse cracking as a function of transverse crack density using the 3-D LSF model. Finally, the validity of the TCDM model was estimated by comparing the NPL model and the experiment results.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room10)

[SY-J4] Two-way coupled modeling of lithium diffusion and diffusion induced finite elastoplastic bending of bilayer electrodes in lithium-ion batteries

Invited

Jun Yin, ○Junqian Zhang （Shanghai University, China）

A fully coupling model for diffusion induced finite elastoplastic bending of bilayer electrodes in lithium-ion batteries is proposed. The effect of mechanical stress on lithium diffusion is accounted for by the mechanical part of chemical potential derived from Gibbs free energy along with use of logarithmic stress and strain. Eight dimensionless parameters, which govern the stress-assisted diffusion and the diffusion induced elastoplastic bending, are identified. It is found that the finite plasticity starting from the interface of bilayer

increases the chemical potential gradient and thereby facilitates lithium diffusion. The full plastic flow makes the abnormal lithium concentration distribution possible that the concentration at the lithium inlet is lower than the concentration at the interface (downstream). The increase in thickness of active layer during charging is much larger than the eigen-stretch due to lithiation, and this excess thickening is found to be caused by the lithiation induced plastic yield.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room10)

[SY-J4] Micro-Scale Model of Thermomechanics in Solidifying Saturated Porous Media

○Michal Benes, Alexandr Zak （Czech Technical University in Prague, Czech Republic）

In the contribution, we discuss the model of solidification of melt occupying pores of the porous medium with grains intact but participating in the heat transfer. The research motivation is given by development of advanced materials as well as by climate changes. The model is based on coupled heat conduction equation and the phase-field. We present the model and several computational studies.

Solidiffication inside the porous medium is accompanied by complex processes affected by the material composition, micro-scale interfaces between phases within the medium, bulk properties of the presented phases, and ambient physical conditions. Volumetric changes of the liquid presented in pores subjected to phase change conditions is one of crucial phenomena. Due to the generic inhomogeneity of volume occupied by the solidifying porous medium, we focus on treating the phase transition at microscale. We have developed a micro-scale model describing mechanical, thermal, and phase change processes within a small sample of a porous medium. The phase change is described in the Lagrangian framework by means of the energy, Navier, and phase-field equations. A coupling of multi-physics and multiple phases is introduced. The model provides spatio-temporal dependencies of primary variables, the resulting forces exerted on grain surfaces by the change in specific volume due to phase transition, and possibly, the mean values of the key quantities useful for upscaling. The role of the model is demonstrated on several computational studies which follow recently published results [1-2].

[1] Žák A., Beneš M. and Illangasekare T.H. Analysis of Model of Soil Freezing and Thawing, IAENG International Journal of Applied Mathematics, Volume 43, Issue 3, pp. 127--134, September 2013

[2] Žák A., Beneš M., Illangasekare T. H., Trautz A. Mathematical Model of Porous Medium Freezing at Micro-Scale, to appear in Communications in Computational Physics, 2018

Plenary Talk | Plenary Talk

[PL4] Plenary Talk 4

Grain boundary sliding, fracture and dislocation motion in ceramics

Chair: Erik Bitzek(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)

Wed. Oct 31, 2018 8:30 AM - 9:20 AM Room1

Yuichi Ikuhara

[PL4] Plenary Talk 4

○Yuichi Ikuhara （The University of Tokyo/Japan Fine Ceramics Center, Japan）

(Wed. Oct 31, 2018 8:30 AM - 9:20 AM Room1)

[PL4] Plenary Talk 4

Grain boundary sliding, fracture and dislocation motion in ceramics

○Yuichi Ikuhara （The University of Tokyo/Japan Fine Ceramics Center, Japan）

Ceramics have been widely used for structural applications because of their superior mechanical properties at high temperatures. It has been known that the behavior of GB sliding is strongly dependent on the GB characters such as misorientation angle between two adjacent crystals and GB plane, however, such effect has not been clarified yet. In addition, this effect in much influenced by dopant segregation at GBs. In this study, in order to clarify the atomistic mechanisms of GB sliding and its dopant effect, bicrystal studies have been performed to find the relationship between the atomic structures, chemistry and GB sliding behavior of Al_2O_3 ceramics. Several kinds of bicrystals including GBs with specific geometrical configuration were fabricated, and some of them were doped by rare-earth elements to enhance the GB segregation.

It has been reported that several oxides can be plastically deformed even at R.T. by dislocation slip like metals. So far, many experimental investigations have been tried for understanding the dislocation-grain boundary interaction, but these experiments were mostly carried out statically, and the fundamental processes are still not well understood yet. In this study, the nanoindentation experiments were conducted for $SrTiO_3$ crystals their bicrystals inside TEM. Several kinds of TEM specimens for in situ nanoindentation experiments were prepared, that are single crystals and bicrystals including various types of GBs. The $SrTiO_3$ single crystals were indented with the sharp diamond tip and successfully observed the dislocation dynamics. In the case of the GBs, the interaction between the introduced lattice dislocations and the GBs were directly observed. The dislocation-GB interaction and its dependence on the GB characters will be discussed in detail.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C5] Symposium C-5

Chair: Christopher Woodward(Air Force Research Laboratory, United States of America)

Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room1

[SY-C5] **Plasticity and Fracture in Transition Metal Carbides**

○Giacomo Po[1], Suneel Kodambaka[2], Jeffrey M Wheeler[3], Davide Sangiovanni[4] （1.University of California Los Angeles, Mechanical Engineering Department, United States of America, 2.University of California Los Angeles, Materials Science and Engineering Department, United States of America, 3.Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Mechanics of Materials and Nanostructures, Swaziland, 4.Department of Physics, Chemistry and Biology, Linköping University, Sweden）

[SY-C5] Atomic Scale Investigation of Plasticity in Laves phases

○Julien Guenole[1], Fatim-Zahra Mouhib[1], Christoffer Zehnder[1], James Gibson[1], Blazej Grabowski[2], Sandra Korte-Kerzel[1] （1.Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Germany, 2.Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany）

[SY-C5] Nucleation of dislocation in ultra-hard ceramic nanoparticles modelled by molecular dynamics and nudged elastic band simulations

○Jonathan Amodeo[1], Emile Maras[2] （1.MATEIS, Univ. Lyon 1, France, 2.SRMP, DEN, CEA, Gif-sur-Yvette, France）

[SY-C5] Multiscale discrete dislocation dynamics modeling of nano-indentation near the grain boundary

○Xu Zhang, Songjiang Lu （School of Mechanics and Engineering, Southwest Jiaotong University, China）

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room1)

[SY-C5] Plasticity and Fracture in Transition Metal Carbides
Invited

○Giacomo Po[1], Suneel Kodambaka[2], Jeffrey M Wheeler[3], Davide Sangiovanni[4] （1.University of California Los Angeles, Mechanical Engineering Department, United States of America, 2.University of California Los Angeles, Materials Science and Engineering Department, United States of America, 3.Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Mechanics of Materials and Nanostructures, Swaziland, 4.Department of Physics, Chemistry and Biology, Linköping University, Sweden）

Current and future applications in hypersonic flight, re-entry vehicles, propulsion, and power production create an insatiable demand for materials capable to perform in severe environments. Materials for these applications must possess a rare combination of properties, which include high specific strength, elevated melting temperature, high thermal conductivity, and low thermal expansion coefficient. Ultra-High Temperature Ceramics are being considered for applications in extreme environments, especially when oxidation is a major concern. Currently, the factor limiting the use of UHTCs as structural materials is their low-temperature brittleness. This talk focuses on the plasticity and fracture mechanisms of the transition metal carbide TaC, one of the highest melting temperature materials known to mankind. *In-situ* micro-pillar compression experiments carried out at different temperatures and orientations reveal unexpected intrinsic ductility of TaC, which contrasts its well-known bulk brittleness. These findings unveil new properties of the material, such as a pronounced non-Schmid behavior and a remarkable temperature/orientation dependence of the yield strength. A variety of multiscale modeling techniques ranging from *ab-initio* to discrete dislocation dynamics simulations are employed to understand the small-scale behavior of TaC. Computer simulations shed light on the room-temperature brittleness of TaC by explaining the link between plastic deformation and fracture.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room1)

[SY-C5] Atomic Scale Investigation of Plasticity in Laves phases
○Julien Guenole[1], Fatim-Zahra Mouhib[1], Christoffer Zehnder[1], James Gibson[1], Blazej Grabowski[2], Sandra Korte-Kerzel[1] （1.Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Germany, 2.Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany）

The strengthening mechanisms in magnesium alloys are strongly related to the complex intermetallic precipitates that spread all over the microstructure. In particular, the hard and brittle Laves phases [1] commonly observed in such alloys exhibit a complex atoms stacking with largely unknown plasticity mechanisms [2].

We propose here a numerical atomistic approach at the cross-road of experiments and *ab initio* simulations, to shed light on the responsible mechanisms for the plasticity in hexagonal Mg_2Ca (C14) Laves phases. Elastic and plastic properties of bulk Laves phase are investigated by both first principle and classical atomistic simulations. Molecular dynamics/statics simulations with a robust MEAM interatomic potential are performed to study the propagation of dislocations, by a combination of nudge-elastic-band (NEB) methods and nano-mechanical tests. In particular, the cross-slip to pyramidal slip planes, the propagation of dislocations in the basal plane by the so called synchroshear mechanism [3,4] and the influence of temperature on slip systems activation, are investigated at the atomic scale. All these results are finally correlated and discussed by considering experimental findings, especially from micro-pillar compression

tests. Our goal is to improve the understanding of the largely unknown plasticity of Laves phases.

References:
[1] - F. Laves and H. Witte, Metallwirtsch. Metallwiss. Metalltech. **15**, 840 (1936).
[2] - M.F. Chisholm, et al., Science **307**, 701 (2005)
[3] - P.M. Hazzledine et al., MRS Proceedings **288**, 591 (1992)
[4] - P.M. Hazzledine and P. Pirouz, Scripta metallurgica et materialia **28**, 1277 (1993).

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room1)

[SY-C5] Nucleation of dislocation in ultra-hard ceramic nanoparticles modelled by molecular dynamics and nudged elastic band simulations

○Jonathan Amodeo[1], Emile Maras[2]　(1.MATEIS, Univ. Lyon 1, France, 2.SRMP, DEN, CEA, Gif-sur-Yvette, France)

Micro- and nano-sized structures have attracted substantial interest due to their special mechanical behavior: they generally show an increased yield strength compared with the bulk material as well as an improved ductility. Among them, nanoparticles (NPs) which are generally used for their shape-dependent functional properties also appear as perfect candidates for submicronic plasticity investigations due to their broad range of sizes and their variety of shapes. While metallic and silicon NPs have been widely investigated since almost two decades, less is known about the strength of ceramic NPs maybe due to the brittleness of their bulk counterparts.

In the light of recent but preliminary in situ TEM observations, we investigate here the mechanical behavior of <100>-oriented MgO nanocubes. First, incipient plasticity mechanisms are investigated using molecular dynamics simulations (MD) of virtual nanocompression tests at constant strain rate. Results show that the plastic deformation of MgO nanocubes starts with the nucleation from the surface of perfect ½<110>{110} dislocations under ultra-high stresses, one order of magnitude larger than what is generally observed in fcc metals. However, as MD simulations can only be carried out at strain rates several orders of magnitude larger than experimental ones,we used the nudged-elastic-band method to calculate the activation energy for the nucleation of the dislocation as a function of stress, particle size and dislocation nucleation site. With the help of the transition state theory, the nucleation stress can then be estimated as a function of temperature and experimental strain rate. We find that due to the large stiffness of the activation energy *vs.*stress curve, the strain rate has a much smaller influence on the nucleation stress than what is found for metallic nanocrystals and therefore, that the nucleation stress estimated using MD is close to that corresponding to experimental strain rate.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room1)

[SY-C5] Multiscale discrete dislocation dynamics modeling of nano-indentation near the grain boundary

○Xu Zhang, Songjiang Lu （School of Mechanics and Engineering, Southwest Jiaotong University, China）

Nano-indentaiton is a convenient method to investigate the mechanical properties of material by utilizing the low-loads and small-scale displacements. However, grain boundary (GB) effect on nano-indentation response needs detailed microstructure and mechanism analysis, which has been a long technique challenge. We developed a three-dimensional multiscale modeling framework, which couples the three-dimensional discrete dislocation dynamics with finite element method, and use it to investigate the GB effects on nano-indentation of aluminum bicrystal. The interaction between dislocations and GB is physically considered by introducing a penetrable GB, where dislocation pile-ups can penetrate through GB and dislocation debris at GB can be re-emitted into grain interior. In the simulation, we confirmed two experimentally observed phenomena, i.e., pop-in events and the dependence of indentation hardness on distance to GB. The pop-in events are correlated with the activation and multiplication of dislocations, especially, the GB pop-in event results from the dislocations penetration through GB. By changing the distances from indenter to GB, the simulation shows that the indentation hardness increases with the decrease of GB-indenter distance. The size effect of nano-indentation results from the geometrically necessary dislocation density distributed within the constraint volume between GB and the indenter.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C6] Symposium C-6
Chair: Jaime Marian(Dept. of Materials Science and Engineering, University of California Los Angeles, United States of America)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room1

[SY-C6] Effect of interstitial solutes on the structure and mobility of screw dislocations in bcc metals
Berengere Lüthi[1], Lisa Ventelon[1], David Rodney[2], Emmanuel Clouet[1], Bernard Legrand[1], Fabienne Berthier[3], ◯Francois Willaime[4] （1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, France, 2.Institut Lumière Matière, CNRS-Université Claude Bernard Lyon 1, France, 3.Synthèse, Propriétés et Modélisation des Matériaux /Institut de Chimie Moléculaire et des Matériaux d'Orsay, Université Paris-Saclay, France, 4.DEN-Département des Matériaux pour le Nucléaire, CEA, Université Paris-Saclay, France）

[SY-C6] Effect of solutes on dislocation motion in dilute hcp and bcc alloys
◯Tomohito Tsuru[1,2], Mitsuhiro Itakura[1], Masatake Yamaguchi[1,2], Tomoaki Suzudo[1], Masato Wakeda[3], Shigenobu Ogata[2,4], Daryl C Chrzan[5] （1.Japan Atomic Energy Agency, Japan, 2.ESISM, Kyoto University, Japan, 3.National Institute for Materials Science, Japan, 4.Osaka University, Japan, 5.University of California, Berkeley, United States of America）

[SY-C6] Investigation of the energy pathway for generation of dislocations in silicon at Σ3 grain boundaries with the kinetic Activation-Relaxation Technique
◯Simen Nut Hansen Eliassen[1], Normand Mousseau[3], Mickaël Trochet[3], Yanjun Li[1], Jesper Friis[2], Inga Gudem Ringdalen[2] （1.Dept. of Materials Science and Engineering, Norwegian Univ. of Science and Technology, Norway, 2.SINTEF Materials and Chemistry, Norway, 3.Dept. of Physics, Univ. de Montréal, Canada）

[SY-C6] Prediction of mechanical twinning in post-perovskite structure
◯Philippe Carrez, Alexandra Goryaeva, Patrick Cordier （Lille University, Lab. UMET UMR-CNRS 8207, France）

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room1)

[SY-C6] Effect of interstitial solutes on the structure and mobility of screw dislocations in bcc metals

Invited

Berengere Lüthi[1], Lisa Ventelon[1], David Rodney[2], Emmanuel Clouet[1], Bernard Legrand[1], Fabienne Berthier[3], ○Francois Willaime[4]　(1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, France, 2.Institut Lumière Matière, CNRS-Université Claude Bernard Lyon 1, France, 3.Synthèse, Propriétés et Modélisation des Matériaux /Institut de Chimie Moléculaire et des Matériaux d'Orsay, Université Paris-Saclay, France, 4.DEN-Département des Matériaux pour le Nucléaire, CEA, Université Paris-Saclay, France）

There is ample experimental evidence of the effects of solute interactions with dislocations, such as Cottrell atmospheres and dynamical strain ageing (DSA). In this work we investigated, using Density Functional Theory (DFT) electronic structure calculations, the interaction between interstitial solute atoms, in particular carbon, and screw dislocation cores in body centered cubic (bcc) metals, in particular iron.
First considering carbon in bcc Fe, our calculations evidence a strong attractive interaction of carbon with screw dislocation cores inducing an unexpected reconstruction towards a hard-core configuration, which is unstable in pure metals. The carbon atoms are at the center of regular trigonal prisms formed by the Fe atoms. Around this decorated core, the 4th nearest neighbor octahedral sites are found to be also highly attractive for carbon. The complex thermodynamic behavior of carbon segregation on these dislocation sites, as function of temperature and bulk carbon concentration, is modelled using mean field and Monte Carlo methods. The parameters of the Hamiltonian, fitted to DFT calculations, account for the C-C repulsions between neighboring sites. It is concluded that in the temperature range corresponding to the occurrence of DSA, the carbon atoms occupy every other prismatic sites, while the other sites are essentially empty. This configuration is then used to study the kink-pair mechanism suggested by in situ straining experiments. The results obtained for the kink-pair formation energy and single kink migration energies are consistent with the activation energy of the end of DSA regime.
The solute segregation on dislocation-core prismatic sites was investigated for other solutes in Fe and for C in other bcc metals. A behavior similar to Fe-C is exhibited for B, N and O in Fe and for C in group 6 metals, Mo and W, but with solute-solute interactions between prismatic sites which can be either attractive or repulsive. By way of contrast, the configuration of lowest energy in group 5 consists of the dislocation in its easy core and the carbon atom in a fifth nearest neighbor octahedral site. We show that this group dependence is consistent with the carbon local environment in the stable stoichiometric carbide structures, namely cubic NaCl-type for group 5 and hexagonal WC-type for group 6.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room1)

[SY-C6] Effect of solutes on dislocation motion in dilute hcp and bcc alloys

○Tomohito Tsuru[1,2], Mitsuhiro Itakura[1], Masatake Yamaguchi[1,2], Tomoaki Suzudo[1], Masato Wakeda[3], Shigenobu Ogata[2,4], Daryl C Chrzan[5]　(1.Japan Atomic Energy Agency, Japan, 2.ESISM, Kyoto University, Japan, 3.National Institute for Materials Science, Japan, 4.Osaka University, Japan, 5.University of California, Berkeley, United States of America）

Unlike fcc metals, where dislocation motion associated with solutes is reproduced by the effect of solute on the stacking fault energy and conventional hardening law, solutes in bcc and hcp metals induce more unique

effects such as softening and dramatic change in plastic deformation. Recently, modeling of dislocations based on first-principles calculations was developed, and the modeling for various crystallographic structure were systemized. Especially for BCC metals, solid-solution model was established based on the thermally-activated process of double-kink nucleation and kink migration related to Orowan's relation. Furthermore, DFT calculations found to have a great role in providing fundamental properties of these kink-related process and reproduced solution softening behavior. While the Burgers vector of the primary slip system in HCP metals is generally dislocation, the slip plane differs depending on the material, which mainly belongs to basal and prismatic plane according to the its stacking fault energy. Solute atoms have a large variety of the influence on dislocation motion resulting in dramatic change in plastic deformation.

In the present study, we implemented first-principles calculations to obtain corresponding data to the fundamental properties of dislocation motion. We will discuss the effect of transmutation product on solid solution softening in BCC tungsten and the change in slip system caused by a specific solute in HCP titanium.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room1)

[SY-C6] Investigation of the energy pathway for generation of dislocations in silicon at $\Sigma 3$ grain boundaries with the kinetic Activation-Relaxation Technique

○Simen Nut Hansen Eliassen[1], Normand Mousseau[3], Mickaël Trochet[3], Yanjun Li[1], Jesper Friis[2], Inga Gudem Ringdalen[2] （1.Dept. of Materials Science and Engineering, Norwegian Univ. of Science and Technology, Norway, 2.SINTEF Materials and Chemistry, Norway, 3.Dept. of Physics, Univ. de Montréal, Canada）

Multicrystalline silicon (mc-Si) is widely used for solar cell applications due to the low production costs and high efficiency. However, the crystallization processes of mc-Si induces different kinds of defects in the structure which reduces the overall conversion efficiency. Regions containing a high density of defects such as dislocations are especially detrimental. The origin of dislocations is an ongoing debate. Previous studies indicates that generation of dislocations in mc-Si can occur at $\Sigma 3$ grain boundaries; however, a detailed atomistic description of the mechanisms governing the generation of dislocations is lacking. To cast light on the mechanisms behind generation of dislocations, we have deployed the kinetic Activation-Relaxation Technique (k-ART), an off-lattice Kinetic Monte Carlo code with an on-the fly cataloging of events. K-ART allows us to construct an extensive description of the energy landscape around defects and obtain the energy barriers of diffusion pathways. Furthermore, this is achievable at a time scale and in a temperature regime relevant to experimental observations. In this work, we have constructed a model structure containing an asymmetric and a symmetric $\Sigma 3$ grain boundary which are joined together to form a kink. We present here an energy pathway for generation of dislocations from the kink with the associated energy barriers, and how the energy barriers is affected when the system is subjected to a shear force.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room1)

[SY-C6] Prediction of mechanical twinning in post-perovskite structure

○Philippe Carrez, Alexandra Goryaeva, Patrick Cordier （Lille University, Lab. UMET UMR-CNRS 8207, France）

The plastic properties of $MgSiO_3$ post-perovskite are believed to be one of the key issues for the understanding of the recorded seismic anisotropy at the bottom of the Earth in a thin layer at the boundary between Earth mantle and Earth core. Indeed, the seismic waves velocities are sensitive to the development of crystallographic preferred orientations directly related to the plastic properties of the phases. Experimental results from high pressure deformation experiments, have unfortunately led to several conflicting interpretations regarding slip systems and dislocation activities in the various investigated post-perovskite material. Whereas, plastic slip in post-pervoskite has attracted much more attention, twinning mechanism has not been addressed despite some experimental evidence on low-pressure analogues such as $CaIrO_3$ compounds.

In this work, we present a twin nucleation model in $MgSiO_3$ and $CaIrO_3$ post-perovskite based on a hierarchical mechanical model of the emission of 1/6<110> partial dislocations. Relying on first-principles calculations, we show that {110} twin wall formation resulting from the interaction of multiple twin dislocations occurs at rather low stresses, suggesting that twinning is a strain producing mechanism as competitive as dislocation activities in our understanding of the development of preferred orientations in post-perovskite materials.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C7] Symposium C-7

Chair: David Rodney(Institut Lumiere Matiere, Universite Lyon 1, France)
Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room1

[SY-C7] Predictive simulations of crystal plasticity: multiscale or cross-scale?

○Vasily V Bulatov[1], Alexander Stukowski[2], Luis A Zepeda-Ruiz[1], Tomas Oppelstrup[1]　(1.Lawrence Livermore National Laboratory, United States of America, 2.Darmstadt University, Germany)

[SY-C7] Molecular dynamics simulations of dislocation avalanche emissions in FCC and BCC crystals

○Javier Varillas[1,2], Jan Očenášek[2], Jorge Alcalá[1]　(1.New Technologies Research Centre, University of West Bohemia in Pilsen, Czech Republic, 2.Department of Materials Science and Metallurgical Engineering, InSup, ETSEIB. Universitat Politècnica de Catalunya, Spain)

[SY-C7] Scrutinizing screw dislocation glide initiation at finite temperatures in BCC metals

○Tomoaki Suzudo[1], Takashi Onitsuka[2], Ken-ichi Fukumoto[2]　(1.Japan Atomic Energy Agency, Japan, 2.Fukui Univ., Japan)

[SY-C7] Uranium plastic deformation: A multiscale approach

○Pavel A. Pokatashkin, Denis K. Ilnitsky, Alexei V. Yanilkin　(Dukhov Research Institute of Automatics (VNIIA), Russia)

[SY-C7] Understanding the grain refinement mechanism in surface mechanical attrition treatment of Fe14Ni18Cr by molecular dynamics simulations

○Ali Rida[1], Matthieu Micoulaut[2], Emmanuelle Rouhaud[1], Ali Makke[1,3]　(1.University of Technology of Troyes , France, 2.Sorbonne Université, France, 3.EPF, Engineering school, France)

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room1)

[SY-C7] Predictive simulations of crystal plasticity: multiscale or cross-scale?

Invited

○Vasily V Bulatov[1], Alexander Stukowski[2], Luis A Zepeda-Ruiz[1], Tomas Oppelstrup[1] （1.Lawrence Livermore National Laboratory, United States of America, 2.Darmstadt University, Germany）

Prediction of crystal plasticity from atomic motion has been regarded over the years as a poster child context for multiscale modeling, given that the relevant scales were inaccessible to direct MD simulations and, at the same time, dislocation lines offer a natural, concise and accurate way to coarse-grain crystal microstructure. The method of Discrete Dislocation Dynamics (DDD) is regarded as a key and most challenging element in the multiscale modeling hierarchy developed to enable such predictions. We will discuss results of a recently completed direct Molecular Dynamic (MD) simulation of dislocation dynamics in which a single crystal of tantalum was compressed at rate 10^5/s. Termed Livermore BigBig (LBB) simulation, LBB is by far the largest MD simulation ever performed. LBB generated a fully dynamic trajectory of over 2.1 billion atoms simulated over 5 microseconds of compressive straining. The simulation generated nearly 80 exabytes of recordable trajectory data a fraction of which was saved on disk in a highly compressed/post-processed form available for further analysis. As opposed to multiscale, LBB simulation can be regarded *cross-scale* being sufficiently large to be statistically representative of collective action of dislocations resulting in the macroscopic flow stress and yet fully resolved to every atomic "jiggle and wiggle". Importantly, LBB is sufficiently large to be used as a critical test of the DDD-based multi-scale approach. To enable an "apples to apples" comparison, we carefully calibrated our DDD model (in ParaDiS) to match our LBB model at the level of single dislocation mobilities, shape and dimensions of the simulation volume, straining rate, temperature, straining axis, positioning and shape of initial dislocation sources, etc. Our first comparisons of the so-calibrated DDD simulations with LBB - which in this case serves as an exact benchmark for comparison - are far from satisfactory suggesting, in particular, that in our DDD model the dislocations do not know how to multiply. The exact origin of the uncovered discrepancies still unclear, we intend to make available to the community all the relevant atomistic simulation data (including the LBB results) thus challenging the DDD practitioners to match our LBB predictions.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room1)

[SY-C7] Molecular dynamics simulations of dislocation avalanche emissions in FCC and BCC crystals

○Javier Varillas[1,2], Jan Očenášek[2], Jorge Alcalá[1] （1.New Technologies Research Centre, University of West Bohemia in Pilsen, Czech Republic, 2.Department of Materials Science and Metallurgical Engineering, InSup, ETSEIB. Universitat Politècnica de Catalunya, Spain）

Plastic deformation in crystalline materials is characterized by intermittent collective dislocation glide processes, or dislocation avalanches [1, 2, 3]. Here we perform a comprehensive set of molecular dynamics (MD) simulations to investigate the influence of strain-rate effects upon the emission of dislocation avalanches in body-centered cubic (BCC) and face-centered cubic (FCC) microcrystals. The MD simulations comprise periodic (representative) cells containing dense dislocation arrangements injected prior to the application of uniaxial displacement. Our results enable assessment of the transition from a continuous deformation mode, developed under a large strain-rate, to the characteristic serrated discontinuous mode

(indicating dislocation-mediated crystal plasticity) under a lower strain rate. In the latter, the stress-strain curves can be essentially probed under strict displacement control, enabling direct comparison with the avalanche-size distributions from quasi-static micropillar compression experiments [3]. Moreover, our findings shed new light on the role of strain hardening and dislocation cross-slip in FCCs as well as on the thermally-activated glide of screw dislocations in BCCs upon the avalanche distributions, including avalanche truncation at large plastic slip events [3].

[1] M. C. Miguel, A. Vespignani, S. Zapperi, J. Weiss and J.-R. Grasso, "Intermittent dislocation flow in viscoplastic deformation", *Nature,* vol. 410, 2001.

[2] R. Maaβ, M. Wraith, J. T. Uhl, J. R. Greer and K. A. Dahmen, "Slip statistics of dislocation avalanches under different loading modes", *Phys. Rev. E,* vol. 91, no. 4, 2015.

[3] J. Alcala, J. Ocenasek, K. Nowag, D. Esqué-de-los-Ojos, R. Ghisleni and J. Michler, "Strain hardening and dislocation avalanches in micrometer-sized dimensions", *Acta Materialia ,* vol. 91, 2015.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room1)

[SY-C7] Scrutinizing screw dislocation glide initiation at finite temperatures in BCC metals

○Tomoaki Suzudo[1], Takashi Onitsuka[2], Ken-ichi Fukumoto[2] （1.Japan Atomic Energy Agency, Japan, 2.Fukui Univ., Japan）

Plasticity of body-centered-cubic (BCC) metals at low temperatures is determined by screw dislocation kinetics. Because the core of screw dislocation in BCC metals has non-planar structure, its motion is complex and unpredictable. For example, although density functional theory (DFT) predicts slip on a {110} plane, the actual slip plane departs from the prediction at elevated temperatures, its mechanism having been a mystery for decades. In the current study, we conducted molecular dynamics simulations at finite temperatures using a recently-developed empirical potential that has the single-hump Peierls barrier for 1/2<111> the screw dislocation jump and examined the dislocation jump process.

In our molecular dynamics, the dislocation glides on the {110} plane with the highest Schmidt's factor, as predicted by DFT at low temperatures, while the dislocation approximately glides on a {112} plane at higher temperatures. Thus, our molecular dynamics simulations successfully reproduced the transition of the slip plane observed in experiments. To examine how the glide-plane transition takes place, we particularly developed a post-analysis tool to scrutinize the initiation of screw dislocation jumps from one Peierls valley to the next with high spatiotemporal resolution. The results indicated that heaved motion of screw dislocation line inside a Peierls valley sometimes causes a double-kink nucleation on a {110} plane with lower Schmidt's factor. Because of the twinning/anti-twinning asymmetry of the core structure, the average slip plane over the long kinetics departed from the original {110} plane and approximately becomes {112}. This suggests that thermal fluctuation of screw dislocation line are responsible for the transition of the slip plane.

We also observed a jerky dislocation motion at low temperatures similar to experiments. Close investigation of this motion using the new post-analysis tool indicates that inertial effect causes the jerky motion, i.e., a previous jump beyond the Peierls barrier can directly cause the double-kink nucleation for the next jump.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room1)

[SY-C7] Uranium plastic deformation: A multiscale approach

○Pavel A. Pokatashkin, Denis K. Ilnitsky, Alexei V. Yanilkin （Dukhov Research Institute of Automatics (VNIIA), Russia）

Uranium is a key element in nuclear technology. We focus on studying plastic deformation of the high-temperature BCC phase. On the one hand, classical molecular dynamics is used for obtaining material parameters, necessary for dislocation dynamics. Dislocation motion involves various mechanisms. The significance of their contribution to plastic response is studied on the other hand.

We show dislocation climb can be observed at nanosecond timescale. Imposing external shear results in gliding of the dislocation, making dislocation climb even more significant. Studying of those mechanisms is performed and quantitative parameters e.g. phonon drag coefficient, activation energy, activation volume are obtained. We emphasize that qualitative results remain the same for all three interatomic potentials considered in our study. Both discrete and continuum dislocation dynamics simulations are performed based on the results obtained from atomistic simulations. Synergy between two approaches of multiscale modeling results in better understanding of uranium plastic deformation.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room1)

[SY-C7] Understanding the grain refinement mechanism in surface mechanical attrition treatment of Fe14Ni18Cr by molecular dynamics simulations

○Ali Rida[1], Matthieu Micoulaut[2], Emmanuelle Rouhaud[1], Ali Makke[1,3] （1.University of Technology of Troyes , France, 2.Sorbonne Université, France, 3.EPF, Engineering school, France）

In surface mechanical attrition treatment the surface of a treated material is submitted to a severe local plastic deformation. This deformation results from the random impacts of spherical shots with high velocity on the surface of the specimen. Therefore, a nanocrystalline layer is generated on the surface. The thickness of this layer can reach a depth of 50 micrometers. The grain refinement mechanisms that lead to the formation of the nanocrystalline layer are still not well understood. In this work, molecular dynamics simulation has been employed to simulate the compression of a single crystal Fe14Ni18Cr at strain rate of $5.10^9\ s^{-1}$ in order to analyze its main plastic deformation mechanisms. Therefore, the relationship between the impacts of the shots and the refinement mechanisms in a grain has been investigated. A combination of dislocation slips and mechanical twinning have been found to be the main refinement mechanisms. High density of dislocations and twins nucleation are observed on the surface. Moreover, the large density of generated twin boundaries modify the monocrystal into lamellar twin-matrix blocks with a nanometer sized thickness. Finally, twin-twin and twin-dislocation interactions lead to the transformation of the twin-matrix blocks to small grains.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C8] Symposium C-8

Chair: Yinan Cui(Mechanical and Aerospace Engineering Department, University of California, Los Angeles, United States of America)

Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room1

[SY-C8] Thermal fluctuations of dislocations reveal the interplay between their core energy and long-range elasticity.

○Pierre-Antoine Geslin[1,2,3], David Rodney[4] （1.Mateis lab, INSA Lyon/CNRS, France, 2.Institute for Materials Research, Tohoku University, Japan, 3.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan, 4.Institut Lumière Matière, Université Lyon 1, France）

[SY-C8] Tension of fluctuating dislocation lines

○Max Boleininger[1], Thomas D Swinburne[2], Laurent Dupuy[3], Sergei L Dudarev[1] （1.Culham Centre for Fusion Energy, UK, 2.Theoretical Division T-1, Los Alamos National Laboratory, United States of America, 3.DEN-Service de Recherches Métallurgiques Appliquées, CEA, France）

[SY-C8] Stress-Dependent Activation Parameters for Cross-Slip in FCC Metals

○Alon Malka-Markovitz, Dan Mordehai （Technion—Israel Institute of Technology, Israel）

[SY-C8] The influence of precipitate size and shape on the strengthening and hardening rate as observed within metallic alloys.

○Benjamin A Szajewski, Joshua Crone, Jaroslaw Knap （Army Research Laboratory, United States of America）

[SY-C8] Molecular dynamics simulations of dislocation dynamics

Eyal Oren, ○Guy Makov （Ben-Gurion University of the Negev, Israel）

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room1)

[SY-C8] Thermal fluctuations of dislocations reveal the interplay between their core energy and long-range elasticity.

Invited
○Pierre-Antoine Geslin[1,2,3], David Rodney[4] (1.Mateis lab, INSA Lyon/CNRS, France, 2.Institute for Materials Research, Tohoku University, Japan, 3.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan, 4.Institut Lumière Matière, Université Lyon 1, France)

Thermal fluctuations of dislocations control their mobility and set the time-scale of thermally activated events such as cross-slip or obstacles by-pass. While dislocation vibrations have been previously investigated using simplified line tension descriptions and numerical dislocation dynamics models, we analyze them by the means of an analytical approach combined with atomistic simulations. Within the framework of the non-singular dislocation theory, we derived an analytical expression for the elastic energy of a weakly perturbed dislocation, which controls the amplitude of the equilibrium thermal fluctuations through the equi-partition theorem. Comparing this analytical prediction with molecular dynamics calculations performed in aluminum shows that a core energy (proportional to the dislocation length) has to be incorporated in addition to long-range elasticity. Adding this contribution allows to reproduce very accurately the fluctuation spectra obtained from molecular dynamics simulations and yields quantitative estimates for the core parameter of the non-singular theory and for the magnitude of the core energy. We also discuss the transferability of these parameters to the bowing-out of a dislocation between obstacles. Finally, a deeper analysis of the time-dependence of the fluctuations yields valuable insights on the dynamical behavior of dislocations, namely their mass and phonon damping.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room1)

[SY-C8] Tension of fluctuating dislocation lines

○Max Boleininger[1], Thomas D Swinburne[2], Laurent Dupuy[3], Sergei L Dudarev[1] (1.Culham Centre for Fusion Energy, UK, 2.Theoretical Division T-1, Los Alamos National Laboratory, United States of America, 3.DEN-Service de Recherches Métallurgiques Appliquées, CEA, France)

Fusion materials will be subjected to high lifetime doses of irradiation at high temperatures. To accurately predict changes in mechanical properties of materials under fusion conditions, we need to simulate complex stochastically-driven evolution of radiation damage defect networks over a broad range of temperature and timescales.

Recent analysis shows that fundamental concepts underpinning defect dynamics require re-examination. In stark disagreement with atomistic simulations, linear elasticity theory predicts that straight dislocations have negative line tension with respect to small fluctuations, suggesting that dislocations are unstable to bow-out. Consequently, a dislocation dynamics model based solely on linear elasticity is unable to cope with stochastic thermal fluctuations.

A consistent treatment of dislocation cores is a prerequisite for correctly describing dislocation line tension in a continuum model. We present a new solution of the discrete Multi-String Frenkel-Kontorova (MSFK) model, which in the continuum limit unifies linear elasticity and the Peierls-Nabarro model for an edge dislocation. The core (misfit) energy and core width are controlled by a single parameter. We find the

continuum displacement fields in agreement with atomistic displacements derived from molecular dynamics simulations of edge dislocations in bcc iron and tungsten. We investigate line tension of the continuum MSFK model with respect to bow-out and find that the misfit energy plays a crucial role in controlling the stochastic line instabilities.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room1)

[SY-C8] Stress-Dependent Activation Parameters for Cross-Slip in FCC Metals

○Alon Malka-Markovitz, Dan Mordehai （Technion—Israel Institute of Technology, Israel）

Cross-slip is a thermally activated process by which screw dislocations can change their glide plane. Quantifying the activation parameters for cross-slip in a general stress field is imperative to model cross-slip in dislocation-based simulations. In most discrete dislocation dynamics (DDD) simulations, only the contribution of the resolved shear stress is considered. Recently, the contributions of Escaig stresses on the primary and cross-slip planes were accounted for. In this work, we propose a model for cross-slip of screw dislocations in Face-Centered Cubic (FCC) metals by employing the line-tension model to calculate the free-energy barrier under a general stress field.

When only Escaig stresses are applied, we show that cross-slip is favorable only when Escaig stress in the primary plane is larger than in the cross-slip plane. The free-energy barrier decreases nonlinearly with Escaig stresses, whereas it decreases stronger with Eacsig stress in the primary plane. Using our model, we show that there is typical length for cross-slip, which is a means to quantify the region that bows-in towards constriction. The typical length scale varies when applying different Escaig stresses on both the primary and the cross-slip planes.

Schmid stresses in the cross-slip plane break the symmetry of the solution, and the partial dislocations bow-out in the cross-slip plane after constricting. The application of Schmid stresses is shown to remove the divergence in the free-energy barrier and cross-slip is possible for all combination of Escaig stress. We propose an Escaig and Schmid stress-dependent closed-form expression for the free-energy barrier for a cross slip in a large range of stresses without any fitting parameters. The proposed expression captures qualitatively the essentials found in atomistic simulations and is in good agreement with previous models. This closed-form activation energy function can be easily implemented in DDD simulations, owing to its simplicity and universality.

Malka-Markovitz A. and Mordehai D., Philos. Mag. 98 (2018) 347-370.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room1)

[SY-C8] The influence of precipitate size and shape on the strengthening and hardening rate as observed within metallic alloys.

○Benjamin A Szajewski, Joshua Crone, Jaroslaw Knap （Army Research Laboratory, United States of America）

The interaction between glissile dislocations and precipitates within a continuum is responsible for marked increases in material strength. Due to their desirable engineering features, dislocation-obstacle interactions have been the subject of theoretical study for many decades. Despite ongoing efforts, these studies have often been limited to crude approximations whose validity is difficult to assess. Towards enhancing our understanding of these complex interactions, we employ a three dimensional coupled dislocation dynamics and finite element method computational scheme to directly compute the strength (i.e. bypass stress) of a variety of dislocation-precipitate interactions. The coupled framework accounts for elastic mismatch between the host matrix and precipitates via the inclusion of elastic image stresses and stress concentrations computed through the finite elements. Our simulations span a range of elastic mismatch, linear obstacle densities, degrees of ellipticity and size. Through our simulations, we demonstrate the influence of these four parameters on both the dislocation-precipitate strength, and hardening rate. We devise a simple mechanical model which yields insight into the results of both our numerical simulations as well as others found within the literature.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room1)

[SY-C8] Molecular dynamics simulations of dislocation dynamics

Eyal Oren, ○Guy Makov （Ben-Gurion University of the Negev, Israel）

Dislocations are of fundamental importance in plasticity and mechanical deformation of solids and their properties are required for understanding of numerous phenomena related to mechanical response. Molecular dynamics simulations allow the study of dislocation motion at the short time and length scales which are difficult to access by experimental means, but require careful convergence for physical meaning. Highly converged simulations were performed on long dislocations in large FCC copper crystal supercells with full periodic boundary conditions, incorporating a dislocation dipole with zero net Burgers vector. Kinematics were studied by accelerating dislocations at constant stress and temperature. The relation between stress and terminal velocity at cryogenic and room temperatures for both screw and edge dislocations was obtained. A transition from viscous behaviour to near sonic asymptotic behaviour was identified and the velocity dependence of the drag force was characterised. At higher stresses a shift into the transonic regimes occurs and the mechanism and stability of this transition is examined. The thermally activated process of cross-slip was simulated multiple times creating statistical data from which the kinetics and activation parameters were calculated. The effects of stresses in the cross slip and in the glide planes on the activation volumes were determined. Finally, the rate controlling step of the cross-slip process was identified producing insight into the cross-slip mechanism.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E5] Symposium E-5

Chairs: Anthony D Rollett(Carnegie Mellon University, United States of America), Evgeniya Kabliman(Austrian Institute of Technology, Austria)

Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room2

[SY-E5] Use of FFT-based micromechanical modeling for analysis of synchrotron-based diffraction experiments

Vahid Tari[1], Ricardo A Lebensohn[2], Reeju Pokharel[2], Rachel E Lim[1], Darren C Pagan[3], Yufeng Shen[1], Joel V Bernier[4], Robert M Suter[1], ○Anthony D Rollett[1]　(1.Carnegie Mellon University, United States of America, 2.Los Alamos National Laboratory, United States of America, 3.Cornell High Energy Synchrotron Source, United States of America, 4.Lawrence Livermore National Laboratory, United States of America)

[SY-E5] Computational Design of Hysteresis-Free and Linear Super-Elastic, and Ultralow Modulus Ferroelastic Materials

○Jiaming Zhu[1], Yipeng Gao[2], Dong Wang[3], Tong-Yi Zhang[4], Yunzhi Wang[2]　(1.City University of Hong Kong, Hong Kong, 2.Ohio State University, United States of America, 3.Xi'an Jiaotong University, China, 4.Shanghai University, China)

[SY-E5] A biphasic continuum model for large deformation visco-elastic mechanics of uncured carbon fibre prepregs

○Amir Hosein Sakhaei, Timothy James Dodwell　(College of Engineering, Mathematics and Physical Sciences, University of Exeter, UK)

[SY-E5] Strong coupling of deformation and microstructure/microchemistry evolution in hot compression tests

○Evgeniya Kabliman[1], Johannes Kronsteiner[1], Ernst Kozeschnik[2]　(1.Light Metals Technologies Ranshofen, Center for Low-Emission Transport, Austrian Institute of Technology, Austria, 2.Institute of Materials Science and Technology, TU Wien, Austria)

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room2)

[SY-E5] Use of FFT-based micromechanical modeling for analysis of synchrotron-based diffraction experiments

Invited

Vahid Tari[1], Ricardo A Lebensohn[2], Reeju Pokharel[2], Rachel E Lim[1], Darren C Pagan[3], Yufeng Shen[1], Joel V Bernier[4], Robert M Suter[1], ○Anthony D Rollett[1] (1.Carnegie Mellon University, United States of America, 2.Los Alamos National Laboratory, United States of America, 3.Cornell High Energy Synchrotron Source, United States of America, 4.Lawrence Livermore National Laboratory, United States of America)

This presentation describes use of image-based modeling to analyze synchrotron-based High Energy Diffraction Microscopy (HEDM) stress-strain experiments. HEDM is both in-situ and non-destructive and was used to measure micromechanical fields such as strain and orientation at the grain scale developed under macroscopic tensile loading of Ti-7Al. Taking the 3D image of the experimentally measured initial microstructure as input, elasto-viscoplastic modeling based on the Micromechanical Analysis of Stress-Strain Inhomogeneities with Fourier transforms (MASSIF) was used to compute the micromechanical fields that develop during loading. To validate the MASSIF calculations, we compared the calculated fields with the ones measured by HEDM. The initial comparisons showed that MASSIF can reproduce the macroscopic stress/strain curve but poor agreement was found between calculated and measured fields at the grain scale. The differences at the grain scale were hypothesized to be caused by the initial residual stress state that was induced during prior material processing, and which was not incorporated in the MASSIF calculation. We used eigenstrain concept to incorporate residual stress in the MASSIF calculation by converting it to an initial eigenstrain field. The results reveal that incorporation of residual stress results in good agreement between calculated and measured fields at the grain scale, thereby validating the computational approach. MASSIF was further used to model an experiment in which a polycrystalline sample of Ti-7Al was cyclically deformed and mapped using boxbeam near field(nf)-HEDM and far field(ff)-HEDM. The ff-HEDM results show a decrease in residual elastic strain over the first cycle followed by a steady increase in (elastic) strain. The initial residual strain in each grain was anti-correlated with the change in that same strain component over the first cycle. The distribution in the von Mises stress, which is a scalar measure of deviatoric stress, broadens as cycles accumulates and develops a long upper tail. Initially, a graph of hydrostatic stress against stress coaxiality angle shows a positive correlation but after about 65 cycles, the trend-line has rotated to a negative correlation. Simulations with MASSIF are used to analyze and understand these results.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room2)

[SY-E5] Computational Design of Hysteresis-Free and Linear Super-Elastic, and Ultralow Modulus Ferroelastic Materials

○Jiaming Zhu[1], Yipeng Gao[2], Dong Wang[3], Tong-Yi Zhang[4], Yunzhi Wang[2] (1.City University of Hong Kong, Hong Kong, 2.Ohio State University, United States of America, 3.Xi'an Jiaotong University, China, 4.Shanghai University, China)

A unique characteristics of ferroelastic materials is their highly non-linear stress-strain curves with plateaus and large hysteresis. We show by computer simulations how to render ferroelastic materials nearly hysteresis-free and linear super-elastic (with an elastic strain limit of 2.7%), and ultralow modulus (<20 GPa) by creating appropriate concentration modulations (CMs) in the parent phase via spinodal decomposition and by pre-straining. The CM causes phase stability modulations, suppresses autocatalysis in nucleation, imposes nano-

confinement on growth and hinders long-range order of transformation strain during martensitic transformation (MT) and, thus, turns the otherwise sharp first-order transition into a broadly smeared, macroscopically continuous transition over a large stress range. The pre-straining yields retained martensitic particles that are stable at the test temperature without applied load and act as operational nuclei in subsequent load cycles, eliminating the stress-strain hysteresis and offering an ultralow apparent Young's modulus. This study demonstrates a novel and universal approach to design new ferroelastic materials with unprecedented properties.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room2)

[SY-E5] A biphasic continuum model for large deformation visco-elastic mechanics of uncured carbon fibre prepregs

○Amir Hosein Sakhaei, Timothy James Dodwell （College of Engineering, Mathematics and Physical Sciences, University of Exeter, UK）

Composite materials are widely used in high value manufacturing industries like aerospace and auto- motive. However, they are often compromised by high costs, long development time, and poor quality due to manufacturing defects. Therefore, numerical simulation for composite manufacturing processes has attracted much attention in academic and industrial communities, with the twin objectives of improving product quality and decreasing production time.

Typically, carbon fibre composite components are made by layering a series of thin carbon fibre layers, pre-impregnated with resin, onto a tool surface. During this lay-up process the stack of plies is consolidated at moderate temperatures and pressures to remove air trapped between layers. The consolidation of composite laminates prior to curing strongly influences the formation of defects which ultimately hinder the components structural integrity.

The deformation of uncured composite laminates is complex. It depends on the individual constitutive behaviour of the plies and interface, as well as the geometric constraints that arise from the layers fitting and moving together. Theoretically, uncured composites can be modelled using detailed finite element calculations in which each layer and interface is defined explicitly. Experimental characterization have led to much better understanding of the shearing, bending, flow and consolidation mechanics of uncured laminate composites. This data has been parameterized largely via simplified heuristic models and have yet to be translated into rigorous 3D continuum models.

At In this study, we have developed a new continuum model for uncured carbon fibres plies to capture the non-linear visco-elastic behaviour of uncured laminates considering shear, bending, flow, and consolidation mechanisms based on the recent experimental characterization results. The model is developed from a biphasic continuum theory allowing for coupling between the solid and fluid responses. It includes the deformation mechanisms of the fibres as an anisotropic hyper-elastic material as well as resin flow through the fibre network. This work is the first part of a larger research effort to develop an efficient multi-scale numerical framework for composite manufacturing process of full scale components.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room2)

[SY-E5] Strong coupling of deformation and microstructure/microchemistry evolution in hot compression tests

○Evgeniya Kabliman[1], Johannes Kronsteiner[1], Ernst Kozeschnik[2]　（1.Light Metals Technologies Ranshofen, Center for Low-Emission Transport, Austrian Institute of Technology, Austria, 2.Institute of Materials Science and Technology, TU Wien, Austria）

When material deformation occurs at elevated temperatures, one has to take into account the simultaneous evolution of grain, sub-grain structure and microchemistry (dissolution and precipitation of phase particles). In the present work, we present current results on the implementation of a computational strong coupling scheme between material deformation and microchemistry/microstructure evolution. For this purpose, we introduce a Dyna2Micro Material Model, which is implemented into a Finite Element Code (LS-DYNA of LSTC) and allows a simultaneous calculation of the (sub)-grain structure and phase kinetics at every integration point and time step. Dynamic processes, such as, work hardening and recovery are calculated by using a dislocation based model (MD^2 Model) implemented into a user defined subroutine, while the phase dissolution and precipitation is calculated by the thermo-kinetic software package MatCalc. Computational efficiency is realized by a new remote control feature implemented in MatCalc specially developed for this project as command interface between the user subroutine and a running MatCalc session. The simulations are checked by simulation of multi-step hot compression tests using a 3D axisymmetric cylindrical model of samples according to the experimental set up. For the material, we choose an Al-Cu-Mg alloy, where precipitation and dissolution of Al_2Cu and Al_2CuMg is considered. The whole simulation process from solidification, pre-heat treatment, deformation and post heat treatment is then controlled by the SProC (Smart Process Control) Toolkit.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E6] Symposium E-6

Chairs: Ying-Jun Gao(Guangxi University, China), Masaki Tanaka(Kyushu Univ., Japan)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room2

[SY-E6] Phase Field Crystal Simulation of Crack Extension and Brittle-Ductile Transition Behavior on Nano-Scale

○Ying-Jun Gao （Guangxi University, China）

[SY-E6] Continuum elasticity and correlations of plastic strain fluctuations in sheared glasses: The effect of hard boundaries

○Muhammad Hassani, Fathollah Varnik （Ruhr-University Bochum, Germany）

[SY-E6] Modeling approaches to tetragonal-to-monoclinic transformations in MgO partially stabilized zirconia

○Michael Budnitzki （TU Bergakademie Freiberg, Germany）

[SY-E6] Delamination cracks in wire-drawn fully pearlitic steels.

○Masaki Tanaka[1], Yelm Okuyama[1], Tatsuya Morikawa[1], Toshiyuki Manabe[2] （1.Kyushu Univ., Japan, 2.Nippon Steel &Sumitomo Corporation, Japan）

[SY-E6] FTMP-based Modeling and Simulations of Inhomogeneous Recovery-Triggered Accelerated Creep Rupture in Lath Martensite Structures

○yasutaka matsubara, tadashi hasebe, yuta amano （Kobe Univ., Japan）

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room2)

[SY-E6] Phase Field Crystal Simulation of Crack Extension and Brittle-Ductile Transition Behavior on Nano-Scale

○Ying-Jun Gao （Guangxi University, China）

Phase field crystal (PFC) method is used to simulate cracks propagation as a function of grain orientation. The results show that when the direction of tensile stress is perpendicular to the grain orientation, the crack exhibits cleaving extension characteristics with straight and smooth edges. As the angle between the grain orientation and the direction of the applied stress changes, the extension of the cracks begins to present a structure with saw teeth on the edge. Then, with the change of the angle increasing, a dislocation is emitted in front of the crack tip. Along with the dislocation slipping, it generates a series of micro holes. These holes further develop and grow to connect each other, and form a crack, which presents a ductile crack growth process. It can be seen that the change of the angle between the direction of the applied stress and the orientation of the grains can lead to a transformation of the ductile-brittle behavior of the fracture.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room2)

[SY-E6] Continuum elasticity and correlations of plastic strain fluctuations in sheared glasses: The effect of hard boundaries

○Muhammad Hassani, Fathollah Varnik （Ruhr-University Bochum, Germany）

Spatial correlations of plastic strain fluctuations in a shear-driven amorphous solid are investigated in the vicinity of a hard wall with a molecular-scale corrugation [1]. Within thin slabs parallel to the wall plane, normalized correlations are enhanced when the slab center is closer to the wall. The amplitude of these correlations, however, is found to be suppressed by the wall. It is shown in this work that the enhancement of the normalized correlations quantitatively matches with the wall-induced enhancement of the elastic propagator within continuum elasticity [1,2]. The decrease of strain amplitude, on the other hand, is shown to originate from molecular scale wall effects on the size of the nearest neighbor cage, explored by particles on intermediate times scales [1]. These results highlight the fundamental role of elasticity for the correlation of plastic activity in glassy systems [3].

[1] M. Hassani, P. Engels and F. Varnik, Wall effects on spatial correlations of non-affine strain in a 3D model glsss (Europhysics Leters 2018, in press).
[2] A. Nicolas and J.-L. Barrat, A mesoscopic model for the rheology of soft amorphous solids, with application to microchannel flows, Faraday Discuss. 167, 567 (2013).
[3] F. Varnik, S. Mandal, V. Chikkadi, D. Denisov, P. Olsson, D. Vagberg, D. Raabe, and P. Schall, Correlations of plasticity in sheared glasses, Phys. Rev. E 89, 040301 (2014).

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room2)

[SY-E6] Modeling approaches to tetragonal-to-monoclinic transformations in MgO partially stabilized zirconia

○Michael Budnitzki （TU Bergakademie Freiberg, Germany）

Partially stabilized zirconia (PSZ) based ceramics are known for their excellent mechanical properties and bio-compatibility. The material's ability to undergo stress-induced phase transitions results in a very high fracture toughness, making it ideal for applications such as dental implants. In MgO-stabilized zirconia (MgO-PSZ) the martensitic phase transformation is restricted to lenticular inclusions of retained tetragonal phase embedded in a cubic matrix.

We use semi-analytical models as well as phase-field methods based on Ginzburg-Landau theory to account for various aspects of microstructure formation. Using phase-field it is possible to directly simulate the phase morphology and investigate the influence of geometric and crystallographic aspects. The semi-analytical model allows to study the effects of material parameters, such as surface energies, on the transformation stress as well as the inelastic strain in the inclusions and allows for the application of homogenization techniques in order to assess the effective constitutive response. Both approaches complement each other in order to achieve a more quantitative understanding of the micromechanics of zirconia.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room2)

[SY-E6] Delamination cracks in wire-drawn fully pearlitic steels.

○Masaki Tanaka[1], Yelm Okuyama[1], Tatsuya Morikawa[1], Toshiyuki Manabe[2] （1.Kyushu Univ., Japan, 2.Nippon Steel &Sumitomo Corporation, Japan）

Wire-drawn fully pearlitic steel was twisted at room temperature. As a result, a delamination crack propagated along the longitudinal direction of the wire. The fracture surface of the delamination crack was compared with the fracture surface obtained by an impact test at 120K, demonstrating that the delamination crack is neither a simple cleavage nor ductile shear one. Backscattered electron and transmission electron microscopy images indicated that the cementite lamellae immediately beneath the delamination crack had vanished. In addition to that, a fine-grained structure was observed. This indicated that the delamination fracture was not a brittle one but a shear one associated with local severe plastic deformation.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room2)

[SY-E6] FTMP-based Modeling and Simulations of Inhomogeneous Recovery-Triggered Accelerated Creep Rupture in Lath Martensite Structures

○yasutaka matsubara, tadashi hasebe, yuta amano （Kobe Univ., Japan）

Against highly complex hierarchical material systems as in high Cr heat-resistant ferritic steels exhibiting inhomogeneous recovery-triggered accelerated creep rupture, the present study tackles a series of problems about their practically-feasible multiscale modeling and simulations based on FTMP. The targeted system here is composed of martensite laths with high-dense dislocations (Scale A), lath blocks/packets (Scale B) embedded within a prior austenitic grain (Scale C). The objectives are (a)reproduction of the experimentally-observed accelerated degradation of the creep strength due to inhomogeneous recovery of the microstructures under relatively low stress conditions, and (b)identification of the minimal conditions for (a)

to occur, focusing on the interactions between Scales A and B. Creep analyses, considering the interior high-dense dislocations evaluated by the spontaneously-evolved incompatibility tensor field in Scale B, are conducted for single lath block models first. They exhibit pronounced local instability due to local recovery brought about by the interaction incompatibility field. Thus-developed models are further combined to construct single packets and embedded packet models, respectively, and the same series of analyses are performed on them. The fluctuating incompatibility field in Scale A, concurrently enhanced by the interaction term, is demonstrated to promote the local recovery. We further clarify the contributions of the projection directions of the incompatibility tensor in evaluating the Scale A dislocation density. The projection to the slip plane normal direction is turned out to play exclusively-dominant roles, implying the critical contribution of the climb-related elementary processes to the enhanced localized recovery. An attempt is also made to replace the above recovery model to improve the consistency of the current approach.

[SY-E7] Symposium E-7

Chairs: Daisuke Matsunaka(Shinshu Univ., Japan), Shiyu Du(Chinese Academy of Sciences, China)
Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room2

[SY-E7] The Activation Parameters for Dislocation Nucleation in Molybdenum Nanoparticles under Compression

Doron Chachamovitz, ○Dan Mordehai （Mechanical Engineering, Technion, 32000 Haifa, Israel）

[SY-E7] Dislocation density-based crystal plasticity analysis for the evolution of atomic vacancies during plastic slip deformation

○Tetsuya Ohashi （Kitami institute of technology, Japan）

[SY-E7] Structural Stability of Long-period Stacking Ordered Magnesium Alloys

○Daisuke Matsunaka[1], Yoji Shibutani[2] （1.Dept. of Mechanical Systems Engineering, Shinshu Univ., Japan, 2.Dept. of Mechanical Engineering, Osaka Univ., Japan）

[SY-E7] **First-principles-based prediction of yield strength in the RhIrNiPdPtCu high entropy alloy**

○Binglun Yin, William A. Curtin （LAMMM, EPFL, Switzerland）

[SY-E7] Metal-coated carbon nanotube reinforced aluminum composites

○Samaneh Nasiri[1,2], Michael Zaiser[1,2] （1.Institute for Materials Simulation WW8, Deptartment of Materials Science, Friedrich-Alexander University Erlangen-Nuernberg, Germany, 2.Cluster of Excellence EAM/FUMIN, Germany）

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room2)

[SY-E7] The Activation Parameters for Dislocation Nucleation in Molybdenum Nanoparticles under Compression

Invited

Doron Chachamovitz, ○Dan Mordehai （Mechanical Engineering, Technion, 32000 Haifa, Israel）

Metallic faceted nanoparticles exhibit ultra-high strength, since their deformation involves the nucleation of dislocations on their surfaces. In this work, we employ molecular dynamics (MD) simulations to study the strength of molybdenum faceted nanoparticles and its relation to the activation parameters for dislocation nucleation [1]. We show that under compression, the nanoparticles yield by nucleating dislocations at the vertices, which are points of stress concentration. For each temperature, the simulation is repeated 30 times with different atomic velocities. Since dislocation nucleation is a thermally-activated process, the calculated strength varies between the different simulations. The strength distribution can be exploited to calculate the activation parameters. We show that the distribution can be approximated by a normal distribution, with a standard-deviation that corresponds directly to the activation volume at the given temperature and stress. Accordingly, the activation volumes are calculated from the MD simulation results at different temperatures and stresses. In addition, the dependence of the most-probable nucleation stress on the temperature is calculated. With the help of classical nucleation theory, the activation free-energy and the activation entropy are calculated. We find that the dependence of the activation free-energy on the stress obeys a power-law near the conditions for spontaneous nucleation, with a critical exponent that is equal ˜1.5. This critical exponent is typical for simple bifurcation problems. In addition, the activation entropies are found to be in the range of 0-15k_B, with some deviations form the Meyer-Neldel compensation rule. Based on the calculated activation parameters, the probabilistic nature of the strength at this scale is discussed.

1. Chachamovitz D, Mordehai D. Sci Rep 2018;8:3915

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room2)

[SY-E7] Dislocation density-based crystal plasticity analysis for the evolution of atomic vacancies during plastic slip deformation

○Tetsuya Ohashi （Kitami institute of technology, Japan）

Density evolution of atomic vacancies during plastic slip deformation is evaluated by crystal plasticity analyses where evolution of dislocation density is calculated by the model of Kocks and Mecking[1] and the dislocation mean free path is given by an effective average distance of forest dislocations and a microstructure length scale[2, 3]. We slightly modified the model by Essmann and Mughrabi[4] for the evolution of atomic vacancy density and implemented to the crystal plasticity software code.
Analysis results[5] show that the vacancy density sometimes reaches at the order of 10^{24} /m^3, which is at the order of 10^{-4} in terms of concentration. Increase rate of the atomic vacancy is shown to depend largely on the microstructure length scale and slip multiplication on different systems.

Reference
1. Mecking H, Kocks U f.; *Acta Metall*. 1981;29:1865-1875.
2. Ohashi T. Dislocation Density-Based Modeling of Crystal Plasticity Finite Element Analysis. In: *Mechanics of Materials. Micromechanics*. Springer Nature Singapore; 2018.

3. Ohashi T, Kawamukai M, Zbib H.; *Int J Plast.* 2007;23(5):897-914.
4. Essmann U, Mughrabi H.; *Philos Mag A.* 1979;40(6):731-756.
5. Ohashi T.; *submitted.*

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room2)

[SY-E7] Structural Stability of Long-period Stacking Ordered Magnesium Alloys

○Daisuke Matsunaka[1], Yoji Shibutani[2] （1.Dept. of Mechanical Systems Engineering, Shinshu Univ., Japan, 2.Dept. of Mechanical Engineering, Osaka Univ., Japan）

Magnesium (Mg) alloys with long-period stacking ordered (LPSO) structures show excellent mechanical performances such as high yield strength and ductility. The LPSO structures consist of periodic arrangement of basal stacking faults (SFs) and enrichment of solute atoms in the vicinity of the SFs. HAADF-STEM measurements observed that the $L1_2$-type clusters of solute atoms are formed and aligned at each SF. The $L1_2$ clusters at each SF have a solute-enriched region of four close-packed planes. As SFs are periodically introduced, each type of the LPSO structures has the specifc close-packed layers between the quadrople solute-enriched layers. While a previous first-principles study showed that the binding energy of solute atoms to SF and the solute-solute pair interaction can describe the formation of the $L1_2$ clusters, the physical origin of the periodic arrangement of the quadrople solute-enriched layers with the $L1_2$ clusters remains controversial.

In order to elucidate the periodic arrangement of the quadrople solute-enriched layers, we investigate interactions mediated by electrons or phonons between the neiboring quadrople solute-enriched layers. The formation energy of the $L1_2$ cluster evaluted by first-principles calculations shows that the electron-mediated interaction is short-range repulsive with respect to the distance of the quadrople solute-enriched layers. On the other hand, we investigate effects of phonon on the inter-planer ordering of the solute-enriched layers using the 1-dimensional chain model with mass change. For heavy mass change, the ordering of the mass changes is stabilized by phonons and the energy gain increases with the concentration of the mass changes, i.e., the short LPSO period is favorable. Thus, a promising mechanism of the inter-planer ordering of the LPSO structures is the phonon-mediated interaction of the quadrople layers where heavy solute atoms are enriched as the $L1_2$ clusters at SFs.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room2)

[SY-E7] First-principles-based prediction of yield strength in the RhIrNiPdPtCu high entropy alloy

○Binglun Yin, William A. Curtin （LAMMM, EPFL, Switzerland）

High entropy alloys (HEAs) are random solid solution alloys with 5 or more components, usually of near equi-composition. HEAs exhibit excellent mechanical properties, including high strength, high ductility, and high fracture toughness [1]. Guiding the design of new HEAs across the vast composition space requires an ability to compute necessary underlying material parameters via first-principle calculations. Here, a methodology is proposed to compute, via density functional theory (DFT), the elemental misfit volumes, as well as alloy lattice constant, elastic constants and stable stacking fault energy, in the fcc noble metal HEA RhIrNiPdPtCu

[2]. These properties are then used in a recently developed solute strengthening model [3, 4] for temperature and strain-rate dependent yield strength, with the prediction of 563 MPa is in excellent agreement with the experimentally measured value of 527 MPa [5]. This methodology links the alloy composition with the yield strength prediction, indicating a general methodological path for exploring new potential high-strength HEAs in this and other alloy classes.

[1] D. B. Miracle and O. N. Senkov, Acta Mater. 122, 448 (2017).

[2] B. Yin and W. A. Curtin, in preparation.

[3] C. Varvenne, A. Luque, and W. A. Curtin, Acta Mater. 118, 164 (2016).

[4] C. Varvenne, G. P. M. Leyson, M. Ghazisaeidi, and W. A. Curtin, Acta Mater. 124, 660 (2017).

[5] S. Sohn, Y. Liu, J. Liu, P. Gong, S. Prades-Rodel, A. Blatter, B. E. Scanley, C. C. Broadbridge, and J. Schroers, Scr. Mater. 126, 29 (2017).

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room2)

[SY-E7] Metal-coated carbon nanotube reinforced aluminum composites

○Samaneh Nasiri[1,2], Michael Zaiser[1,2] (1.Institute for Materials Simulation WW8, Deptartment of Materials Science, Friedrich-Alexander University Erlangen-Nuernberg, Germany, 2.Cluster of Excellence EAM/FUMIN, Germany)

Carbon nanotubes (CNT) possess excellent mechanical properties in terms of axial elastic stiffness and rupture strength. It is therefore an obvious question whether these properties can be harnessed for structural applications by using such nanoparticles as fillers in low-melting lightweight metals such as Al or Mg nanocomposite. To this end, homogeneous dispersion of CNT in the metal matrix and strong interfacial bonding are essential factors since agglomerated nanoparticles with weak bonding into the surrounding metal matrix might act as flaws which actually deteriorate, rather than improve, the mechanical properties of composites. However, good dispersion and strong interfacial bonding are hindered by the low affinity of CNT to Al or Mg. To overcome this problem, interface engineering approaches such as coating CNT with an appropriate metal such as Nitweight , or by decorating them with metal nanoparticiles, may offer a promising approach towards the efficient fabrication of lightweight metal-CNT nanocomposites.

In this work we study how metal coated or metal decorated carbon nanotubes affect the mechanical properties of aluminium/CNT composites. In particular we look at the pullout behaviour of pristine as well as Ni coated or Ni decorated CNT from an aluminium matrix. Our result shows that Ni coating produces an extended interface ("intephase") where a significant amount of energy is dissipated during CNT pull-out, leading to a high pull-out force. We then investigate the interaction of embedded CNT with and without coating/decoration with cracks and with dislocations during simulated tensile tests. We discuss the results in view of promising approaches for engineering CNT-metal interfaces such as to achieve high strength and high toughness of the metal-CNT composites.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E8] Symposium E-8

Chairs: Hao Wang(Institute of Metal Research, CAS, China), Jun-Ping Du(Kyoto University, Japan)
Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room2

[SY-E8] **Effect of hydrogen on the vacancy diffusion in metals**
○Jun-Ping Du[1,2], W.T. Geng[3], Kazuto Arakawa[4], Shigenobu Ogata[2,1] （1.Elements Strategy Initiative for Structural Materials, Kyoto University, Japan, 2.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 3.University of Science and Technology Beijing, China, 4.Department of Materials Science, Faculty of Science and Engineering, Shimane University, Japan）

[SY-E8] Promotional effects of anisotropic strain on vacancy mobility in tungsten: the independence on the sign of strain
○Zhong Zhu Li, Yu Hao Li, Hong Bo Zhou, Guang Hong Lu （Department of Physics, Beihang University, China）

[SY-E8] **Ab initio investigation on the stacking fault energy and the c/a ratio in hexagonal metals and alloys**
○Gang Zhou, Hao Wang, Dong sheng Xu, Rui Yang （Institute of Metal Research, Chinese Academy of Sciences, China）

[SY-E8] Role of vacancies and grain boundaries of 2D materials for the catalytic ammonia synthesis
○Qinye Li[1], Lizhong He[1], Chenghua Sun[2,3], Xiwang Zhang[1] （1.Monash University, Australia, 2.Swinburne University of Technology, Australia, 3.Dongguan University of Technology, China）

[SY-E8] First-principles Investigation on the Stability and Oxygen Adsorption Behavior of a $Ti_2AlNb/TiAl$ Interface
○Yue Li, Jianhong Dai, Yan Song （School of Materials Science and Engineering, Harbin Institute of Technology at Weihai, China）

[SY-E8] **DFT predictions of hydrogen storage properties of Mg_7TiX_2 (X= F, O, S, P and Cl)**
○Yuying Chen, Jianhong Dai, Yan Song （School of Materials Science and Engineering, Harbin Institute of Technology at Weihai, China）

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room2)

[SY-E8] Effect of hydrogen on the vacancy diffusion in metals

○Jun-Ping Du[1,2], W.T. Geng[3], Kazuto Arakawa[4], Shigenobu Ogata[2,1]　(1.Elements Strategy Initiative for Structural Materials, Kyoto University, Japan, 2.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 3.University of Science and Technology Beijing, China, 4.Department of Materials Science, Faculty of Science and Engineering, Shimane University, Japan)

Hydrogen can be either an intentional constituent or unwelcome impurity in metals. The fact that excess hydrogen can enhance greatly the self-diffusion of atoms in metals has been explained by the appearance of superabundant vacancies, because the vacancy formation energy decreases substantially with increasing H concentration, while individual vacancy diffusion is supposed to be slowed down due to the increased jumping energy barrier of H-vacancy complexes based on the previous first-principles studies. Here, performing first-principles calculations of appearance probability of possible H-vacancy configurations and activation energy of possible vacancy jumping pathways in combination with molecular dynamics (MD) simulations, we found at certain H concentrations and temperatures, the diffusivity of vacancy in face-centered cubic Cu can be accelerated by H, which is caused by H-enhanced diffusion attempt frequency and environmental H-assisted vacancy diffusion pathway. The MD simulations demonstrated that the promoting effect of H can also be found in dynamical processes. The uncovered H-vacancy diffusion processes in metals can advance our understanding of the H behavior in metals.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room2)

[SY-E8] Promotional effects of anisotropic strain on vacancy mobility in tungsten: the independence on the sign of strain

○Zhong Zhu Li, Yu Hao Li, Hong Bo Zhou, Guang Hong Lu　(Department of Physics, Beihang University, China)

Tungsten (W) is one of the most promising candidates for the plasma facing materials (PFMs) in future fusion devices. Vacancy is the typical defect in W, and plays key role in the microstructure and mechanical properties of W. Vacancies can aggregate to form voids by migrating, and further lead to swelling, hardening and embrittlement of W. Therefore, the behaviors of vacancy in W have attracted many attentions. Generally, the presence of vacancy is accompanied with the disappearance of normal W atom, and induces local lattice distortion and forms stress field. Thus, one can expect that the external strain/stress field should have effect on vacancy behaviors in W, while little work focuses on this aspect so far.
Here, we have investigated the migration of vacancy in W under strain using a first-principles method in combination with the activation volume tensor and thermodynamic models. In general, vacancy inevitably induces local tensile stress field, tending to contract the lattice. Thus, it is considered that the mobility of vacancy responds to strain "monotonically", i.e., the migration energy of vacancy will decrease (increase) with the increasing tensile (compressive) strain. The mobility of vacancy in W under triaxial strain follows this rule. Surprisingly, we have discovered that the vacancy mobility can always be promoted by anisotropic (biaxial) strain in W, independent of the sign of strain. In a wide range of strain values, the vacancy mobility is enhanced in the strained W. This anomalous behavior is found to be caused by an unusual variation of the vacancy activation volume tensor induced by anisotropic strain, which is originated from the Poisson effect. Further, it is found that the diffusivity of the vacancy in W with 5% tensile (compressive) biaxial strain will be increased by 3 (2) orders at 600K based on the Arrhenius equation. Meanwhile, the onset temperature for

vacancy diffusion will also be markedly reduced by biaxial strain. Consequently, our finding suggests that anisotropic strain will significantly enhance vacancy mobility in W and promote the formation and growth of hydrogen/helium bubbles.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room2)

[SY-E8] Ab initio investigation on the stacking fault energy and the *c/a* ratio in hexagonal metals and alloys

○Gang Zhou, Hao Wang, Dong sheng Xu, Rui Yang （Institute of Metal Research, Chinese Academy of Sciences, China）

For structural materials with hexagonal close-packed structures, the stacking fault energy and the ratio of *c/a* are key factors which have strong correlation with many properties, such as the critical shear stress of dislocations and deformation twinning. We thus employed high-throughput *ab initio* calculations to investigate the stacking fault energy and the *c/a* ratio in hexagonal metals, Mg, Ti, Zr, Be and Zn, as well as in alloyed Mg and Ti. The result indicates that the ratio of the unstable stacking fault energy on the prism plane over that on the basal plane, γ^p/γ^b, is primarily relevant to the *c/a* ratio. In Be, Mg and Zn, γ^p/γ^b increases with *c/a* leading to increasing preference of basal slip, whereas in Ti and Zr, γ^p/γ^b changes unperceivably with *c/a* leading to the preference of prism slip. In alloyed Mg and Ti, alloying varies both the stacking fault energy and the *c/a* ratio and certain alloying elements significantly affect -slip preference in Mg, while alloying exhibits negligible influence on -slip preference in hexagonal Ti.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room2)

[SY-E8] Role of vacancies and grain boundaries of 2D materials for the catalytic ammonia synthesis

○Qinye Li[1], Lizhong He[1], Chenghua Sun[2,3], Xiwang Zhang[1] （1.Monash University, Australia, 2.Swinburne University of Technology, Australia, 3.Dongguan University of Technology, China）

Ammonia has been extensively synthesized by human beings, dominatedly by Haber-Bosch process at high temperature and high pressure. It results in large amount of carbon emisson and energy consumption. This work aims to investigate the role of vacancies and grain boundaries for catalysts design used in ammonia synthesis. They are employed as active sites for the design of single-atom catalyst design. As revealed by DFT calculations, single Fe/Co/Mo atoms can actively adsorb on these defects and offer high performance for N2 activation. Fe-doped MoN2 has been identified as an excellent catalyst for nitrogen reduction.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room2)

[SY-E8] First-principles Investigation on the Stability and Oxygen Adsorption Behavior of a $Ti_2AlNb/TiAl$ Interface

○Yue Li, Jianhong Dai, Yan Song （School of Materials Science and Engineering, Harbin Institute of Technology at Weihai, China）

The stability of a interface between O-phase Ti_2AlNb (1 -1 0) surface and B2-phase TiAl (2 1 -1) surface was studied by first principles calculations to investigate the atomic matching behavior. A coherent twin boundary with extremely small misfit degree was found, The calculated formation energy and the electronic structure illustrate that the interaction is strong. The adsorption of a single oxygen atom at the interface was estimated thermally stable by adsorption energy. The present research indicates the existence of O/B2 interface may lead to influences on both the mechanical strength and the oxidation resistance of Ti_2AlNb alloys.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room2)

[SY-E8] DFT predictions of hydrogen storage properties of Mg_7TiX_2 (X= F, O, S, P and Cl)

○Yuying Chen, Jianhong Dai, Yan Song （School of Materials Science and Engineering, Harbin Institute of Technology at Weihai, China）

Stability and reversibly de/hydrogenation properties of presumed Mg_7TiX_2 (X= F, O, S, P and Cl) were predicted using Density Functional Theory. Hypothetical Mg_7TiX_2 and its hydride are energetically stable with respect to the individual elements involved and they may be synthesized experimentally. The stability of alloy highly relate to the formation energy of Mg-X compound because that distance of Ti-X is large than that of Mg-X. The considered systems possess preferable hydrogen adsorbing capacity, and their hydrogen adsorption energies lie in the range from -0.5 eV to -0.05 eV. The dehydrogenation of the $Mg_7TiX_2H_{14}$ were calculated and found that H-Mg bond and Ti-Mg bond have significant effect on dehydrogenation process. The study of desorption energy of X atoms found that P atoms are less stable than H atoms and will escape from system before H atoms that lead system collapse, thus Mg_7TiP_2 is not available to hydrogen storage. Our studies indicated that Mg_7TiX_2 (X= F, O, S and Cl) can realize reversible hydrogen storage properties.

Keywords: Density Functional Theory; Hydrogen Storage; Stability; Reversibility; Mg_7TiX_2.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F5] Symposium F-5
Chair: Ingo Steinbach(Ruhr-University Bochum, Germany)
Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room3

[SY-F5] Solidification microstructure formation by phase-field simulation with multi-GPU acceleration
○Tomohiro Takaki[1], Shinji Sakane[1], Munekazu Ohno[2], Yasushi Shibuta[3], Takayuki Aoki[4] （1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.The University of Tokyo, Japan, 4.Tokyo Institute of Technology, Japan）

[SY-F5] **Phase-field study of eutectic colony formation in NiAl-34Cr**
○Michael Kellner[1,2], Johannes Hötzer[1,2], Markus Linnenberg[1], Marco Seiz[1], Britta Nestler[1,2] （1.Institute of Applied Materials - Computational Materials Science (IAM-CMS), Karlsruhe Institute of Technology, Germany, 2.Institute of Digital Materials Science (IDM), Karlsruhe University of Applied Science, Germany）

[SY-F5] Solidification analysis by non-equilibrium phase field model using thermodynamics data estimated by machine learning
○Sukeharu Nomoto[1], Hiroshi Wakameda[1], Masahito Segawa[1], Toshiyuki Koyama[2], Akinori Yamanaka[3] （1.ITOCHU techno-Solutions Coorporation, Japan, 2.Materials Design Innovation Engineering, Nagoya Univ., Japan, 3.Department of Mechnical Systems Engneering, Tokyo University of Agriculture and Technology, Japan）

[SY-F5] Phase field modeling of deformation twinning in β-metastable titanium alloys
○Juba Hamma[1], Benoît Appolaire[2], Yann Le Bouar[1], Alphonse Finel[1] （1.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay F-92322 Châtillon, France, 2.IJL, UMR 7198 CNRS-Université de Lorraine, 54000 Nancy, France）

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room3)

[SY-F5] Solidification microstructure formation by phase-field simulation with multi-GPU acceleration

Invited

○Tomohiro Takaki[1], Shinji Sakane[1], Munekazu Ohno[2], Yasushi Shibuta[3], Takayuki Aoki[4] （1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.The University of Tokyo, Japan, 4.Tokyo Institute of Technology, Japan）

Accurate prediction of material microstructures is crucial for the production and design of high performance material. Phase-field method has emerged as a powerful numerical model for predicting the formation process of complicated material microstructure. Now, it is well accepted as the most accurate and promising model for microstructure formation in the mesoscale. On the other hand, a large computational cost due to the diffuse interface is a major drawback, and usually the phase-field simulation is limited to the small domain. To overcome this drawback, we need a high-performance computing for the phase-field simulation.

In this talk, we introduce our recent progresses in the high-performance phase-field simulation using multi-GPU acceleration. Here, we focus on the dendritic solidification where the microstructure is formed through the competitive growth among multiple dendrites. We introduce the phase-field simulations of dendrite competitive growth during directional solidification of a binary alloy in single crystal [1], bicrystal [2], and polycrystal [3]. In addition, the liquid flow drastically changes the solidification microstructure. We also introduce the large-scale phase-field simulations of dendrite growth with liquid flow [4-6]. The above all simulations have been performed by the GPU supercomputer TSUBAME at the Tokyo Institute of Technology.

[1] T. Takaki, S. Sakane, M. Ohno, Y. Shibuta, T. Shimokawabe, T. Aoki, Acta Materialia 118 (2016) 230-243.
[2] T. Takaki, S. Sakane, M. Ohno, Y. Shibuta, T. Shimokawabe, T. Aoki, ISIJ Int. 56(8) (2016) 1427-1435.
[3] T. Takaki, M. Ohno, Y. Shibuta, S. Sakane, T. Shimokawabe, T. Aoki, J. Crystal Growth 442 (2016) 14-24.
[4] S. Sakane, T. Takaki, R. Rojas, M. Ohno, Y. Shibuta, T. Shimokawabe, T. Aoki, J. Crystal Growth 474 (2017) 154-159.
[5] T. Takaki, R. Rojas, S. Sakane, M. Ohno, Y. Shibuta, T. Shimokawabe, T. Aoki, J. Crystal Growth 474 (2017) 146-153.
[6] T. Takaki, R. Sato, R. Rojas, M. Ohno, Y. Shibuta, Comp. Mater. Sci. 147 (2018) 124-131.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room3)

[SY-F5] Phase-field study of eutectic colony formation in NiAl-34Cr

○Michael Kellner[1,2], Johannes Hötzer[1,2], Markus Linnenberg[1], Marco Seiz[1], Britta Nestler[1,2] （1.Institute of Applied Materials - Computational Materials Science (IAM-CMS), Karlsruhe Institute of Technology, Germany, 2.Institute of Digital Materials Science (IDM), Karlsruhe University of Applied Science, Germany）

The properties of a material are mainly defined by their chemical composition and by their underlying microstructure. Therefore, the development of tailored microstructures is crucial for the applicability in high-performance materials with specified properties. Depending on the material properties and process conditions, multi-scale microstructures evolve during the directional solidification of eutectics. Beside the microscopic eutectic lamellar and/or fibrous structures, macroscopic structures like eutectic colonies occur at certain process conditions. Eutectic colonies are mainly observed in ternary systems when the

composition of the alloy is in the vicinity of a binary eutectic reaction. The formation of colonies is driven by microscopic instabilities in a macroscopic planar solidification front, due to the impurities by the third component that diffuse from the two solidifying phases into the liquid.

To simultaneously investigate the formation processes of micro- and macroscopic structures in their complex spatial arrangement, two- and three-dimensional large-scale phase-field simulations based on a Grand potential formalism are conducted for the high-performance material NiAl-34Cr. By systematic variations of the solidification velocity beyond the stability range the underlying mechanisms leading to the formation of eutectic colonies are studied. Further the interactions and the coherences between the eutectic rod-like structure of NiAl-34Cr and the arrangement of the eutectic colony are investigated. Especially the contact zones between the colonies are of interest, as these are indicated to be the weak points for the applicability. In additional studies the stability of the colonies for different temperature gradients and off-eutectic melt compositions is observed.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room3)

[SY-F5] Solidification analysis by non-equilibrium phase field model using thermodynamics data estimated by machine learning

○Sukeharu Nomoto[1], Hiroshi Wakameda[1], Masahito Segawa[1], Toshiyuki Koyama[2], Akinori Yamanaka[3]
 （1.ITOCHU techno-Solutions Coorporation, Japan, 2.Materials Design Innovation Engineering, Nagoya Univ., Japan, 3.Department of Mechical Systems Engneering, Tokyo University of Agriculture and Technology, Japan）

A multi-phase field (MPF) model coupled with finite interface dissipation proposed by Steinbach et al. is applied to simulate the dendritic solidification in Fe-Cr-Ni-Mo-C steel. Thermodynamic calculation using CALPHAD database is replaced by machine learning prediction procedure in this MPF program. Solidification calculations are performed in a case of quinary system: Fe-16Cr-2Mo-10Ni-0.08C. We confirm that the microstructure evaluated by using machine learning parameter is good agreement with one directly coupled with CALPHAD database. Furthermore, this calculation is also confirmed to be approximately five times faster than the direct CALPHAD calculation method.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room3)

[SY-F5] Phase field modeling of deformation twinning in β-metastable titanium alloys

○Juba Hamma[1], Benoît Appolaire[2], Yann Le Bouar[1], Alphonse Finel[1]   (1.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay F-92322 Châtillon, France, 2.IJL, UMR 7198 CNRS-Université de Lorraine, 54000 Nancy, France）

Recently, new β-metastable titanium alloys, so-called "TRIP/TWIP titanium alloys" (TRIP for TRansformation Induced Plasticity and TWIP for TWinning Induced Plasticity), have been developed to exhibit improved mechanical properties at ambient temperature. These properties are attributed to very complex microstructures engendered by the mechanical destabilization of the initial bcc phase (β) in the course of the deformation. Indeed, the microstructure features numerous twins following the peculiar {332}<113>

twinning mode of the β phase, specific to β-titanium alloys, as well as the orthorhombic (α") phase ensued from concomitant displacive transformations. Moreover, experimental observations revealed the possible activation of secondary deformation mechanisms, i.e. the formation of secondary twins and/or α" inside primary twins of the β phase.

To get a better understanding of the formation of the complex microstructures described above, we propose a numerical model using the phase field method. This method provides a thermodynamically consistent framework to couple the mechanisms at the origin of the microstructure evolution. As a first step of modeling the evolution of the β-metastable titanium alloys microstructure upon deformation, we focus on the {332}<113> twinning mode of the bcc phase β. In this work, we propose a phase-field model relying on (i) a finite strain formalism; and (ii) the possibility of taking into account the activation of secondary twinning inside primary twins. We will show with simple calculations the capabilities of the model to describe the {332}<113> twin growth. A comparison with a model formulated in a small strain formalism will also be presented to show the influence of the geometrical non-linearities introduced in the finite strain framework.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F6] Symposium F-6
Chair: Benoit Appolaire(Institut Jean Lamour, Univ. de Lorraine, France)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room3

[SY-F6] Atomistically informed full-field simulation of tempered martensite:Quenching, tempering and mechanical characterization

○Ingo Steinbach （Ruhr-University Bochum, Germany）

[SY-F6] **Characterisation and modelling of drawn martensite**

○Marius Gintalas[1], Miguel A. Santajuana[2], Carlos Garcia-Mateo[2], David San-Martin[2], Jose A. Jiménez[2], Wim Van Haver[3], Pedro E. J. Rivera-Diaz-del-Castillo[4] （1.The University of Cambridge, Department of Materials Science &Metallurgy, 27 Charles Babbage Road, Cambridge CB3 0FS, UK, 2.Materalia research group, Department of Physical Metallurgy, Spanish National Centre for Metallurgical Research (CENIM-CSIC), Avda. Gregorio del Amo 8, Madrid E-28040, Spain, 3.NV Bekaert SA, Bekaertstraat 2, Zwevegem B-8550, Belgium, 4.The University of Lancaster, Department of Engineering, Engineering Building, Lancaster University, Gillow Ave, Bailrigg, Lancaster LA1 4YW, UK）

[SY-F6] 3D modeling of microstructure evolution in Ni-based superalloys under creep loading

○Maeva Cottura[1], Benoît Appolaire[1], Alphonse Finel[2], Yann Le Bouar[2] （1.Institut Jean Lamour , France, 2.LEM - CNRS/Onera, France）

[SY-F6] Phase field study of the effect of coherency strains and applied load in material couples

○Sourav Chatterjee, Nele Moelans （Department of Materials Engineering, KU Leuven, Belgium）

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room3)

[SY-F6] Atomistically informed full-field simulation of tempered martensite:Quenching, tempering and mechanical characterization

Invited

○Ingo Steinbach （Ruhr-University Bochum, Germany）

A scale bridging modelling and simulation strategy of virtual production and virtual testing is presented which starts with parametrization of continuum constitutive relations by quantum mechanical calculations at the atomistic scale. These models are integrated into a full-field framework at the scale of microstructures in technical materials. The phase-field method is employed to simulate the microstructure evolution during processing: virtual production. Finally micromechanical simulations of deformation and damage evolution till catastrophic failure are performed utilizing the full information about the microstructure, composition and residual stresses resulting from the production route: virtual testing. The approach is applied to tempered martensite, describing the evolution of the microstructure under quenching, tempering and testing.

The quenching simulation reproduces the martensite transformation under consideration of the Kurdjumov-Sachs relationship. Based on these results, tempering is simulated. Diffusion is enabled at elevated temperatures and cementite carbides are nucleated, which decreases carbon composition in the martensite, which also decreases the tetragonal distortion. A virtual tension test provides then information about strain hardening, damage as well as the macroscopic response of the material to the loading. Different microstructures, as resulting from different alloy composition and different tempering conditions are compared regarding their mechanical performance.

[1] Atomistically Informed Extended Gibbs Energy Description for Phase-Field Simulation of Tempering of Martensitic Steel, Oleg Shchyglo, Thomas Hammerschmidt, Miroslav Čak, Ralf Drautz, Ingo Steinbach, Materials 9 (8), 669

[2] Microstructure Design of Tempered Martensite by Atomistically Informed Full-Field Simulation: From Quenching to Fracture, Efim Borukhovich, Guanxing Du, Matthias Stratmann, Martin Boeff, Oleg Shchyglo, Alexander Hartmaier, Ingo Steinbach, Materials 9 (8), 673

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room3)

[SY-F6] Characterisation and modelling of drawn martensite

○Marius Gintalas[1], Miguel A. Santajuana[2], Carlos Garcia-Mateo[2], David San-Martin[2], Jose A. Jiménez[2], Wim Van Haver[3], Pedro E. J. Rivera-Diaz-del-Castillo[4] （1.The University of Cambridge, Department of Materials Science &Metallurgy, 27 Charles Babbage Road, Cambridge CB3 0FS, UK, 2.Materalia research group, Department of Physical Metallurgy, Spanish National Centre for Metallurgical Research (CENIM-CSIC), Avda. Gregorio del Amo 8, Madrid E-28040, Spain, 3.NV Bekaert SA, Bekaertstraat 2, Zwevegem B-8550, Belgium, 4.The University of Lancaster, Department of Engineering, Engineering Building, Lancaster University, Gillow Ave, Bailrigg, Lancaster LA1 4YW, UK）

There has been an extensive work on microstructural refinement via severe plastic deformation, which leads to improved strength in metallic materials. However, due to the complexity of the microstructural changes involved, the mechanisms responsible for the strength enhancement of the cold deformed marteniste have not been completely revealed. This work summarises advanced experimental and modelling activities carried out on heavily drawn martensite. These include slow heating high resolution dilatometry, high resolution transmission electron microscopy and high resolution X-ray diffraction conducted with both synchrotron and lab x-ray sources. The purpose of employing various characterisation techniques is to collect data to gain a comprehensive understanding on the microstructural evolution with respect to applied strain. The modelling work aims to propose a novel martensite strength model to describe the relationship between microstructure and mechanical properties, including the effects of applied strain upon severe plastic deformation. The strengthening model is validated using stress-strain data of martensite drawn at various strain levels.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room3)

[SY-F6] 3D modeling of microstructure evolution in Ni-based superalloys under creep loading

○Maeva Cottura[1], Benoît Appolaire[1], Alphonse Finel[2], Yann Le Bouar[2] （1.Institut Jean Lamour , France, 2.LEM - CNRS/Onera, France）

Many materials used in everyday life have a complex internal structure organized at different scales with a texture of grains, and a complex pattern of thermodynamic phases at lower scale. This microstructure strongly impacts the movement of crystalline defects in the materials and therefore controls the mechanical behaviour. The phase field method has emerged as a well-suited method for tackling microstructure evolutions during phase transformations when elastic coherency stresses are generated. In addition, in many materials and especially at high temperature, the microstructure evolution is coupled with plasticity, and there is currently a great research effort to extend the phase field method to take this coupling into account. In this context, we will show how to couple a classical phase field model (for the description of the phase transformation) with a crystal plasticity model based on dislocation densities. The latter model uses a storage-recovery law for the dislocation density of each glide system and a hardening matrix to account for the short-range interactions between dislocations. The proposed model will be applied to study rafting of ordered precipitates observed in Ni-based superalloys. We will present 3D calculations of microstructure evolution under [100], [110] and [111] creep loading as well as different shear creep tests.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room3)

[SY-F6] Phase field study of the effect of coherency strains and applied load in material couples

○Sourav Chatterjee, Nele Moelans （Department of Materials Engineering, KU Leuven, Belgium）

We investigate the role of coherency strains and applied load on phase growth and morphological evolution in binary diffusion couples using the phase field method. We employ the Kim-Kim-Suzuki model for the chemical contribution in the free energy. The elastic energy contribution to the free energy is evaluated using a suitable interpolation scheme considering the elastic heterogeneity between the different phases. When

elastic stresses are considered, we observe bending and splitting of the phase layers for mechanically constrained, partially constrained and relaxed systems. The interface remains planar in the absence of elastic stresses. In addition, we study the role of volume fraction of the phases and finite size of the system on the microstructure evolution.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F7] Symposium F-7

Chair: Tomohiro Takaki(Kyoto Institute of Technology, Japan)
Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3

[SY-F7] A Cosserat crystal plasticity and phase field theory for grain boundary migration

○Benoit Appolaire[1,2], Anna Ask[3], Samuel Forest[3], Kais Ammar[3] （1.Institut Jean Lamour, Univ. de Lorraine, France, 2.LEM, CNRS-Onera, France, 3.Centre des Materiaux, Mines ParisTech, France）

[SY-F7] Phase-field modeling of precipitation growth and ripening during heat-treatment conditions in Ni-base superalloys

○Michael Fleck, Felix Schleifer, Markus Holzinger, Yueh-Yu Lin, Uwe Glatzel （Metals and Alloys, University Bayreuth, Germany）

[SY-F7] Two-dimensional Simulation of Cyclic Phase Transformation in Fe-C-Mn-Si Alloy using Non-equilibrium Multi-Phase-Field Model

○Masahito Segawa[1], Nomoto Sukeharu[1], Akinori Yamanaka[2] （1.ITOCHU Techno-Solutions Corporation, Japan, 2.Division of Advanced Mechanical Systems Engineering, Institute of Engineering, Tokyo University of Agriculture and Technology, Japan）

[SY-F7] Prediction of the microstructure evolution in Electron Beam Melting Alloy 718 through phase field modelling

○Chamara Kumara[1], Dunyong Deng[2], Johan Moverare[2], Per Nylén[1] （1.Department of Engineering Science, University West, Sweden, 2.Department of Management and Engineering, Linköping University, Sweden）

[SY-F7] Phase-field simulation of solidification morphology in laser powder deposition of Fe-B alloys

○Xiaoxia Li, Xiangge Qin （School of Materials Science and Engineering, Jiamusi Univ., China）

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3)

[SY-F7] A Cosserat crystal plasticity and phase field theory for grain boundary migration

Invited

○Benoit Appolaire[1,2], Anna Ask[3], Samuel Forest[3], Kais Ammar[3] （1.Institut Jean Lamour, Univ. de Lorraine, France, 2.LEM, CNRS-Onera, France, 3.Centre des Materiaux, Mines ParisTech, France）

Elaborating a unified field framework to model concurrent viscoplastic deformation and recrystallization and grain growth in metal polycrystals has remained a formidable issue. In this work, we will present such a unified framework relying on the enhancement of a Cosserat crystal plasticity model with an order parameter to account for diffuse, mobile grain boundaries in analogy with phase field models. The Cosserat directors are taken to represent the lattice orientation of the grains. In order to introduce an evolution law for reorientation during grain boundary migration, the skew-symmetric part of the Cosserat deformation tensor is associated with a dissipative stress. The formulation in terms of the Cosserat deformation provides a natural way to couple reorientation due to deformation and reorientation due to grain boundary migration. In the absence of displacements and for a particular choice of free energy function the model can be considered a generalization to three dimensions of the Kobayashi-Warren-Carter (KWC) orientation phase field model (2000, 2003).

The proposed 3D anisotropic constitutive framework couples the changing orientation at a material point due to migrating grain boundaries (which is essential to the KWC model) to the lattice reorientation due to displacements and plastic slip. Due to the coupling of the Cosserat directors and the elastic reorientation, the bulk rotation of the grains which is inherent to the KWC model (and considered an artefact here although it can nevertheless be desirable in certain cases) can be controlled and even suppressed.

In this contribution, we will explain the main features of this framework and we will illustrate its capabilities with several cases that could not be handled convincingly by other models.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3)

[SY-F7] Phase-field modeling of precipitation growth and ripening during heat-treatment conditions in Ni-base superalloys

○Michael Fleck, Felix Schleifer, Markus Holzinger, Yueh-Yu Lin, Uwe Glatzel （Metals and Alloys, University Bayreuth, Germany）

We develop a phase-field model for the simulation of chemical diffusion limited microstructure evolution, with a special focus on precipitation growth and ripening in multi-component alloys. Further, the model accounts for elastic effects, which result from the lattice-misfit between the precipitate particles and the parent matrix-phase. To be able to simulate particle growth and ripening in one dimension, we introduce an extra optional driving-force term, which mimics the effect of the curved particle/matrix interface in one dimension. As a case study, we consider the gamma'-precipitation growth and ripening under the influence of realistic heat treatment time-scales in the multi-component Ni-base single crystalline cast alloy CMSX-4. The respectively required temperature-dependent thermodynamic and kinetic input parameters are obtained from CALPHAD calculations using the commercial software-package ThermoCalc. The required temperature-dependent elastic parameters are measured in-house at the chair of Metals and Alloys, using resonance ultrasound spectroscopy for the anisotropic and inhomogeneous stiffness-tensor and high temperature X-ray defraction for the lattice misfit.

We study the kinetics of growth and ripening of statistically many interacting precipitated particles as function of the temperature and time in one and two dimensions, with the explicit consideration of up to 8 independent chemical components. Furthermore, the model is applied to calculate the detailed shape-evolution of a few interacting gamma'-particles in two and three dimensions with periodic boundary conditions. Relations to the shapes of gamma'-particles in respectively heat treated experimental microstructures are discussed.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3)

[SY-F7] Two-dimensional Simulation of Cyclic Phase Transformation in Fe-C-Mn-Si Alloy using Non-equilibrium Multi-Phase-Field Model

○Masahito Segawa[1], Nomoto Sukeharu[1], Akinori Yamanaka[2]　(1.ITOCHU Techno-Solutions Corporation, Japan, 2.Division of Advanced Mechanical Systems Engineering, Institute of Engineering, Tokyo University of Agriculture and Technology, Japan）

Multi-phase-field (MPF) method incorporating CALPHAD database has attracted much attention as a powerful numerical tool for simulating microstructure evolutions in various metallic materials. Transformation modes and diffusion behavior of substitutional solute atoms strongly depend on temperature and chemical compositions of the alloy especially in multi-component steels, i.e. an Fe-C-Mn ternary alloy. Therefore, we need to use a robust MPF model which can simulate the transition of transformation mode and the complex diffusion behavior. Recently, the MPF model with finite interface dissipation has been proposed (Hereafter, the MPF model is called as the non-equilibrium MPF (NEMPF) model). The attractive advantages of the NEMPF model are its computational efficiency and flexibility for simulating microstructure evolutions under strong non-equilibrium interface condition without the equal chemical potential assumption. In the previous study, we investigated the cyclic $\gamma \rightarrow \alpha$ and $\alpha \rightarrow \gamma$ transformations in Fe-C-Mn-Si alloys using the NEMPF model coupled with CALPHAD database. The one-dimensional simulations of the cyclic phase transformation revealed that the switching of the polarities of Mn and Si spikes formed at the α / γ interface caused the stagnant stage where the phase transformation was suppressed. In this study, the two-dimensional simulation of cyclic phase transformation in Fe-C-Mn-Si alloy is performed using the NEMPF model in order to gain a deeper understanding of the mechanism of the stagnant stage and the transition of transformation modes.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3)

[SY-F7] Prediction of the microstructure evolution in Electron Beam Melting Alloy 718 through phase field modelling

○Chamara Kumara[1], Dunyong Deng[2], Johan Moverare[2], Per Nylén[1]　(1.Department of Engineering Science, University West, Sweden, 2.Department of Management and Engineering, Linköping University, Sweden）

Electron Beam Melting (EBM) is a powder bed additive manufacturing process where powder material is being melted selectively by a layer-by-layer approach using an electron beam. It has some unique features when it comes to manufacturing of components in high-performance superalloys such as alloy 718 that are commonly used in gas turbines. EBM has high deposition rate due to high beam energy and speed, comparatively low residual stresses and limited problems with oxidation. However, due to the layer-by-layer melting approach and high powder bed temperature, the resultant microstructure of as-built EBM Alloy 718

is observed to have a microstructure gradient starting from the top of the sample. The aim of this study was to use modelling to create a deeper understanding of microstructure development during EBM and the homogenization that occurs during manufacturing in Alloy 718. A multi-component phase field modelling approach combined with thermodynamic modelling was used to predict the experimentally observed microstructure gradient. Of particular interest was to study the element segregation during the solidification and the subsequent "in-situ" homogenization heat treatment that occur due to the elevated powder bed temperature. The predicted element composition was then used in thermodynamic modelling to predict the changes in the CCT and TTT diagrams for Alloy 718. This helps to explain the observed phase evolution within the microstructure. The results indicate that the approach can be a valuable tool both for creating process understanding and for process development including subsequent homogenization and heat treatment.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3)

[SY-F7] Phase-field simulation of solidification morphology in laser powder deposition of Fe-B alloys

○Xiaoxia Li, Xiangge Qin （School of Materials Science and Engineering, Jiamusi Univ., China）

Laser melting deposition is a complicated physical and chemical metallurgical process. In this paper, the phase field model of alloy solidification is coupled to laser melting deposition process, and a finite element model of heat transfer is established. By studying the variation of the spacing of dendrite Fe_2B of Fe-B alloy powder under the conditions of laser melt deposition, the robustness and accuracy of the coupled model were verified. Experiments show that under different temperature gradient conditions, the size and spacing of the dendrite Fe_2B of the cross-section morphology of the Fe-B alloy deposited by laser melting deposition have changed significantly. The quantitative phase field simulation of the heat transfer finite element model under local steady state conditions confirms this behavior. This work demonstrates the potential of the phase-field method to simulate laser melting deposition techniques and analyze the potential of alloy solidification under complex heat transfer conditions.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F8] Symposium F-8

Chair: Martin Diehl(Max-Planck-Institut fuer Eisenforschung GmbH, Germany)
Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3

[SY-F8] From state parameter-based microstructure modeling to temperature and strain rate-dependent yield stress

○Ernst Kozeschnik （Institute of Materials Science and Technology, TU Wien, Austria）

[SY-F8] **Modelling of grain boundary segregation and precipitation in multi-component Al alloys subjected to heat treatment**

○Dongdong Zhao[1], Sylvain Gouttebroze[2], Jesper Friis[3], Yanjun Li[1] （1.Norwegian University of Science and Technology (NTNU), 7491, Trondheim , Norway, 2.SINTEF Materials and Chemistry, 0314 Oslo, Norway, 3.SINTEF Materials and Chemistry, 7491 Trondheim, Norway）

[SY-F8] Modeling the microstructure and electrical conductivity evolution during aging of Al-Mg-Si alloys

○Yijiang Xu, Yanjun Li （Norwegian University of Science and Technology , Norway）

[SY-F8] Thermo-kinetic modeling of long-term precipitate evolution in heat-resistant alloys

○Jae-Hyeok Shim[1], Magdalena Speicher[2], Mahesh Chandran[3], Woo-Sang Jung[1] （1.Korea Institute of Science and Technology, Korea, 2.Materials Testing Institute, Germany, 3.Indo-Korea Science and Technology Centre, India）

[SY-F8] **Simultaneous Transformation Kinetics Model for Additive Manufacturing**

○Narendran Raghavan, Srdjan Simunovic, John Turner （Oak Ridge National Laboratory , United States of America）

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3)

[SY-F8] From state parameter-based microstructure modeling to temperature and strain rate-dependent yield stress

Invited

○Ernst Kozeschnik （Institute of Materials Science and Technology, TU Wien, Austria）

In the past 20 years, significant progress has been made in the development of state parameter-based modeling approaches for the simulation of microstructure evolution, in particular, with respect to precipitation kinetics, recrystallization, recovery, grain growth, dislocation density evolution in the course of thermo-mechanical treatment, as well as the mutual interactions of all mechanisms. Once, the relevant state parameters and their evolution are known, it is straightforward, however not trivial, to deduct from these the stress strain response of the microstructure as a function of temperature and strain rate. In this presentation, an overview of these models is given as well as some implementation details in the thermokinetic software package MatCalc. Finally, an example is discussed, where the precipitation microstructure and its interaction with deformation in the course of compression testing is simulated and compared to corresponding experimental data.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3)

[SY-F8] Modelling of grain boundary segregation and precipitation in multi-component Al alloys subjected to heat treatment

○Dongdong Zhao[1], Sylvain Gouttebroze[2], Jesper Friis[3], Yanjun Li[1] （1.Norwegian University of Science and Technology (NTNU), 7491, Trondheim , Norway, 2.SINTEF Materials and Chemistry, 0314 Oslo, Norway, 3.SINTEF Materials and Chemistry, 7491 Trondheim, Norway）

A newly developed modelling framework which accounts for grain boundary (GB) segregation and precipitation in multi-component Al alloys subjected to cooling and subsequent heat treatments is presented. Within this framework, both the equilibrium and non-equilibrium segregation mechanisms are considered to predict the solute and vacancy segregations towards GBs. In the model of non-equilibrium segregation, GBs are considered as ideal sinks for vacancy annihilation. The CALPHAD (CALculations pf PHAse Diagrams) approach is implemented to supply the important thermodynamic and kinetic data of multi-component Al alloys as input for the model. The present framework is expected to predict the solute and vacancy segregations at GBs in multi-component Al alloys during typical heat treatment (e.g. quenching, ageing) processes. It is shown that the variation of vacancy and solute segregation behavior at GBs as a function of heat treatment or microstructure variables, i.e. solution/ageing temperature, cooling rate, grain size, can be well described within the present model. Based on the segregation of solute elements, preliminary precipitation behavior at GBs and bulk are predicted using the Kampmann-Wagner numerical approach. The simulation results have been compared with experimental observations. This work is supposed to provide a preliminary theoretical understanding towards the GB segregation and precipitation in multi-component Al alloys subjected to various cooling and subsequent heat treatment processes.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3)

[SY-F8] Modeling the microstructure and electrical conductivity evolution during aging of Al-Mg-Si alloys

○Yijiang Xu, Yanjun Li （Norwegian University of Science and Technology , Norway）

Aging is commonly performed after forming process to obtain better mechanical properties and electrical conductivity of Al-Mg-Si alloys (AA6xxx series) applied in the electrical wire. In this work, the nucleation, growth, coarsening and dissolution of different precipitate phases (Mg_xSi_y) during aging treatment is simulated based on a Kampmann-Wagner Numerical (KWN) type precipitation model. By coupling with the CALPHAD, the thermodynamics of the metastable precipitate phases is well treated. Furthermore, the precipitation model is linked to an electrical conductivity model to predict the evolution of electrical conductivity based on the volume fraction, size and spatial distribution of different precipitates, solid solution level, etc. The modeling results are compared to the transmission electron microscopy (TEM) experimental results and electrical conductivity measurements. It is revealed that the present model can well address the influence of alloy composition, aging temperature and aging time on the microstructure and electrical conductivity of Al-Mg-Si alloys.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3)

[SY-F8] Thermo-kinetic modeling of long-term precipitate evolution in heat-resistant alloys

○Jae-Hyeok Shim[1], Magdalena Speicher[2], Mahesh Chandran[3], Woo-Sang Jung[1] （1.Korea Institute of Science and Technology, Korea, 2.Materials Testing Institute, Germany, 3.Indo-Korea Science and Technology Centre, India）

There is an urgent need to improve the thermal efficiency of fossil fuel power plants by raising the operation temperature and pressure in order to reduce CO_2 emission as well as the cost of fuel. Plant operation at higher temperatures inevitably requires the development of heat-resistant alloys with a higher creep strength. There has recently been an increasing interest in applying advanced heat-resistant alloys to fossil fuel power plants in order to raise their operation temperature. The important role of precipitation in the achievement of good creep properties of heat-resistant alloys has long been recognized. One of the most effective ways for improving the creep properties is to uniformly distribute fine precipitates with a good long-term stability at elevated temperatures. The experimental investigation of the long-term precipitate evolution behavior in heat-resistant alloys have not often been performed, although it is important in understanding the creep properties. In addition to experimental approaches, there have recently been a few attempts to simulate the precipitation kinetics in heat-resistant alloys. The purpose of this study is to simulate the long-term precipitate evolution in various heat-resistant alloys such as ferritic/martensitic and austenitic steels and nickel alloys using the MatCalc software, which operates based on the classical nucleation theory and evolution equations derived from the thermodynamic extremum principle that maximizes the dissipation rate of the total Gibbs energy of the system. The simulation results, such as the precipitation sequence and the precipitate size, will be compared with experimental observations.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3)

[SY-F8] Simultaneous Transformation Kinetics Model for Additive Manufacturing

○Narendran Raghavan, Srdjan Simunovic, John Turner （Oak Ridge National Laboratory , United States of America）

Metal additive manufacturing is disrupting the traditional approaches in the manufacturing sector. However, there are uncertainties associated with the qualification of fabricated components owed to the difficulty in predicting the process-structure relationship in the PSPP linkage. Understanding the process-structure linkage includes understanding the (a) liquid-solid phase transformation and (b) solid-solid phase transformation. Previously solidified layers are affected by the thermal cycles during the melting of the subsequent layers. During processing in AM, the conditions are highly non-isothermal, non-equilibrium and understanding this highly transient condition is crucial to understand the precipitation kinetics. The temperature of the substrate can also be varied in the machine. This affects the solid-state phase transformation of a given alloy system. Multiple phases can simultaneously precipitate from the product phase as a function of thermal cycle. In this work, we develop a model based on simultaneous transformation kinetics theory and the developed phenomenological model is then coupled with the numerical thermal model to predict the solid-state phase transformation and volume fraction of multiple phases as a function of thermal cycles and processing conditions. Numerical thermal model is used to predict the thermal cycles as a function of input processing conditions. The thermal cycle is then discretized into set of small isothermal steps. The extent of simultaneous precipitation/dissolution of the phases will be calculated at each of the discretized time step. Volume fraction of each of the phases is then updated and similar procedure is repeated for rest of the discretized isothermal time steps. Appropriate thermodynamic framework, database will be used to calculate the thermodynamic properties as a function of alloy system and is used as the input to the model. It is a semi-empirical model and the input from experimental results are used to calibrate the model. Some of the other calibration parameters include nucleation site densities and surface energies. Advantages and limitations of this approach will be discussed in detail.

Symposium | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[SY-N1] Symposium N-1

Chair: Danny Perez(Los Alamos National Laboratory, United States of America)
Wed. Oct 31, 2018 9:45 AM - 10:45 AM Room4

[SY-N1] Increasing the power of accelerated molecular dynamics methods and plans to exploit the coming exascale

○Arthur F Voter （Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, United States of America）

[SY-N1] Atomistic processes at interfaces on extended timescales

○Jutta Rogal[1] （1. Ruhr University Bochum, Germany）

(Wed. Oct 31, 2018 9:45 AM - 10:45 AM Room4)

[SY-N1] Increasing the power of accelerated molecular dynamics methods and plans to exploit the coming exascale

Invited

○Arthur F Voter （Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, United States of America）

Many important materials processes take place on time scales that far exceed the roughly one microsecond accessible to molecular dynamics simulation. Typically, this long-time evolution is characterized by a succession of thermally activated infrequent events involving defects in the material. In the accelerated molecular dynamics (AMD) methodology, known characteristics of infrequent-event systems are exploited to make reactive events take place more frequently, in a dynamically correct way. For certain processes, this approach has been remarkably successful, offering a view of complex dynamical evolution on time scales of microseconds, milliseconds, and sometimes beyond. We have recently made advances in all three of the basic AMD methods (hyperdynamics, parallel replica dynamics, and temperature accelerated dynamics (TAD)), exploiting both algorithmic advances and novel parallelization approaches. I will describe these advances, present some examples of our latest results, and discuss what should be possible when exascale computing arrives in roughly four years.

(Wed. Oct 31, 2018 9:45 AM - 10:45 AM Room4)

[SY-N1] Atomistic processes at interfaces on extended timescales

Invited

○Jutta Rogal[1] （1. Ruhr University Bochum, Germany）

Obtaining atomistic insight into the fundamental processes during phase transformations and their dynamical evolution up to experimental timescales remains one of the great challenges in materials modelling. In particular, if the mechanisms of the phase transformations are governed by so-called rare events the timescales of interest will reach far beyond the applicability of regular molecular dynamics simulations. In addition to the timescale problem the simulations provide a vast amount of data in the high-dimensional phase space. A physical interpretation of these data requires the projection into a low-dimensional space and the identification of suitable reaction coordinates.

In this presentation, I will give an example of our analysis of the atomistic processes at a complex phase boundary during a solid-solid phase transformation. The migration of the phase boundary proceeds via concerted multi-atom processes on a complex energy landscape. Here, we employ an adaptive kinetic Monte Carlo (AKMC) approach together with driven adiabatic free energy dynamics (d-AFED) to investigate such processes at the interface between the body-centered cubic and A15 phase in molybdenum.

Symposium | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[SY-N2] Symposium N-2

Chair: Erik Bitzek(FAU Erlangen-Nuernberg, Germany)
Wed. Oct 31, 2018 11:15 AM - 12:15 PM Room4

[SY-N2] *Modeling Microstructure Evolution in Rapid Solidification Phenomena Using Structural Phase Field Crystal Models*

○Nikolas Provatas （McGill University, Canada）

[SY-N2] The Phase Field Method: Crystal Structures and Facets

○Peter Voorhees[1], Eli Alster[1], Nana Ofuri-Opoku[1,3], David Montiel[2], Katsuyo Thornton[2], James Warren[3] （1.Northwestern University, United States of America, 2.University of Michigan, United States of America, 3.National Institute for Standards and Technology, United States of America）

[SY-N2] Using free energy calculations and statistical mechanics to probe the brittle to ductile transition of bcc metals

○Thomas Swinburne[1] （1.CINaM, CNRS/Aix-Marseille Univ., France）

(Wed. Oct 31, 2018 11:15 AM - 12:15 PM Room4)

[SY-N2] *Modeling Microstructure Evolution in Rapid Solidification Phenomena Using Structural Phase Field Crystal Models*

Invited
○Nikolas Provatas （McGill University, Canada）

This talk will study several closely connected density functional type theories that employ both short and long range, rotationally invariant, multi-point particle interactions. Collectively, these models give rise to a class of *structural phase field crystal* (*XPFC*) models. These XPFC models allow for numerous microstructural phenomena to be studied that couple important physics emergent at the atomic scale with phase transformation kinetics occurring on diffusional time scales. Results from recent solidification studies conducted using XPFC modelling in pure materials and alloys will be presented and compared to experiments and other theory. These include multi-step nucleation in solidification, void formation in nano-confined liquid pools during rapid cooling, solute drag, and dislocation-assisted nucleation in solid-state precipitation in alloys. Coupling of the base phase field theory with heat transfer will also be demonstrated for the study of latent heat effects in solidification. We close by discussing coarse graining methods for deriving practical phase field theories from phase field crystal models for meso-scale modelling applications.

(Wed. Oct 31, 2018 11:15 AM - 12:15 PM Room4)

[SY-N2] The Phase Field Method: Crystal Structures and Facets

○Peter Voorhees[1], Eli Alster[1], Nana Ofuri-Opoku[1,3], David Montiel[2], Katsuyo Thornton[2], James Warren[3]
（1.Northwestern University, United States of America, 2.University of Michigan, United States of America, 3.National Institute for Standards and Technology, United States of America）

Phase field crystal (PFC) method allows the atomic scale motion and defect formation to be determined on diffusive timescales. A major challenge with the method is to devise free energy functions that can yield complicated crystal structures. We introduce a phase-field crystal model that creates an array of complex three- and two-dimensional crystal structures via a numerically tractable three-point correlation function. This approach successfully yields energetically stable simple cubic, diamond cubic, simple hexagonal, graphene layers, and CaF2 crystals, as well as the particularly complex and technologically important perovskite crystal structure. Highly anisotropic interfaces play an important role in the development of material microstructure. We examine the capability of the PFC model to quantitatively describe faceted interfaces by coarse graining the PFC model to attain both its complex amplitude formulation, and its corresponding phase field limit. Using this formulation, we find that the model yields Wulff shapes with missing orientations, the transition to missing orientations, and facet formation. We demonstrate, in two dimensions, how the resultant model can be used to study the growth of crystals with varying degrees of anisotropy in the phase-field limit.

(Wed. Oct 31, 2018 11:15 AM - 12:15 PM Room4)

[SY-N2] Using free energy calculations and statistical mechanics to probe the brittle to ductile transition of bcc metals

Invited

○Thomas Swinburne[1] （1.CINaM, CNRS/Aix-Marseille Univ., France）

The fracture response of bcc metals is known to be controlled by dislocation mobility, which in turn is dependent on the slow, thermally activated nucleation of kink pairs on screw dislocations. We present a general, efficient scheme to calculate free energy barriers in large crystalline systems[1] which we apply to the kink nucleation process, finding significant anharmonic contributions at low homologous temperatures. A statistical mechanical approach is then used to study kink-limited dislocation motion through a field of obstacles[2]. We identify a crossover obstacle density below which the activation energy for plastic flow is half the free energy barrier for kink pair nucleation. Our results show striking agreement with fracture experiments across a wide range of bcc metals and are applied to interpret experimental data on irradiation induced embrittlement.

[1] TD Swinburne and M-C Marinica, Physical Review Letters 120 (13), 135503
[2] TD Swinburne and SL Dudarev, Physical Review Materials 2 (7), 073608

[SY-N3] Symposium N-3

Chair: Arthur F. Voter(Los Alamos National Lab, United States of America)
Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room4

[SY-N3] Kinetics of Fivefold-Twinned Nanowire Growth
○Kristen Fichthorn （Penn State University, United States of America）

[SY-N3] Accelerated quantum molecular dynamics simulations of chemistry under extreme conditions
○Romain Perriot, Marc Cawkwell, Enrique Martinez （Los Alamos National Laboratory, United States of America）

[SY-N3] Hydrogen diffusion in TiH_x: insights from PRD accelerated QMD
○Ivan Novoselov[1,2], Alexey Yanilkin[1] （1.Dukhov Research Institute of Automatics, Russia, 2.Moscow Institute of Physics and Technology, Russia）

[SY-N3] Shape fluctuation of metallic nanoclusters: observations from long-timescale simulations
○Rao Huang[1], Li-Ta Lo[2], Arthur F. Voter[2], Danny Perez[2] （1.Xiamen University, China, 2.Los Alamos National Lab, United States of America）

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room4)

[SY-N3] Kinetics of Fivefold-Twinned Nanowire Growth

Invited

○Kristen Fichthorn （Penn State University, United States of America）

There has been significant emphasis recently on the synthesis of fivefold-twinned Ag and Cu nanowires, which are considered to be excellent candidates for transparent conductors in flexible and stretchable electronic devices. A fundamental understanding of nanowire growth is important in achieving optimal syntheses. Nanowires grow from fivefold-twinned seeds and our work shows that likely shapes for these structures include {111} end facets and "notches", {100} side facets, and {110} facets between the notches and the ends. We find that the density of islands on the {111} facets of growing wires is lower than that on {100} facets and that islands are likely to nucleate on {111} facets near {110}-{111} facet boundaries. Our climbing-image nudged-elastic band calculations of diffusion barriers based on embedded-atom method potentials indicate that diffusion in the {111} notches and on the {110} "steps" is significantly faster than diffusion on {100} facets. Thus, these structures become "superhighways" that channel atom diffusion to the wire ends to increase wire aspect ratios. Small islands facilitate trapping of atoms on {111} facets. We use finite Markov chains to model nanowire growth and to predict net atom fluxes from nanowire sides to the ends. These simulations predict anisotropic nanowires similar to those seen experimentally.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room4)

[SY-N3] Accelerated quantum molecular dynamics simulations of chemistry under extreme conditions

○Romain Perriot, Marc Cawkwell, Enrique Martinez （Los Alamos National Laboratory, United States of America）

Atomistic simulations are a key component to understand reaction chemistry in materials; for instance, the detonation chemistry of energetic materials under pressure, which is characterized by rapid breaking and remaking of covalent bonding, and where intermediate products and reaction rates are difficult to characterize in experiments.

While accurate methods exist to study systems of relevant size with explicit electronic contributions critical to the description of bonds, e.g. density functional tight-binding (DFTB), the timescale of the simulation is often limited to a few hundreds of picoseconds. This restrains the study to systems in which reactions occur relatively quickly. In the case of detonation chemistry, this implies high pressure and temperature. In order to consider less extreme conditions, one can benefit from the rare occurrence of chemical reactions to use accelerated molecular dynamics methods such as parallel replica dynamics (PRD).

In this work, we describe efforts to combine the DFTB code LATTE, developed at LANL, with the PRD method, in order to perform accelerated QMD (AQMD) simulations of reactive chemistry. AQMD was first applied to the study of liquid benzene, a prototypical reactive hydrocarbon that has been studied both experimentally and theoretically. AQMD allowed to perform simulations reaching several nanoseconds, and thus the observation of reactions at pressures below 20 GPa. Importantly, these simulations unraveled the precursor reaction to polymerization: the formation of Diels-Alder dimers.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room4)

[SY-N3] Hydrogen diffusion in TiH$_x$: insights from PRD accelerated QMD

$^\bigcirc$Ivan Novoselov[1,2], Alexey Yanilkin[1] (1.Dukhov Research Institute of Automatics, Russia, 2.Moscow Institute of Physics and Technology, Russia)

TiH$_x$ is of practical interest due to high volume concentration of hydrogen, and for many applications its diffusion properties should be established with confidence. We investigate the mechanisms of diffusion, and calculate corresponding rates in the framework of quantum molecular dynamics (QMD). However, time scales accessible to conventional QMD are very limited. It therefore can be employed only at very high temperatures, where no experimental data is available. In order to explore diffusion at lower temperatures, we accelerate QMD simulations via parallel replica dynamics algorithm (PRD). Application of PRD allows to reveal different mechanisms of hydrogen diffusion in TiH$_x$, and also makes it possible to perform direct comparison with experiment

---

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room4)

[SY-N3] Shape fluctuation of metallic nanoclusters: observations from long-timescale simulations

Invited

$^\bigcirc$Rao Huang[1], Li-Ta Lo[2], Arthur F. Voter[2], Danny Perez[2] (1.Xiamen University, China, 2.Los Alamos National Lab, United States of America)

Metallic nanoclusters are functional materials with many applications owing to their unique physical and chemical properties, which are sensitively controlled by their shapes and structures. An in-depth understanding of their morphology stability is therefore of crucial importance. It has been well documented by transmission electron microscopy (TEM) studies that metallic nanoclusters can interconvert between different isomers. However, the relevant mechanisms remain elusive because the timescales of such shape fluctuations are too short to be resolved experimentally and yet too long for conventional atomistic simulations. By employing a recently introduced Accelerated Molecular Dynamics method, Parallel Trajectory Splicing, we present simulations that reached timescales of milliseconds and thus provide a clear description of the dynamic process of the experimentally observed shape fluctuation in metallic nanoclusters. We observe transformations back and forth between face-centered-cubic (fcc) and structures with five-fold symmetry (decahedron or icosahedron). These transitions occur following either by a partial-dislocation-mediated twinning mechanism or by a surface-reconstruction driven process. The identified pathway is in remarkable agreement with the existing microscopy results and serves as further evidence that shape fluctuation can occur directly through thermal activation, without involving melting or other external factors.

[SY-N4] Symposium N-4

Chair: Laurent Karim Beland(Queen's University, Canada)
Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room4

[SY-N4] Multiscale diffusion method for simulations of long-time defect evolution with application to dislocation climb

○Kristopher Baker[1], William Curtin[2] (1.Knolls Atomic Power Laboratory, United States of America, 2.Swiss Federal Institute of Technology, Switzerland）

[SY-N4] Accelerated Quantum Molecular Dynamics

○Enrique Martinez Saez[1], Christian Negre[2], Romain Perriot[2], Danny Perez[2], Eduard Kober[2], Marc Cawkwell[2], Arthur F. Voter[2], Anders Niklasson[2] (1.Material Science and Technology Division, MST-8,Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America, 2.Theoretical Division, T-1, Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America）

[SY-N4] On the effect of hydrogen on vacancy diffusion

○Sebastian Echeverri Restrepo[1], Anthony T Paxton[2] (1.Department of Metallic Materials &Ceramics, SKF, Netherlands, 2.Department of Physics, King's College London, UK）

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room4)

[SY-N4] Multiscale diffusion method for simulations of long-time defect evolution with application to dislocation climb

Invited

○Kristopher Baker[1], William Curtin[2] （1.Knolls Atomic Power Laboratory, United States of America, 2.Swiss Federal Institute of Technology, Switzerland）

In many problems of interest to materials scientists and engineers, the evolution of crystalline extended defects (dislocations, cracks, grain boundaries, interfaces, voids, precipitates) is controlled by the flow of point defects (interstitials/substitutional atoms and/or vacancies) through the crystal into the extended defect. Accurate modeling of this process requires atomistic methods in and around the extended defect, but the flow of point defects into and out of the extended defect region can be treated by coarse-grained methods. This talk presents a multiscale algorithm to provide this coupling, which was first documented in the manuscript "Multiscale diffusion method for simulations of long-time defect evolution with application to dislocation climb," published in 2016 in the *Journal of the Mechanics and Physics of Solids*, Number 92, pages 297-312. Specifically, direct accelerated molecluar dynamics (AMD) of extended defect evolution is coupled to a diffusing point defect concentration field that captures the long spatial and temporal scales of point defect motion in the presence of the internal stress fields generated by the evolving extended defect. The algorithm is applied to study vacancy absorption into an edge dislocation in aluminum where vacancy accumulation in the core leads to nucleation of a double-jog that then operates as a sink for additional vacancies; this corresponds to the intial stages of dislocation climb modeled with explicit atomistic resolution. The method is general, so it can be applied to many other problems associated with nucleation, growth, and reactions due to accumulation of point defects in crystalline materials.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room4)

[SY-N4] Accelerated Quantum Molecular Dynamics

○Enrique Martinez Saez[1], Christian Negre[2], Romain Perriot[2], Danny Perez[2], Eduard Kober[2], Marc Cawkwell[2], Arthur F. Voter[2], Anders Niklasson[2] （1.Material Science and Technology Division, MST-8,Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America, 2.Theoretical Division, T-1, Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America）

The accurate study of the long-term evolution of rare events is extraordinarily challenging as computations are arduous and quantum-based molecular dynamics simulation times are limited to, at most, hundreds of ps. Here, the Extended Lagrangian Born-Oppenheimer molecular dynamics formalism is used in conjunction with Parallel Replica Dynamics to obtain an accurate tool to describe the long-term dynamics of reactive benzene. Langevin dynamics has been employed at different temperatures to calculate the first reaction times in a periodic benzene sample at different pressures. We have also studied the long-term behavior of vacancy complexes, which compare satisfactorily with experimental observations. Our coupled engine runs for times on the order of ns (two to three orders of magnitude longer than traditional techniques) and is capable of detecting reactions characterized by rates significantly lower than we could study before.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room4)

[SY-N4] On the effect of hydrogen on vacancy diffusion

○Sebastian Echeverri Restrepo[1], Anthony T Paxton[2] (1.Department of Metallic Materials &Ceramics, SKF, Netherlands, 2.Department of Physics, King's College London, UK)

Although it is widely recognised that even small amounts of hydrogen (H) can cause embrittlement in iron (Fe) and in (high strength) steels, the fundamental mechanisms that cause it are not yet completely understood. To contribute to a better understanding of the fundamental behaviour of hydrogen in metals, in the present work we used parallel replica dynamics (PRD) to study the effect that different amounts of atomic H have in the diffusion of a single vacancy in body centred cubic (BCC) Fe. Using PRD we calculated, for the first time, the diffusion of hydrogen vacancy complexes at temperatures and time scales that are not reachable using classical methods. These calculations showed that the diffusivity of a vacancy-H complex is not only dependent of the migration barriers, but also that the addition of one H atom reduces the diffusivity of a vacancy in BCC Fe and the subsequent addition of more H atoms has the opposite effect.

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O5] Symposium O-5

Chairs: Hitoshi Washizu(University of Hyogo, Japan), Sophie Loehle(TOTAL Marketing &Services, Solaize, France)

Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room5

[SY-O5] **On the formation of superlubricious layers during boundary lubrication of diamond and diamond-like carbon**

○Michael Moseler[1,2] （1.Fraunhofer Institute for Mechanics of Materials IWM, Germany, 2.University of Freiburg, Germany）

[SY-O5] **Unveiling the chemical reactions involved in moisture-induced weakening of adhesion between aluminum and epoxy resin: a hybrid quantum-classical simulation study**

○Shuji Ogata, Masayuki Uranagase （Dept. of Physical Science and Engineering, Nagoya Institute of Technology, Japan）

[SY-O5] **Efficient evaluation of adhesion free energy between a liquid and polymer-grafted substrate**

○Masayuki Uranagase, Shuji Ogata （Nagoya Institute of Technology, Japan）

[SY-O5] **Ultimate response of confined fluids under extreme conditions: a Molecular Dynamics analysis**

○Alejandro Porras-Vazquez, Laetitia Martinie, Philippe Vergne, Nicolas Fillot （INSA Lyon, France）

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room5)

[SY-O5] On the formation of superlubricious layers during boundary lubrication of diamond and diamond-like carbon

Invited

○Michael Moseler[1,2] (1.Fraunhofer Institute for Mechanics of Materials IWM, Germany, 2.University of Freiburg, Germany)

Ultralubricity and superlubricity has been observed for diamond and tetrahedral amorphous carbon (ta-C) coatings lubricated with water and unsaturated organic friction modifiers, respectively. Although spectroscopic characterization suggests that lubricity is connected to the formation of oxygen-containing surface layers, the underlying tribo-chemical mechanisms and the detailed structures of these layers remain elusive. This talk presents atomistic calculations on various scales that elucidate the mechano-chemical processes for the formation of oxygen functional groups and aromatic protective layers [1,2].

In the first part of this talk, quantum molecular dynamcis calculations are presented that shed light on friction regimes for diamond lubricated by water and the different characteristic layers in the different regimes [1]. We find four universal friction regimes that are active on all low-index diamond surfaces: cold-welding&amorphisation, ether cold-welding without amorphisation, H/OH-termination, H/OH-termination with water layer coverage. In addition four special regimes are found: aromatic Pandey surface reconstruction for (111), ether/keto passivation for (110) and (001) as well as two mild cold-welding regimes for (110).

In the second part, combined experiments and multiscale simulations are presented that unveil the tribochemical mechanism leading to superlubricity of ta-C/ta-C tribopairs lubricated by unsaturated fatty acids [2]. Experiments show that superlow friction can be achieved by lubrication with unsaturated fatty acids. Atomistic simulations reveal that, due to the simultaneous presence of a carboxylic group and a C=C double bond, unsaturated fatty acids can concurrently chemisorb on both ta-C surfaces and bridge the tribogap. The resulting, sliding-induced mechanical strain triggers a cascade of molecular fragmentation reactions that release passivating hydroxyl, keto, hydrogen and olefinic groups to the ta-C surfaces. These findings provide design principles for novel organic friction modifiers that promote the formation of superlubricious amorphous carbon layers.

[1] T.Kuwahara, G.Moras, M.Moseler, **Phys. Rev. Lett.** 119 096101 (2017)

[2] T.Kuwahara, P.A.Romero, S.Makowski, V.Weihnacht, G.Moras, M.Moseler, under consideration (2018)

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room5)

[SY-O5] Unveiling the chemical reactions involved in moisture-induced weakening of adhesion between aluminum and epoxy resin: a hybrid quantum-classical simulation study

○Shuji Ogata, Masayuki Uranagase （Dept. of Physical Science and Engineering, Nagoya Institute of Technology, Japan）

Epoxy resin is commonly used as an adhesive for bonding metals. Recent industrial demands, e.g., light-weight multi-material cars and highly reliable pressure sensors, motivate researchers to improve the reliability and durability of bonded materials. One critical issue regarding adhesive bonding is the weakening of its bonding strength by the water that migrates from a moist environment along the interface. When bonding naturally surface-oxidized aluminum with epoxy resin, the adhesion strength reduces by about 40 % in a moist environment. Surface treatment techniques, such as sealing with polyvinyl chloride, only delay such adhesion weakening.

Despite the importance of this issue, adhesion weakening is not well understood. To understand the mechanisms at the electronic structure level, we perform atomic dynamics simulations on various Al and epoxy resin interface systems with water molecules inserted in the contact region. In accordance with experimental conditions, the Al layer is surface oxidized to a depth of 10 Åwhile the bisphenol-A type epoxy molecule has both OH and ether groups. Shear deformations are simulated using the hybrid quantum-classical method in which about 1,500 atoms at the contact region are treated with density-functional theory.

For the first time, calculated adhesion strengths compare well with the experimental values. Former simulations gave one order of magnitude larger adhesion strength than the experimental value. Three types of chemical reactions that affect the adhesion strength are found to occur depending on the terminal functional groups of the Al oxide surface and the water layer formation. Separate calculations confirm small barrier energies for all the reaction processes.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room5)

[SY-O5] Efficient evaluation of adhesion free energy between a liquid and polymer-grafted substrate

○Masayuki Uranagase, Shuji Ogata （Nagoya Institute of Technology, Japan）

Relating to recent rapid advancement in substrate-decoration technique such as the one using the Self-Assembled Monolayers, there exist strong demands to predict the adhesion free energy between a complex liquid and polymer-grafted substrate. In principle, the adhesion free energy can be evaluated through the molecular simulation by integrating the work required to separate the liquid from the substrate. In former methods for the work of adhesion, a planar shape potential is introduced and the work of adhesion is calculated through integrating the force exerted on the potential from liquid molecules when liquid molecules are separated from the solid surface by gradually shifting the potential origin. These methods work well for sufficiently flat solid substrate. However, they are inefficient for a polymer-grafted substrate because it becomes necessary to shift the potential over a long distance.
 Motivated by that, we propose a novel method to efficiently evaluate the work of adhesion of the interface between a liquid and a polymer-grafted surface. In the present method, a set of spherical potentials whose centers are set at the atomic positions of either polymer or substrate are introduced instead of a planar

potential. It enables efficient separation of the liquid molecules from the polymer-grafted substrate. Moreover, potential-parameter update schemes are carefully chosen to suppress sharp variation in the force exerted on the potential and thereby to minimize the number of integration points.

The present method is applied to the interface between a water and a gold substrate on which poly(ehtylene oxide)s (PEOs) are grafted. Then, we find that the work of adhesion tends to become large at the intermediate density of PEO. This tendency is related to the number of water molecules accessible to oxygen atoms in PEO.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room5)

[SY-O5] Ultimate response of confined fluids under extreme conditions: a Molecular Dynamics analysis

○Alejandro Porras-Vazquez, Laetitia Martinie, Philippe Vergne, Nicolas Fillot （INSA Lyon, France）

In order to control energy losses in mechanical systems, the study of friction in lubricated contacts has to be approached. Depending on the operating conditions and its chemical nature, the confined fluid can exhibit a limiting shear stress at high pressure [1, 2]. The physical origins of this phenomenon and its implications to friction are currently not completely understood [3]. In this study, an extensive Molecular Dynamics analysis of the shearing behavior of different types of molecules is performed. The behavior of the confined sheared system is explored and compared to the fluid bulk state. One of the main conclusion is that flow profile results from two competing forces in the molecular system, which is linked to the weakest interfaces being sheared. Additionally, the saturated shear stress response is found to be related to the concept of atomic mobility. With increasing pressure, the relaxation time of the material is increased. Thus, atomic mobility can be saturated for a range of high pressures, diffusion would not be allowed, and a solid-like behavior is displayed. Finally, a link between flow and friction behavior is discussed.

[1] Martinie, L. and Vergne, P., "Lubrication at extreme conditions: a discussion about the limiting shear stress concept", Tribol. Lett., 63, 2016.

[2] Ewen, J. P., Gattinoni, C., Zhang, J., Heyes, D. M., Spikes, H. A. and Dini D., "On the effect of confined fluid molecular structure on nonequilibrium phase behaviour and friction", Phys. Chem. Chem. Phys., 2017.

[3] Ndiaye, S. N., Martinie, L., Philippon, D., Devaux, N. and Vergne, P., "A Quantitative Friction-Based Approach of the Limiting Shear Stress Pressure and Temperature Dependence", Tribol. Lett., 65, 2017.

[SY-O6] Symposium O-6

Chairs: Yoshitaka Umeno(The University of Tokyo, Japan), Yoshinori Shiihara(Toyota Technological Institute,Japan)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room5

[SY-O6] Modeling the plastic deformation of a metal crystal induced by contact with a rough rigid surface
○Lucia Nicola[1,2] (1.Delft University of Technology, Netherlands, 2.University of Padova, Italy)

[SY-O6] On the potential use of liquid crystals as 'smart' lubricants - an MD simulation study
○Kerstin Falk[1], Konstantinos Gkagkas[2], Gianpietro Moras[1], Michael Moseler[1,3] (1.Dept. of Tribology, Fraunhofer IWM, Freiburg, Germany, 2.Toyota Motor Europe, Technical Center, Zaventem, Belgium, 3.Dept. of Physics, University of Freiburg, Germany)

[SY-O6] **Sliding on physisorbed cetyltrimethylammonium bromide (CTAB)**
○Johannes Laurin Hoermann, Lars Pastewka (University of Freiburg, Germany)

[SY-O6] Atomistic simulations of amines as organic friction modifiers
Rafael Pereira de Matos[1], Sophie Loehlé[2], Clotilde Minfray[1], ○Manuel Cobian[1] (1.LTDS ECL, Universite de Lyon, France, 2.TOTAL Marketing &Services, Solaize, France)

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room5)

[SY-O6] Modeling the plastic deformation of a metal crystal induced by contact with a rough rigid surface

Invited
○Lucia Nicola[1,2]　(1.Delft University of Technology, Netherlands, 2.University of Padova, Italy)

When rough bodies are pressed against each other, a small contact area has to support all the load. This is why plastic deformation occurs even at moderate nominal contact pressure. Although indentation of elastic bodies by self-affine rough indenters has been studied extensively, little attention has so far been devoted to plasticity. This is mostly because capturing plasticity as well as contact with a self-affine rough surface is computationally quite challanging. Here, we succeed in achieving this goal by using Green's function dislocation dynamics, a modeling technique that combines discrete dislocation plasticity (DDP) with Green's function molecular dynamics (GFMD). As usual in DDP, plasticity is studied by tracking the nucleation and glide of each dislocation in the metal crystal. The dislocation image fields are instead calculated with GFMD, which allows to describe the self-affine rough surface using wavelenghts spanning from 5 nanometers to 100 micrometers.

Simulations are performed varying various parameters of the surface roughness, including the Hurst exponent and the root-mean-square height. Results show that the plastic response is size-dependent. An important implication of the size-dependence is that, when bodies deform plastically, it is not possible to scale observables such as contact pressure and contact area with crystal size or root-mean-square height, as typically done for elastic contact problems.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room5)

[SY-O6] On the potential use of liquid crystals as 'smart' lubricants - an MD simulation study

○Kerstin Falk[1], Konstantinos Gkagkas[2], Gianpietro Moras[1], Michael Moseler[1,3]　(1.Dept. of Tribology, Fraunhofer IWM, Freiburg, Germany, 2.Toyota Motor Europe, Technical Center, Zaventem, Belgium, 3.Dept. of Physics, University of Freiburg, Germany)

Liquid crystals (LC) - well-known for their application in LC-displays - have recently raised interest also for lubrication applications: favorable friction properties (specific friction of the order 0.005) have been experimentally observed in different systems [1]. The special behavior is attributed to the anisotropic viscosity and compressibility, which LC exhibit in semi-ordered phases (i.e. nematic or smectic phase). The LC molecules' elongated shape allows them to align with the shear, which could simultaneously reduce friction and increase load support. Moreover, the complex phase behavior and dynamic properties might also be exploited to design novel tribological systems with tunable or self-regulating friction, so-called 'smart' lubricants [2,3].

Here, we present a molecular dynamics simulations study of different LC lubricated model tribo-systems with the aim to characterize the LC rheological properties and investigate possible tuning mechanisms on a microscopic level. Shearing simulations of LC lubricating films with different structure characteristics, i.e. preferential molecule orientation, were performed for varying loads and shear rates. The response of the systems (velocity profiles, local viscosity and shear force) was evaluated and correlated to the fluid film

structure, which is influenced by the flow. Of particular interest are situations, where the inherent equilibrium structure of the LC film (induced by surface boundary conditions or external fields) is different from the shear direction, due to the competing forces for aligning the LC molecules in different directions.

[1] T. Amann, C. Dold and A. Kailer, Tribology International 65 (2013), p. 3
[2] C. Tadokoro, T. Nihira and K. Nakano, Tribol Lett 56 (2014), p. 239
[3] S. Itoh, Y. Imura, K. Fukuzawa andH. Zhang, Langmuir 31 (2015), p. 11360

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room5)

[SY-O6] Sliding on physisorbed cetyltrimethylammonium bromide (CTAB)

○Johannes Laurin Hoermann, Lars Pastewka （University of Freiburg, Germany）

In solution, amphiphilic surfactants can form physisorbed boundary films on immersed surfaces. A film's structure and thereby its lubrication performance depend on numerous properties of all involved substances, such as the surface's potential, as well as surfactant and background electrolyte concentration. We investigate the dependency of the coefficient of friction on adsorption film topography in exemplary contact systems by means of classical all-atom molecular dynamics. For this purpose, the present study focuses on cationic CTAB at idealized aqueous solution-gold interfaces. Recent parametrizations of CTAB, originally intended for micelle modeling in bulk solution, are combined with representations of simple gold surfaces. The stability of differently shaped pre-assembled surface aggregates at various effective surfactant concentrations are compared against expected behavior as documented by abundant experimental contributions. We finally present friction tests in simple shear geometries of surfaces covered with pairwise identical CTAB film morphologies.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room5)

[SY-O6] Atomistic simulations of amines as organic friction modifiers

Rafael Pereira de Matos[1], Sophie Loehlé[2], Clotilde Minfray[1], ○Manuel Cobian[1] （1.LTDS ECL, Universite de Lyon, France, 2.TOTAL Marketing &Services, Solaize, France）

Amines molecules can be used as organic friction modifiers OFM in a
lubricated contact working under in mixed/boundary regime.
Several experimental studies have been already done using steel against
steel contact. Our aim is to propose
a computational simulation protocol to have a better understanding of
what happens at atomic scale in the contact.
We study some physical properties (density, diffusivity) of amines
blended in Poly Alpha Olephin PAO using
molecular dynamics MD simulations employing the OPLS force field.
Green-Kubo formalism gives us access to diffusion coeficients of amines
in the oil.
Then, we present ab-initio (DFT+U based) study of the adsorption of

this OFM on alpha-hematite Fe2O3 surface {01-12}.
The interactions between the amine molecule and the surface will be
analysed and used to fit Lennard-Jones potential
to model the interaction and open the way to new simulations using
molecular dynamics.
We will conclude presenting simulations of the friction process
applying stress and shear and computing a
numerical coefficient of friction.

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O7] Symposium O-7

Chairs: Lucia Nicola(Delft University of Technology, Netherlands), Shuji Ogata(Nagoya Institute of Technology, Japan)

Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5

[SY-O7] Toward Exascale Atomistic Simulations of Interfaces

○Aiichiro Nakano （Univ. of Southern California, United States of America）

[SY-O7] Molecular Dynamics Simulation Study on the Structure, Role, and Formation Mechanism of Tribofilms of Silicon-Based Materials in Water

○Yusuke Ootani[1], Jingxiang Xu[1], Naoki Takahashi[1], Koshi Adachi[2], Momoji Kubo[1] （1.Institute for Materials Research, Tohoku University, Japan, 2.Department of Mechanical Systems Engineering, Graduate School of Engineering, Tohoku University, Japan）

[SY-O7] Influence of Tribo-Film Structure Generated from MoDTC at DLC/DLC Interface on Friction Behavior : A Molecular Dynamics Simulation

○Masahiro Saito[1], Jingxiang Xu[1], Yusuke Ootani[1], Nobuki Ozawa[1], Koshi Adachi[2], Momoji Kubo[1] （1.Institute for Materials Research, Tohoku Univ., Japan, 2.Graduate School of Engineering, Tohoku Univ., Japan）

[SY-O7] **Shear-induced amorphization of silicon and diamond yields liquid-like amorphous solids**

○Gianpietro Moras[1], Andreas Klemenz[1], Thomas Reichenbach[1], Adrien Gola[2], Hiroshi Uetsuka[3], Michael Moseler[1,4], Lars Pastewka[1,5] （1.Fraunhofer Institute for Mechanics of Materials IWM, Germany, 2.Institute for Applied Materials, Karlsruhe Institute of Technology, Germany, 3.Asahi Diamond Industrial Co. Ltd., Japan, 4.Institute of Physics, University of Freiburg, Japan, 5.Department of Microsystems Engineering, University of Freiburg, Germany）

[SY-O7] A new damage implementation for Smooth Particle Hydrodynamics and its application to simulating the wear response of metals.

○Alban de Vaucorbeil, Christopher Hutchinson （Monash University, Australia）

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5)

[SY-O7] Toward Exascale Atomistic Simulations of Interfaces

Invited

○Aiichiro Nakano （Univ. of Southern California, United States of America）

Under the U.S. Department of Energy, Aurora/A21 early science program, our group will be one of the 10 initial users of the Nation's first exaflop/s computer that can perform 10^{18} mathematical operations per second, when it is introduced in 2021. To make quantum molecular dynamics (QMD) and reactive molecular dynamics (RMD) simulations exa-scalable, we have developed an extension of the divide-and-conquer algorithmic framework called divide-conquer-recombine. On today's supercomputing platform, for instance, the framework has achieved over 98% of the perfect speedup on 786,432 IBM Blue Gene/Q processors for 40 trillion electronic degrees-of-freedom QMD in the framework of density functional theory and 68 billion-atom RMD. Production simulations include (1) 16,616-atom QMD simulation of rapid hydrogen production from water using metallic alloy nanoparticles, (2) 6,400-atom nonadiabatic QMD simulation of photoexcitation dynamics for efficient solar cells, and (3) 112 million-atom RMD simulation of metacarbon synthesis by high temperature oxidation of SiC nanoparticles. We will discuss tribology and interfacial applications such as frictional heating of energetic molecular crystals.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5)

[SY-O7] Molecular Dynamics Simulation Study on the Structure, Role, and Formation Mechanism of Tribofilms of Silicon-Based Materials in Water

○Yusuke Ootani[1], Jingxiang Xu[1], Naoki Takahashi[1], Koshi Adachi[2], Momoji Kubo[1] （1.Institute for Materials Research, Tohoku University, Japan, 2.Department of Mechanical Systems Engineering, Graduate School of Engineering, Tohoku University, Japan）

It is known that silicon-based materials such as silicon carbide have low friction coefficients in water lubrication system. A tribofilm formed at a sliding interface is considered to reduce the friction coefficient, however detailed mechanism is still unclear because in-situ observation of the atomic scale sliding interface is difficult. Therefore, in this work, we investigated the structure, role and formation mechanism of the tribofilm of silicon-based materials by using molecular dynamics method. We performed sliding simulations of a SiO_2 substrate, which is a model of a native oxide layer of silicon-based materials, in water environment. We found that hydrolysis reaction of Si-O bond in SiO_2 surfaces occurred at contact areas of the surfaces as, Si-O + H_2O →Si-OH + OH. The hydrolysis reaction was mediated by proton transfer process. Since the hydrolysis reaction dissociated Si-O bonds, Si-O bond network of the SiO_2 surfaces became sparse, and then, several SiO_2 clusters were removed from the surfaces as wear debris. The wear debris were dissolved in the water layer between two surfaces, forming a colloidal silica layer. On the other hand, the water molecules penetrated into the sparse SiO_2 surfaces and hydrate the surfaces, forming a hydrophilic silica gel layers on the SiO_2 surfaces. Therefore, at the sliding interface, the colloidal silica layer was sandwiched by two silica gel layers. The colloidal silica layer prevents the contact of the surfaces and reduces a friction force, whereas the hydrophilic silica gel layer holds the colloidal silica layer at the sliding interface. Thus, the colloidal silica and silica gel layer that formed by hydrolysis reaction reduces the friction coefficient of silicon-based materials in water lubrication systems.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5)

[SY-O7] Influence of Tribo-Film Structure Generated from MoDTC at DLC/DLC Interface on Friction Behavior : A Molecular Dynamics Simulation

○Masahiro Saito[1], Jingxiang Xu[1], Yusuke Ootani[1], Nobuki Ozawa[1], Koshi Adachi[2], Momoji Kubo[1] （1.Institute for Materials Research, Tohoku Univ., Japan, 2.Graduate School of Engineering, Tohoku Univ., Japan）

Diamond-like carbon (DLC) has excellent friction properties such as low friction and high wear resistance. Thus, it is used as a solid lubricant material for engine parts. For this application, it is expected that DLC is used with the MoDTC friction modifier. When MoDTC is used as additives, a tribo-film of MoS_2 layers is formed at a sliding interface during friction, leading to low friction. It is known that frictional property of this system depends on many factors such as composition of additives, a structure of DLC, and so on. Thus, to improve the friction property, it is required to understand effects of these factors on friction behavior of the tribo-film. However, the friction behavior is unknown because *in situ* observation of the sliding interface is difficult. Thus, in order to investigate the friction behavior, we performed molecular dynamics simulation by using reactive force field, which takes into account the chemical reactions. In this study, we analyzed the influence of the defects in the MoS_2 layers on friction behavior of DLC by using a DLC/MoS_2 layers/DLC model. Here, we investigated the influence of the defects by comparing the friction behavior of the MoS_2 layers with and without grain boundaries. The friction simulation of the model without grain boundaries shows that the DLC/MoS_2 interface is the sliding interface. On the other hand, the simulation of the model with grain boundaries shows that the MoS_2/MoS_2 interface is the sliding interface since C-S bonds is formed between DLC and MoS_2 around grain boundaries. In addition, the MoS_2 layers with grain boundaries show higher friction force because the sliding between the MoS_2 layers is inhibited when a grain boundary attacks another grain boundary in neighboring layers. Then, we found that these friction behaviors caused by grain boundaries in the MoS_2 are major factors that increase friction force in this system. We will report the influence of other defects at the conference.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5)

[SY-O7] Shear-induced amorphization of silicon and diamond yields liquid-like amorphous solids

○Gianpietro Moras[1], Andreas Klemenz[1], Thomas Reichenbach[1], Adrien Gola[2], Hiroshi Uetsuka[3], Michael Moseler[1,4], Lars Pastewka[1,5] （1.Fraunhofer Institute for Mechanics of Materials IWM, Germany, 2.Institute for Applied Materials, Karlsruhe Institute of Technology, Germany, 3.Asahi Diamond Industrial Co. Ltd., Japan, 4.Institute of Physics, University of Freiburg, Japan, 5.Department of Microsystems Engineering, University of Freiburg, Germany）

Silicon and diamond are brittle materials with the same crystal structure but opposite density change upon melting. Using molecular dynamics simulations, we show that both crystals can respond to shear deformation by undergoing mechanical amorphization. The resulting amorphous material has liquid-like structure, is denser than the crystal in silicon and less dense than the crystal in diamond. As a result, as normal pressure

increases, amorphization, which is often related to nanoscale wear, is enhanced in silicon but suppressed in diamond. Moreover, shear-induced amorphization of silicon yields a high-density, ductile amorphous material at pressures much lower than the polyamorphic transition (~14 GPa) observed upon hydrostatic compression. These results are potentially relevant for the friction properties of other crystals that densify upon melting and show polyamorphism, like germanium and ice.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5)

[SY-O7] A new damage implementation for Smooth Particle Hydrodynamics and its application to simulating the wear response of metals.

○Alban de Vaucorbeil, Christopher Hutchinson （Monash University, Australia）

Simulations of materials and structures submitted to wear, machining, forming, forging, and impacts, to name but a few, often involve large deformations, damage, and failure. These phenomena are challenges for usual computational tools such as finite element modeling. When large deformations occur, finite element methods have limitations due to the need to remesh which is computationally expensive and sometimes fails. Therefore, mesh-free methods such as Smooth Particle Hydrodynamics (SPH) are more suitable for these applications.

The use of SPH for the simulations of wear, tribology, and impacts problems in solids has recently gained momentum as large deformations and instability phenomena such as damage and fracture could be easily handled. However, little work exists on the implementation of damage in SPH. This is thought to be due to the approximation problems around surfaces. As damage and fracture develops in solids, this creates new surfaces around which the SPH approximation breaks down.

In this presentation, we present the results of simulations of wear response to show case a new implementation of damage in SPH that solves some of the problems due to the approximation break-downs close to surfaces. This implementation is built as an upgrade of the SPH package for solids available within LAMMPS called Smooth Mach Dynamics.

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O8] Symposium O-8

Chairs: Tianbao Ma(Tsinghua University, China), Yang Wang(Institute for Materials Research, Tohoku University, Japan)
Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room5

[SY-O8] Friction mechanism of nanostructured steel in lubricant: A coarse-grained molecular dynamics study

○Yoshitaka Umeno Umeno, Atsushi Kubo, Yuta Sudo （The University of Tokyo, Japan）

[SY-O8] Coarse-Grained Molecular Dynamic Simulation on the Wear Mechanism of Polymer Brush with Different Chain Topologies

○Zhongmin Liu, Shuichi Uehara, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Material Research,Tohoku Univ., Japan）

[SY-O8] Molecular Dynamics Simulation Study on Friction of Bottlebrush Polymer with a Cationic Anchor Block Adsorbed on Substrate

○Shuichi Uehara, Zhongmin Liu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Materials Research, Tohoku Univ., Japan）

[SY-O8] Temperature dependent dynamics simulation of traction fluid by molecular dynamics method

○Eiji Tomiyama[1,2], Takeshi Iwasaki[3], Hitoshi Washizu[2] （1.Research Organization for Information Science and Technology, Japan, 2.Graduate School of Simulation Studies, Univ. of Hyogo, Japan, 3.Lubricants Research Laboratory, Idemitsu Kosan Co., Ltd., Japan）

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room5)

[SY-O8] Friction mechanism of nanostructured steel in lubricant: A coarse-grained molecular dynamics study

○Yoshitaka Umeno Umeno, Atsushi Kubo, Yuta Sudo （The University of Tokyo, Japan）

Intensive studies have been dedicated to the problem of boundary lubrication in recent years. Experimental studies have demonstrated a significant reduction in friction coefficients of steel that has nanostructured surfaces. It is conjectured that nanostructured metals have a large density of sites with strong attraction to lubricant molecules, resulting in reduced friction. The detailed mechanism of the phenomenon however remains unclear.

To reveal the mechanism of lubrication between metal surfaces, atomic- or molecular-level investigations are required for the effect of metal-molecule interaction on boundary lubrication. Coarse-grained molecular dynamics (CGMD) is a useful and efficient simulation method to tackle such problems. Indeed, a CGMD study of shear flow of lubricant molecules between metal surfaces showed that the more molecules were adsorbed on the surfaces, the lower the friction coefficient became. Nevertheless, molecular-level mechanisms are not fully understood regarding the experimentally presented effect of the surface nanostructure on the friction coefficient or the nature of structural ordering in shear flow.

In this study, we performed CGMD simulations with the aim to reveal the molecular-level friction mechanism in boundary lubrication between nanostructured steel surfaces. As lubricant molecules, polyethylene (nonpolar) and fatty acid (polar) were modeled by the coarse-grained method representing methylene (CH_2) and carboxyl (COOH) groups by individual particles. The effect of the surface nanostructure was mimicked by distributing atoms producing stronger attraction with the molecular groups. The effect of alignment of the strong potentials on the friction coefficient is apparent in the case of polar molecules. In both polar and nonpolar lubricants, the nanostructure enhances critical shear stress for separation of adsorbed lubricants from the surface. These results suggest salient influence of the surface nanostructure on the friction coefficient.

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room5)

[SY-O8] Coarse-Grained Molecular Dynamic Simulation on the Wear Mechanism of Polymer Brush with Different Chain Topologies

○Zhongmin Liu, Shuichi Uehara, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Material Research,Tohoku Univ., Japan）

As a low friction material, polymer brush has attracted attention in many areas because of its good frictional properties and biological compatibility. The frictional properties of polymer brush are improved by different chain topologies. However, the effects of the chain topologies on the wear of polymer brush are still not clear. To reduce the wear of the polymer brush, it is required to understand the wear behaviors and mechanism of different topological polymer brush. However, in-situ observation of the sliding interface at the molecular scale is difficult. Thus, we investigated the wear mechanism of polymer brush with different topological chain by using coarse-grained molecular dynamics (CGMD) method.

 We perform friction simulations of linear polymer brush, cyclic polymer brush where the polymer chains have

cyclic structure, and crosslinked polymer brush where the polymer chains are connected with the neighboring polymer chain with crosslinker to understand the effect of chain topologies on the wear. We found that cyclic polymer brush and crosslinked polymer brush had smaller number of dissociation than linear polymer brush because the cyclic polymer brush and crosslinked polymer brush showed smaller frictional forces than that of linear polymer brush. We found that the cyclic polymer brush and crosslinked polymer brush had less interpenetrating beads than that of linear polymer brush. Therefore, the cyclic polymer brush and crosslinked polymer brush have smaller entanglements, leading to the low frictional force. We conclude that chain topologies of polymer brush can improve the wear resistance because they suppress the interpenetration at the sliding interface.

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room5)

[SY-O8] Molecular Dynamics Simulation Study on Friction of Bottlebrush Polymer with a Cationic Anchor Block Adsorbed on Substrate

○Shuichi Uehara, Zhongmin Liu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Materials Research, Tohoku Univ., Japan）

In recent years, concentrated polymer brush (CPB), which is constructed by grafting polymer chains onto a substrate with high density, has been developed. CPB has attracted much attention for application to low friction materials as artificial joints because of its high wear resistance and biocompatibility. However, the graft of polymer chains onto substrate is complicated and takes much cost. As an alternative method analogous to CPB, bottlebrush polymer (BBP) known as macromolecules with polymeric side chains is candidate for low friction materials. Previous studies have revealed that BBPs with a cationic anchor block adsorbed on a negatively charged surface swell, which produces low friction force. However, the detail of friction mechanism of BBP is not clear. Furthermore, the effects of sliding speed and side chain length on friction properties are also unknown because the in-situ observation of the sliding interface is difficult. Thus, computational simulation is required. Herein, to reveal the mechanism during friction of BBP consisting of a cationic anchor block, we developed a coarse-grained molecular dynamics code which can consider chemical specificity of each monomer, and performed friction simulation in water solvent. The low friction coefficient was observed at the low load, but friction coefficient was increased at high load. We found that, at low load, water beads which coordinate to the side chain of BBP suppressed contact between BBPs on the counter surfaces, because side chains of BBP prefer to interact with the water beads. This swelling state of BBP facilitates shear between the opposite substrates. With high load, water beads were removed from the sliding interface, which reduces the number of water beads around BBP. Therefore, the contact between BBPs on a counter surface leads to high friction coefficient. The effects of side chain length and sliding speed on the friction properties will be discussed on the day.

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room5)

[SY-O8] Temperature dependent dynamics simulation of traction fluid by molecular dynamics method

○Eiji Tomiyama[1,2], Takeshi Iwasaki[3], Hitoshi Washizu[2] （1.Research Organization for Information Science and Technology, Japan, 2.Graduate School of Simulation Studies, Univ. of Hyogo, Japan, 3.Lubricants Research Laboratory, Idemitsu Kosan Co., Ltd., Japan）

Traction drive is a mechanism that transmits power by a rotor and lubricating oil. In order to evaluate the characteristics of the fluid molecules in the traction drive, we construct a simulation method to apply shear to the fluid confined between solids using LAMMPS, a molecular dynamics simulator.

In this simulation, conditions are set as follows. The boundary condition of the system is a periodic boundary condition in the horizontal direction. Fluid is composed of a single hydrocarbon compound and the number of atoms is about ten thousand. The solids are a model metal surface imitating (100) plane of α-iron, and thier atomic motion is frozen. The force field parameter of fluid molecules uses the Dreiding force field. Apply a pressure of 0.8 GPa to 1.24 GPa in the direction perpendicular to the solid atoms. Furthermore, a constant slip of relative sliding speed 1 m/s to 50 m/s is applied. Then, the simulation time on the order of nanoseconds is passed and the steady state is set. With the above setting, an ensemble of constant pressure / constant shear state is created.

The temperature dependency of the coefficient of traction is evaluated by changing the temperature of the fluid from -20 ˚C to 140 ˚C. The coefficient of traction also change with the change of temperature, and the tendency is at least qualitatively consistent with the experimental values.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A5] Symposium A-5

Chair: Sinisa Dj Mesarovic(Washington State University, United States of America)
Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room6

[SY-A5] Parameters to consider in the modelling of dislocation boundary evolution
　　　○Grethe Winther Winther （Technical University of Denmark, Denmark）

[SY-A5] Data Mining of Indentation Induced Dislocation Microstructures
　　　○Dominik Steinberger[1], Shyamal Roy[1], Dan Mordehai[2], Stefan Sandfeld[1] （1.Chair of Micromechanical Materials Modelling, TU Bergakademie Freiberg, Germany, 2.Department of Mechanical Engineering, Technion - Israel Institute of Technology, Israel）

[SY-A5] Lattice continua for polycrystal grains: Climb and glide of dislocations, diffusion and grain boundary kinematics.
　　　○sinisa Dj Mesarovic （Washington State University, United States of America）

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room6)

[SY-A5] Parameters to consider in the modelling of dislocation boundary evolution

Invited

○Grethe Winther Winther （Technical University of Denmark, Denmark）

An essential part of the development of theory and simulations of microstructure evolution is the parameters used as input as well as the output, which should be comparable to experimental observations. An overview of the experimentally observed dislocation boundary evolution in metals of medium to high stacking fault energy are presented with emphasis on such parameters. In particular, the spatial distribution of boundaries in terms of boundary planes, spacings and misorientation angles are considered as a function of crystallographic grain orientation, deformation mode and strain. Based on the experimental observations relations to crystal plasticity and the Burgers vectors available for boundary formation are discussed.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room6)

[SY-A5] Data Mining of Indentation Induced Dislocation Microstructures

○Dominik Steinberger[1], Shyamal Roy[1], Dan Mordehai[2], Stefan Sandfeld[1] （1.Chair of Micromechanical Materials Modelling, TU Bergakademie Freiberg, Germany, 2.Department of Mechanical Engineering, Technion - Israel Institute of Technology, Israel）

In general, data mining is the process of discovering patterns in large data sets, with the most common tasks being, anomaly detection, association rule learning, clustering, classification, regression and summarization. Within materials science, the most popular application so far is materials discovery, one of the goals of the well-known Materials Genome Initiative (https://www.mgi.gov).

In order to understand the convoluted interactions of dislocations that define the mechanical properties of metals to a large degree, a lot of data has been and is being generated, be it via experiments or simulations. Due to the complexity of the dislocation microstructure and its discrete nature aforementioned algorithms can not be applied ad-hoc. Thus, developing methods that enable their use are highly desirable.

In this presentation we want to outline the key aspects of the data mining framework for dislocation microstructures that we are currently developing. Among others, we will show examples of how quantitative comparisons of dislocation data—be it from experimental or computational methods—can be done. Aforementioned framework will be applied to a dataset consisting of hundreds of realizations of a numerical indentation experiment realized with discrete dislocation dynamics. Rate coefficient beneath the indenter will be extracted for the dislocation densities commonly found in continuous dislocation dynamics models. The resulting microstructures will be analyzed for common patterns and their correlation with the intially emerging structure to enable predicting the characteristics of the final state from the first initial steps.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room6)

[SY-A5] Lattice continua for polycrystal grains: Climb and glide of

dislocations, diffusion and grain boundary kinematics.

○sinisa Dj Mesarovic （Washington State University, United States of America）

At high temperatures, the interior of each grain in a polycrystal suffers: (1) dislocation glide, (2) climb, and (3) diffusion of vacancies. Grain boundaries undergo: (4) growth/disappearance, as a result of vacancy diffusion, and, (5) crystallographic reorientation/mismatch, as a result of dislocations arriving to the boundaries either by glide or by climb. All the above deformation mechanisms are naturally described in the lattice continuum framework, whereby the lattice represents the material. Climbing edge dislocations are lattice sink/source which must be reflected in the continuity equation and the transport theorem. The interacting kinematics of dislocation glide and climb requires dual definition of crystallographic slip fields: the true slip and the apparent slip. The transport theorem for grains with lattice growing or disappearing lattice at different grain boundary faces results in the direct formulation of the boundary condition for vacancy diffusion flux in terms of the boundary velocity (different from the lattice velocity). The field equations for each grain are derived by means of the principle of virtual power. Additional boundary conditions result from the relative motion of the adjacent crystal faces: Change of tilt and twist angle and surface elastic mismatch are derived from the geometry of dislocations arriving to the boundary. The resulting polycrystal initial/boundary value problem consists of elasticity-plasticity-diffusion field equations in each crystalline domain with moving boundaries, coupled through the boundary conditions.

Mesarovic, S.Dj. 2018 Physical foundations of mesoscale continua. In Meso-scale models: From micro-physics to macro-interpretation. Springer lecture notes. To appear.

Mesarovic, S.Dj. 2017 Dislocation creep: Climb and glide in the lattice continuum. *Crystals* **7**(8), 243.

Mesarovic, S.Dj. 2016 Lattice continuum and diffusional creep. *Proc. R. Soc. A* **472**, 20160039.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A6] Symposium A-6
Chair: Emma Griffiths(University of Cape Town, South Africa)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room6

[SY-A6] Design of patchy nanoparticles via the self-assembly of triblock terpolymers in selective solvents
○Eliot Fried, Nicolás Moreno （Okinawa Institute of Science and Technology, Japan）

[SY-A6] Nanoporous Composites: Giving Polymers Strength and Helping Metals Move
○Emma Griffiths[1], Jana Wilmers[2], Swantje Bargmann[2], BD Reddy[1] （1.University of Cape Town, South Africa, 2.University of Wuppertal, Germany）

[SY-A6] Multiscale modeling of advanced materials for hybrid organic-inorganic solar cells
○Alexander E. Kobryn （Nanotechnology Research Center, National Research Council Canada, Canada）

[SY-A6] From cellulose and lignin to kerogen: molecular simulations of a geological process
○Roland PELLENQ[1], Pierre-Louis Valdenaire[1], Christophe Bichara[3], Franz Ulm[1], Jean-Marc Leyssale[2] （1.<MSE>2, MIT- CNRS - AMU, United States of America, 2.ISM, CNRS - Bordeaux U., France, 3.CINaM, CNRS - Aix-Marseille U., France）

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room6)

[SY-A6] Design of patchy nanoparticles via the self-assembly of triblock terpolymers in selective solvents

Invited

○Eliot Fried, Nicolás Moreno （Okinawa Institute of Science and Technology, Japan）

The hierarchical self-assembly of triblock terpolymers in solution is a successful bottom-up methodology for constructing functional patchy nanoparticles with prescribed topology and shape. Currently, the design of such nanoparticles requires an iterative process to identify the experimental phase parameters needed to produce any target pattern. The broad use of this technology is therefore cumbersome and limited by an incomplete understanding of the mechanisms underlying patch transition. A detailed understanding of how thermodynamics and kinetics influence the topology of the assemblies is also missing. In this work, we present a set of rules for programming desired shapes of the nanoparticles and predicting the pathways by which they assemble. We investigate systematically the interplay between entropic and enthalpic parameters governing the self-assembly of ABC triblock copolymers in a selective solvent for the C block. We use a computational modeling at the mesoscale and thereby encompass the length and time scales associated with the motion and assembly of the polymer coils, while accurately approximating the chemically driven interactions. The phase diagram predicted by our model is consistent with experimentally identified characteristic nanoparticle shapes. We find that the effective volume fraction of the soluble block determines the size of a particle and the distribution of its patches via steric interactions. Moreover, we find that the relative fraction of the patch-forming block and its affinity with the core of a articles dictates the number and shape of its patches. As a major outcome, we construct a morphologically-based library of nanoparticles. That library can be used to hierarchically design mesoscale aggregates with specific morphologies. Our results provide insight regarding the mechanisms that determine nanometer scale objects in synthetic and naturally occurring systems.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room6)

[SY-A6] Nanoporous Composites: Giving Polymers Strength and Helping Metals Move

○Emma Griffiths[1], Jana Wilmers[2], Swantje Bargmann[2], BD Reddy[1] （1.University of Cape Town, South Africa, 2.University of Wuppertal, Germany）

An important benefit of electroactive polymers is their large strain response due to certain stimuli such as an electric current. However, for sufficient mechanical use in electrochemical systems, they lack the necessary strength and stiffness. Metals on the other hand have sufficient strength and stiffness but are unable to function as piezoelectric materials [1]. By creating a metal-polymer composite, however, a stronger material with large strain capacity is created that can withstand larger actuation forces. Specifically, using polymer impregnated nanoporous structures, with their exceptional mechanical properties providing a reinforcing base [2,3], creates a composite material with superior actuator properties by having both sufficient strength and strain capabilities.

This work presents the chemoelectromechanical response of a gold-polymer nanocomposite model. A representative volume element is modelled using a linear version of the chemoelectromechanical theory developed by Wilmers et al. [4] and is implemented through a staggered explicit-implicit finite element

simulation in ABAQUS. Additionally the theory is enhanced by introducing an implicit solvent model to capture the effects of the crowding of ions due to saturation within the material. The micromechanical response of the composite is explored under an imposed electric field and thus providing information to be used in the optimization of microstructures for sensory and actuation applications.

References
[1] Stenner, Shao, Mameka, Weissmüller, J. Piezoelectric Gold: Strong Charge-Load Response in a Metal-Based Hybrid Nanomaterial, Adv. Funct. Mater. 26, 2016
[2] Griffiths, Bargmann, Reddy, Elastic behaviour at the nanoscale of innovative composites of nanoporous gold and polymer, Extreme Mech. Lett. 17, 2017
[3] Soyarslan, Bargmann, Pradas, Weissmüller, J. 3D stochastic bicontinuous microstructures: Generation, topology and elasticity Acta Mater. 149, 2018
[4] Wilmers, McBride, Bargmann, Interface elasticity effects in polymer-filled nanoporous metals, J. Mech. Phys. Solids 99, 2017

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room6)

[SY-A6] Multiscale modeling of advanced materials for hybrid organic-inorganic solar cells

○Alexander E. Kobryn （Nanotechnology Research Center, National Research Council Canada, Canada）

When it comes to talk about alternatives to non-renewable sources of energy, photovoltaics is one of the most promising choices for converting solar light into electricity with the use of solar cells. At present, there is wide variety of solar cell devices on the market and this variety will continue to grow because of the race for better conversion efficiency and the final product sustainability. Within recent years, the seemingly clear boundaries between photovoltaics of inorganic and organic solar cells have started to fade by the advent of metal-halide hybrid organic-inorganic perovskites (OIP). They are very promising candidates for future photovoltaic applications because they have wide-direct band gap, which can be tuned by either changing the organic cation, the metal atom, or the halide. Their power conversion efficiency now reached over 22%. At the same time, the level of our understanding of the origin of such performance is still insufficient. We believe that thin film morphology is a key factor determining the performance of bulk heterojunction organic solar cells, because of its influence on charge separation, charge transport and recombination losses in donor-acceptor blends. With this respect, we present both descriptive and predictive multiscale modeling of electronic and structural properties of blends of PCBM or hybrid OIP of the type $CH_3NH_3PbX_3$ (X=Cl, Br, I) with P3HT, P3BT or squaraine SQ2 dye sensitizer, including adsorption on TiO_2 clusters. Here, the multiscale nature of modeling means that in a set of simple hierarchical approaches we combine different methods for different scales (quantum mechanical, microscopic, mesoscopic) interpreted independently and that the information obtained at one level is transmitted to the next level as a required input. If necessary, new information is sometime transmitted back to the previous level for a feedback control. As the result, we arrive at a very reliable methodology that allows computing the microscopic structure of blends on the nanometer scale and getting insight on miscibility of its components at various thermodynamic conditions. The calculated nanoscale morphologies serve as an instrument in rational design of hybrid OIP. They are used in collaboration with experts who actually make prototypes or devices for practical applications.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room6)

[SY-A6] From cellulose and lignin to kerogen: molecular simulations of a geological process

○Roland PELLENQ[1], Pierre-Louis Valdenaire[1], Christophe Bichara[3], Franz Ulm[1], Jean-Marc Leyssale[2]
 （1.<MSE>2, MIT- CNRS - AMU, United States of America, 2.ISM, CNRS - Bordeaux U., France, 3.CINaM, CNRS - Aix-Marseille U., France）

The process by which organic matter decomposes deep underground to form petroleum and its underlying kerogen matrix has so far remained a no man's land to theoreticians, largely because of the geological (Millions of years) timescale associated with the process. Using a replica exchange accelerated molecular dynamics method initially developed in the context of the micro- to milli-second timescale for protein folding, we simulate the full transformation of cellulose and lignin (the main components of wood) into kerogen under prevailing geological conditions. We observe in sequence (i) the fragmentation of the cellulose crystal and production of water, (ii) the development of an aliphatic macromolecular phase, (iii) its aromatization, and (iv) its aggregation into a stiff porous aromatic carbon upon expulsion of the fluid phase. The composition of the solid residue along the maturation pathway strictly follows what is observed for natural type III kerogens and for artificially matured samples under closed conditions, providing further evidence of a kinetically controlled, irreversible, decomposition process in which the aliphatic (immature) phase is a metastable intermediate.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A7] Symposium A-7

Chair: Michael Zaiser(FAU University of Erlangen-Nuremberg, Germany)

Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6

[SY-A7] Mathematical challenges for a mesoscale theory of dislocations

○Thomas Hochrainer （TU Graz, Austria）

[SY-A7] **Dislocation multiplication in the discrete-continuum transition regime**

○Katrin Schulz[1], Markus Sudmanns[1], Kolja Zoller[1], Peter Gumbsch[1,2] （1.Karlsruhe Institute of Technology, Germany, 2.Fraunhofer Institute for Mechanics of Materials, Germany）

[SY-A7] The fundamental instability of dislocation transport equations

○Michael Zaiser, Ronghai Wu （FAU University of Erlangen-Nuremberg, Germany）

[SY-A7] 2D continuum theory of dislocations

○Istvan Groma （Eotvos Lorand University, Hungary）

[SY-A7] Continuum dislocation dynamics for finite deformation mesoscale plasticity

○Anter El-Azab （Purdue University, United States of America）

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6)

[SY-A7] Mathematical challenges for a mesoscale theory of dislocations

Invited

○Thomas Hochrainer （TU Graz, Austria）

During the last two decades, dislocation research saw a revival driven by new experimental techniques for small scale testing, high resolution characterization and the rise of large scale discrete dislocation simulations. This also stimulated intensive research in mesoscale theories of dislocations. Great advances were achieved on continuum models of dislocation interactions for strongly simplified straight-dislocation systems and continuum dislocation dynamics of single slip deformation. However, a transfer of the employed averaging methods to fully three-dimensional multiple slip deformation remains a challenge for various reasons.

In the current talk we shall highlight some challenges appearing on different levels of continuum dislocation modelling. At the most fundamental level it is yet unclear what continuum measures are suited for characterizing 3D networks of dislocations. The alignment tensors successfully used for dislocation distributions in single slip seem to be of limited value in networks consisting mostly of junctions and reaction products. It is likewise an open question how to describe the kinematics of dislocation networks, where reactions and junction formation or break-up imply permanent changes in the topology of the network and the characteristics of dislocations. Closely related is the challenge of capturing the averaged energetics, kinematics and dissipation of these dislocation interactions.

To overcome the named challenges possibly requires new mathematical tools or at least the adoption of concepts from other areas of physics and mathematics which were not yet (fully) exploited in dislocation theory. We shall discuss several ideas where we might find new impulses and promising tools for further successes in developing a mesoscale theory of dislocations. Expected key areas include discrete and differential topology, gradient flows, rough energy landscapes, and temporal and spatial statistics.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6)

[SY-A7] Dislocation multiplication in the discrete-continuum transition regime

○Katrin Schulz[1], Markus Sudmanns[1], Kolja Zoller[1], Peter Gumbsch[1,2] （1.Karlsruhe Institute of Technology, Germany, 2.Fraunhofer Institute for Mechanics of Materials, Germany）

The striving for advanced materials with well-defined microstructures has led to an increasing effort towards a physically based description of the motion of dislocations as the cause of plastic deformation. Several dislocation based continuum theories have been introduced, but only recently rigorous techniques have been developed for performing meaningful averages over systems of moving, curved dislocations, yielding evolution equations for a dislocation density tensor, see [1].

Regarding a self-consistent coarsening of dislocation modeling in order to construct an efficient numerical implementation, several issues have to be solved including calculation of the stress field of a system of dislocations, representation of dislocation interactions and reactions as well as boundary conditions. Accurate solutions have been found for one and two dimensional systems [2, 3]. However, the analysis and

understanding of dislocation networks in three dimensions involves additional challenges such as the representation of dislocation multiplication.

In this presentation, we discuss the implications of a homogenization of dislocation interactions and reactions in the discrete-continuum transition regime. Based on the analysis of 3d discrete dislocation structures, we present a coarse-grained continuum formulation for dislocation multiplication due to cross-slip and glissile reaction events. The formulation is validated by the comparison with discrete dislocation dynamics simulations and discussed in the context of a continuum limit as lower application limit of a continuum approach.

[1]Hochrainer, T.; Sandfeld, S.; Zaiser, M.; Gumbsch, P.: Continuum dislocation dynamics: Towards a physical theory of crystal plasticity. *J. Mechan. Phys. Solids.* 63 (2014), p. 167-178.

[2] Schmitt, S., Gumbsch, P., Schulz, K.: Internal Stresses in a Homogenized Representation of Dislocation Microstructures. *J. Mechan. Phys. Solids*, 84 (2015), p. 528-544.

[3] Schulz, K., Sudmanns, M., Gumbsch, P.: Dislocation-Density based Description of the Deformation of a Composite Material. Modell. Simul. Mater. Sci. Eng., 25 (2017), 064003.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6)

[SY-A7] The fundamental instability of dislocation transport equations
○Michael Zaiser, Ronghai Wu （FAU University of Erlangen-Nuremberg, Germany）

We analyze the stability of transport equations which describe dislocation dynamics in terms of fluxes of dislocation densities defined on scales above the dislocation spacing. We demonstrate that such transport equations exhibit a generic instability which emerges as soon as a dislocation flux function, which in the simplest case is identical with the shear strain rate on a given slip system, has a negative derivative with respect to the flowing dislocation density. The criterion for instability is equivalent to the condition that the stress required to sustain plastic flow at a given rate is an increasing function of dislocation density. We conclude that dislocation patterning of some kind is an almost trivial, and practically unavoidable, consequence of dislocation transpoort in conjuction with work hardening. Implications for the theory and interpretation of different types of dislocation patterns, and for density-based simulations of plastic flow in general, are discussed.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6)

[SY-A7] 2D continuum theory of dislocations
○Istvan Groma （Eotvos Lorand University, Hungary）

During the past 20 years, by a systematic course graining of the equation of motion of straight parallel edge dislocations a 2D continuum theory of dislocation has been developed. It is able to account for many important feature of the collective properties of dislocations, like size effect, hardening due to precipitates, dislocation density distribution next to boundaries, and dislocation patterning. The predictions of the theory

are directly compared to discrete dislocation dynamics simulations.

In spite of the success of the theory there are several open issues need to be addressed for further developing the current theory. In the talk the problems "blocking" the extension of the theory are discussed:

1. Do we need a continuum theory?

2. Why still in 2D? What we can learn from it?

3. Should we course grain the equations of motion of the dislocations or the energy of the discrete system to derive the continuum theory?

3. Numerical determination of the dislocation dislocation correlation function. Problems related to the the finite size effect observed.

4. What to do next to boundaries?

5. Phase field approach. Issues related to the nontrivial mobility function one has to introduce.

6. Slow, power law relaxation of the dislocation system.

7. How to incorporate stochastic effects.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6)

[SY-A7] Continuum dislocation dynamics for finite deformation mesoscale plasticity

○Anter El-Azab （Purdue University, United States of America）

Many dislocation dynamics simulation models were developed to understand plastic deformation of metals most of which are based on small deformation kinematics. In this talk, I will present a density-based dislocation dynamics model within the framework of finite deformation of crystals, focusing on crystal mechanics and the dislocation transport equations at finite deformation. The geometric coupling and non-linearity of the dislocation transport on various slip systems will be explained. The relevant crystal mechanics, thermodynamics, and constitutive closure questions will also be discussed. Collaboration: Giacomo Po, University of California-Los Angeles; Grethe Winther, Technical University of Denmark.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A8] Symposium A-8
Chair: Thomas Hochrainer(TU Graz, Austria)
Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room6

[SY-A8] Pattern formation in doubly curved thin shells
○Eleni Katifori[1], Desislava Todorova[1], Octavio Albarran[2], Lucas Goehring[2] （1.University of Pennsylvania, United States of America, 2.Max Planck Institute, Germany）

[SY-A8] Phase-field model for microstructure change in $L1_0$ type ordering with lattice distortion
○Ryuichiro Oguma[1], Long-Qing Chen[2], Syo Matsumura[3] （1.Fukuoka Univ., Japan, 2.The Pennsylvania State Univ., United States of America, 3.Kyushu Univ., Japan）

[SY-A8] Coupling multi-component phase field models for oxide systems to thermodynamic databases - breaking the curse of dimensionality
○Inge Bellemans[1], Nico Vervliet[2], Lieven De Lathauwer[2,3], Nele Moelans[4], Kim Verbeken[1] （1.Department of Materials, Textiles and Chemical Engineering, Ghent University , Belgium, 2.Department of Electrical Engineering, KU Leuven, Belgium, 3.Group Science, Engineering and Technology, KU Leuven - Kulak, Belgium, 4.Department of Materials Engineering, KU Leuven, Belgium）

[SY-A8] A Sharp Phase Field Method
○Alphonse FINEL[1], Yasunori YAMADA[2], Yann LE BOUAR[1], Benoît DABAS[1], Benoît APPOLAIRE[1], Tetsuo MOHRI[2] （1.Laboratoire d'Etude des Microstructures, CNRS, ONERA, France, 2.Institute for Materials Research, Tohoku University, Japan）

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room6)

[SY-A8] Pattern formation in doubly curved thin shells

Invited

○Eleni Katifori[1], Desislava Todorova[1], Octavio Albarran[2], Lucas Goehring[2]　(1.University of Pennsylvania, United States of America, 2.Max Planck Institute, Germany)

Pattern formation in thin elastic shells has attracted increasing interest in both fundamental studies and practical applications. Examples include biological systems and engineering applications, such as the fabrication of flexible microelectronics. In this talk we explore the mechanical instabilities of an intrinsically curved thin shell deposited on a liquid surface. Here, the pattern formation is not a direct result of externally imposed strain, but is due to the geometric incompatibility between a curved, stiff membrane and an (initially flat) liquid substrate. We observe several types of instabilities, including a wrinkle-to-fold transition from periodic sinusoidal solutions to morphologies that combine sinusoidal wrinkles and folds; a transition from dimples (geometric inversions) to periodic sinusoidal solutions; and a transition from flat bands with zero Gaussian curvature, to dimpled periodic patterns. We show that whe wrinkling patterns can be described via an effective theory of liquid crystalline smectics at intermediate length scales. This insight allows better understanding of the wrinkling patterns seen in such systems, with which we explain pattern breaking into domains, the properties of domain walls and wrinkle undulation. We compare our predictions with numerical simulations and experimental observations. We investigate how the global geometry of the curved shells and their elastic properties control the transitions between the various morphologies. Last, we discuss various new strategies for creating and controlling patterns in thin elastic shells with natural curvature.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room6)

[SY-A8] Phase-field model for microstructure change in $L1_0$ type ordering with lattice distortion

○Ryuichiro Oguma[1], Long-Qing Chen[2], Syo Matsumura[3]　(1.Fukuoka Univ., Japan, 2.The Pennsylvania State Univ., United States of America, 3.Kyushu Univ., Japan)

Domain structures consisting of multiple off-phase variants are generally formed in ordering process in binary alloy systems. The $L1_0$ type order is formed in AB type alloys on the basis of an *fcc* lattice. The crystal structure is tetragonal. Therefore three orientational variants can be formed depending on which of <100> directions corresponds to c-axis and two translational variants are possible for each of them; six distinct crystallographic variants exist in this type of order. The present authors previously developed a phase-field formulation for ordering process of $L1_0$ type in binary alloys, taking into account the symmetry of the crystal structure. In the $L1_0$ structure the *fcc* lattice is divided into four simple cubic sublattices. The atomic occupation probabilities on the sublattices are represented by three independent order parameters and a composition parameter. If the state of order of atomic arrangement is represented by a point in the three dimensional Euclidean space spanned by the three order parameters, the six equivalent variants are defined by the six tips of a regular octahedron centered on the origin for the disordered state. A mean-field free energy is defined in a form of Landau type expansion with the order parameters and the composition parameter. In this presentation we further consider the effect of the lattice distortion. An elastic energy is introduced with eigen strains according to Khachatrian's method. The interface energy automatically reflects the direction of c-axis and satisfies symmetries of cubic, tetragonal and orthorhombic structures. Kinetic equations for time-evolution of the order parameters and the concentration are derived from the Ginzburg-

Landau type thermodynamical potential. Formation of domain structures was simulated by treating the kinetic equations numerically in a three-dimensional cell scheme. The microstructures obtained are compared with experimental results of TEM observation.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room6)

[SY-A8] Coupling multi-component phase field models for oxide systems to thermodynamic databases - breaking the curse of dimensionality

○Inge Bellemans[1], Nico Vervliet[2], Lieven De Lathauwer[2,3], Nele Moelans[4], Kim Verbeken[1]　(1.Department of Materials, Textiles and Chemical Engineering, Ghent University , Belgium, 2.Department of Electrical Engineering, KU Leuven, Belgium, 3.Group Science, Engineering and Technology, KU Leuven - Kulak, Belgium, 4.Department of Materials Engineering, KU Leuven, Belgium）

An important focus in creating more realistic phase field models is the incorporation of the thermodynamic driving forces in multicomponent multiphase-field models by coupling to thermodynamic databases. This coupling, which aims at retrieving Gibbs energies and chemical potentials, becomes increasingly intricate as the number of components/chemical elements in the system increases. This is caused by the fact that the number of elements in a tensor increases exponentially with the number of dimensions, and so do the computational and memory requirements. The exponential dependency (and the problems that are caused by it) is called the curse of dimensionality.

Alternatives need to be investigated for the storage and handling of the thermodynamic data required for the phase field simulations. A possible solution for this might be the use of a canonical polyadic decomposition on the tensors containing the thermodynamic data. In this way, the huge tensors are approximated well by compact multilinear models or decompositions. Tensor decompositions are more versatile tools than the linear models resulting from traditional matrix approaches.

This solution promises to be suitable for this challenge and has been applied to a quaternary and quinary metal-oxide system in a multicomponent multiphase-field model which incorporates facetted and dendritic growth and can also treat the boundaries as an open boundary where the melt is locally in equilibrium with the atmosphere at a certain partial oxygen pressure. The results and improvements in computational requirements are compared for various methods to couple to a thermodynamic database.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room6)

[SY-A8] A Sharp Phase Field Method
Invited
○Alphonse FINEL[1], Yasunori YAMADA[2], Yann LE BOUAR[1], Benoît DABAS[1], Benoît APPOLAIRE[1], Tetsuo MOHRI[2]　(1.Laboratoire d'Etude des Microstructures, CNRS, ONERA, France, 2.Institute for Materials Research, Tohoku University, Japan）

Phase field modelling offers an extremely general framework to predict microstructural evolutions in complex systems. However, its computational implementation requires a discretisation scheme with a grid spacing

small enough to preserve the diffuse character of the theory. We present a new formulation in which the interfaces are resolved with essentially one grid point with no pinning on the grid and an accurate rotational invariance, allowing to multiply the accessible linear dimensions by an order of magnitude or, conversely, to reduce the computational time by almost three orders of magnitude. We show that this Sharp Phase Field Method (S-PFM) reproduces interfacial kinetic properties with a very high accuracy. Then, we apply the model to a situation where conserved and non-conserved fields are coupled. Finally, to couple S-PFM to elastic fields, we propose a new elastic solver that efficiently treats strong elastic heterogeneities and that is mathematically stable.

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I5] Symposium I-5

Chairs: Stephen M Foiles(Sandia National Laboratories, United States of America), Mitra L Taheri(Drexel University, United States of America)

Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room7

[SY-I5] **Heterogeneous disconnections nucleation mechanisms during grain boundary migration**

○Nicolas Combe[1,2], Frederic Mompiou[1], Marc Legros[1]　(1.CEMES Toulouse, France, 2.Univ. Toulouse, UPS, France)

[SY-I5] **Motion of Grain Boundaries Based on Disconnections**

○Chaozhen Wei[1,2], Luchan Zhang[5], Yang Xiang[2], Jian Han[4], Spencer Thomas[4], kongtao Chen[4], David J. Srolovitz[3,1]　(1.HKUST Jockey Club Institute for Advanced Study, Hong Kong University of Science and Technology, Hong Kong, 2.Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong, 3.Materials Science and Engineering, Mechanical Engineering and Applied Mechanics, Computer and Information Science, University of Pennsylvania, United States of America, 4.Materials Science and Engineering, University of Pennsylvania, United States of America, 5.Department of Mathematics, National University of Singapore, Singapore)

[SY-I5] **Dislocation-mediated boundary motion, dislocation-boundary interaction, and their effect on the mechanical behavior in fcc materials**

○Bob Svendsen[1,2], Jaber Rezaei Mianroodi[2], Juan Li[3], Christoph Kirchlechner[3], Gerhard Dehm[3]　(1.Material Mechanics, RWTH Aachen University, Germany, 2.Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Germany, 3.Structure and Nano-/Micromechanics of Materials, Max-Planck-Institut für Eisenforschung GmbH , Germany)

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room7)

[SY-I5] Heterogeneous disconnections nucleation mechanisms during grain boundary migration

Invited

$^{\circ}$Nicolas Combe[1,2], Frederic Mompiou[1], Marc Legros[1]　(1.CEMES Toulouse, France, 2.Univ. Toulouse, UPS, France)

In specific conditions, grain boundary (GB) migration occurs in polycrystalline materials as an alternative vector of plasticity compared to the usual dislocation activity. The shear-coupled GB migration, the expected most efficient GB based mechanism, couples the GB motion to an applied shear stress. The migration of the GB occurs through the nucleation and motion of disconnections.

We report a detailed theoretical study of the elementary mechanisms occurring during heterogeneous disconnections nucleation. Using molecular simulations, the absorption of a $1/2[110]$ edge bulk dislocation in a symmetric $\Sigma{17}(410)$ $[001]$ tilt GB generates an immobile disconnection in the GB. We show that the shearing of this GB induces its migration and reveals a new GB migration mechanism through the nucleation of a mobile disconnection from the immobile one. Energy barriers and yield stress for the GB migrations are evaluated and compared to the migration of a perfect GB. As expected, the migration of imperfect GB is easier than the one of perfect GB. An immobile disconnection in a BG can thus operate as a source of disconnections driving the GB migration.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room7)

[SY-I5] Motion of Grain Boundaries Based on Disconnections

$^{\circ}$Chaozhen Wei[1,2], Luchan Zhang[5], Yang Xiang[2], Jian Han[4], Spencer Thomas[4], kongtao Chen[4], David J. Srolovitz[3,1]　(1.HKUST Jockey Club Institute for Advanced Study, Hong Kong University of Science and Technology, Hong Kong, 2.Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong, 3.Materials Science and Engineering, Mechanical Engineering and Applied Mechanics, Computer and Information Science, University of Pennsylvania, United States of America, 4.Materials Science and Engineering, University of Pennsylvania, United States of America, 5.Department of Mathematics, National University of Singapore, Singapore)

We propose a novel approach to simulate the evolution of polycrystalline microstructures based upon a disconnection model for grain boundary (GB) kinetics. The model incorporates surface tension, applied stress, and jumps in chemical potential across GBs. The model also includes disconnection nucleation and mobility. Disconnections are line defects that lie solely with GB and are characterized by both a Burgers vector and a step height, as set by the GB bicrystallography. We first derive a continuum equation of motion for individual GBs and then for GB triple junctions (TJ) within a polycrystalline microstructure that rigorously accounts for conservation of disconnection Burgers vectors and step heights and couples the GBs meeting at the TJ. We then implement this model in a continuum simulation of GB dynamics without TJs, with TJs and in a polycrystalline microstructure. The resultant simulations provide clear demonstrations of the importance of including a crystallography-respecting microscopic model of microstructure evolution and the intrinsic coupling between stress, capillarity, and microstructure connectivity in microstructure evolution.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room7)

[SY-I5] Dislocation-mediated boundary motion, dislocation-boundary interaction, and their effect on the mechanical behavior in fcc materials

Invited

○Bob Svendsen[1,2], Jaber Rezaei Mianroodi[2], Juan Li[3], Christoph Kirchlechner[3], Gerhard Dehm[3] （1.Material Mechanics, RWTH Aachen University, Germany, 2.Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Germany, 3.Structure and Nano-/Micromechanics of Materials, Max-Planck-Institut für Eisenforschung GmbH , Germany）

In the current work, mechanisms for dislocation-mediated motion of and deformation at coherent boundaries in fcc materials is investigated along with the resulting mechanical behavior.

On the modeling side, molecular dynamics (MD) simulations are carried out on bulk single and bi-crystal Cu, the latter containing two Σ3(111) boundaries. These are subject to loading conditions varying between shear loading parallel to the boundaries and perpendicular uniaxial loading. In the case of pure shear loading, MD results demonstrate that <112> shearing on Σ3(111) results in monotonic flow depending on the shear sign, whereas <110> shearing leads to oscillatory flow. As it turns out, this difference in behavior can be related to corresponding changes in the coincidence site lattice (CSL). In particular, in the case of <112> shearing, new potential boundary positions in the CSL occur every three atomic layers. Depending on the shear sign, however, one of these positions is closer to the current boundary position than the other. Since less energy is required for the boundary to shift to the closer position, the boundary moves to this position. In contrast, <110> shearing results in new potential boundary positions in the CSL having the same distance to the current boundary. Consequently, none of these is favored energetically, resulting in oscillatory motion of the boundary between these.

On the experimental side, nano-indentation experiments with 2m sized spherical indenter tips are used to study the impact of coherent Σ3(111) boundaries on the yield strength distribution in copper. The indents are performed either inside a grain or close to a coherent Σ3(111) boundary aligned normal to the sample surface. The force-displacement curves show elastic loading following Hertz´s predictions until a sudden displacement burst - a "pop-in" - is observed. The maximum shear stress beneath the indenter tip at the pop-in force is interpreted as yield stress. The statistical behavior of the yield stress is analyzed via cumulative probability (CP) plots. The CP plots show a significantly lower average yield stress at the boundary with respect to the single grains and an extremely narrow distribution at the boundary. The later finding suggests that the mechanism responsible for dislocation source activation is omnipresent at the boundaries.

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I6] Symposium I-6

Chairs: Garritt Tucker(Colorado School of Mines, United States of America), Chuang Deng(University of Manitoba, Canada)

Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room7

[SY-I6] Migration mechanisms of faceted vicinal grain boundaries
○Sherri Hadian[1], Blazej Grabowski[1], Mike W Finnis[2], Jörg Neugebauer[1] （1.Max-Planck-Institut fuer Eisenforschung, Germany, 2.Imperial College London, UK）

[SY-I6] Multiscale model for the structure and energy of low-angle general grain boundaries in Al, Cu and Ni
○Shuyang Dai[1], Yang Xiang[2], David Joseph Srolovitz[3] （1.Wuhan University, China, 2.Hong Kong University of Science and Technology, Hong Kong, 3.University of Pennsylvania, United States of America）

[SY-I6] The influence of normal stress on the structural transformation and migration of grain boundaries
○Chuang Deng, Mohammad Aramfard （University of Manitoba, Canada）

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room7)

[SY-I6] Migration mechanisms of faceted vicinal grain boundaries

Invited

○Sherri Hadian[1], Blazej Grabowski[1], Mike W Finnis[2], Jörg Neugebauer[1] (1.Max-Planck-Institut fuer Eisenforschung, Germany, 2.Imperial College London, UK)

We report molecular dynamics simulations and their analysis for grain boundaries vicinal to the Sigma 7 symmetric tilt boundary of the type {1 2 3} in aluminium. When minimized in energy at 0K a grain boundary of this type exhibits nano-facets that contain kinks. We observe that at higher temperatures of migration simulations, given extended annealing times, it is energetically favorable for these nano-facets to coalesce into a large terrace-facet structure. Therefore we initiate the simulations from such a structure and study as a function of applied driving force and temperature how the boundary migrates. We find the migration of a faceted boundary can be described in terms of the flow of steps. The migration is dominated at lower driving force by the collective motion of the steps incorporated in the facet, and at higher driving forces by the step detachment from the terrace-facet junction and propagation of steps across the terraces. The velocity of steps on terraces is faster than their velocity when incorporated in the facet, and very much faster than the velocity of the facet profile itself, which is almost stationary. A simple kinetic Monte Carlo model matches the broad kinematic features revealed by the molecular dynamics. Since the mechanisms seem likely to be very general on kinked grain boundary planes, the step flow description is a promising approach to more quantitative modeling of general grain boundaries.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room7)

[SY-I6] Multiscale model for the structure and energy of low-angle general grain boundaries in Al, Cu and Ni

○Shuyang Dai[1], Yang Xiang[2], David Joseph Srolovitz[3] (1.Wuhan University, China, 2.Hong Kong University of Science and Technology, Hong Kong, 3.University of Pennsylvania, United States of America)

We present a multiscale model to describe the structure and the energetics for various grain boundaires. The model incorporates both the anisotropy elasticity in each grain and the first-principle calculation informed interaction between two grains across the grain boundary, i.e., the generalized stacking-fault energy based upon the disregistry. The force balance between these two contributions determines the structure. We apply this approach to determine the structure and energetics of several twist grain boudnaries and tilt grain boundaries in FCC metals such as Cu, Al and Ni.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room7)

[SY-I6] The influence of normal stress on the structural transformation and migration of grain boundaries

Invited

○Chuang Deng, Mohammad Aramfard (University of Manitoba, Canada)

It is now widely accepted that stress plays important roles on the kinetics of grain boundaries. Past studies on grain boundary kinetics by atomistic simulation mainly focused on those under shear deformation by recognizing that shear coupling is one of the most fundamental modes of grain boundary motion. However, grain boundaries in polycrystalline materials under realistic loading conditions rarely experience pure shear deformation and stresses with both shear and normal components are more common. In this work, we used molecular dynamics simulations to investigate (1) how normal stress would influence the ground state structures of a few types of special CSL grain boundaries and (2) how such structural change would further influence the modes and energy barrier for migration in those grain boundaries.

We found that while both constant and cyclic normal stresses can facilitate the transition in grain boundary structure among its metastable states, the influences of tension and compression are not the same and vary among different types of grain boundaries. It is also found that the macroscopic strain caused in the materials due to the structural transformation in grain boundaries under cyclic stress can be well described by Coble creep, which implies a possible new mechanism of Coble creep that has been overlooked before. Furthermore, the grain boundary structural transformation can either lower or raise the energy barrier for grain boundary migration depending on the grain boundary type, which can be explained by the relative easiness of atomic shuffling in each grain boundary based on their DSC lattice.

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I7] Symposium I-7

Chairs: Nicolas Combe(CEMES Toulouse, France), Brandon Runnels(University of Colorado Colorado Springs, United States of America)
Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room7

[SY-I7] Insights into recrystallisation: atomistic simulations of the properties of grain boundaries in heavily deformed material
　　○Chris P Race （University of Manchester, UK）

[SY-I7] Continuum Dislocation Dynamic Based Grain Fragmentation Modeling for Severe Plastic Deformation in FCC Metals
　　○Ali Al-Hadi I. Kobaissy[1], Georges Ayoub[2], Mu'Tasem Shehadeh[1] （1.Department of Mechanical Engineering, American University of Beirut, Lebanon, 2.Department of Industrial and Manufacturing Systems Engineering, University of Michigan-Dearborn, United States of America）

[SY-I7] Atomistic Investigation on Interaction of Stress-Assisted Grain Boundary Motion with Crack
　　○Mohammad Aramfard, Chuang Deng （Univ. Manitoba, Canada）

[SY-I7] **Effect of grain boundary structure on its Dynamic Response using Molecular Dynamics**
　　○Saryu Fensin[1], Timothy Frolov[2] （1.Los Alamos National Lab, United States of America, 2.Lawrence Livermore National Laboratory, United States of America）

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room7)

[SY-I7] Insights into recrystallisation: atomistic simulations of the properties of grain boundaries in heavily deformed material

Invited
○Chris P Race （University of Manchester, UK）

A critical process in the development of a desirable microstructure in polycrystalline metals is that of recrystallisation, in which new grains of defect-free material nucleate and grow within the defect-laden microstructure of deformed material.

Thus, recrystallisation involves the creation and migration of grain boundaries between pristine and highly defective crystal. The structure and properties of these grain boundaries will be strongly affected by the plastic deformation in the defective grain. Furthermore, the driving force for their migration will be the elimination of the deformation defects. This force will be larger in magnitude and different in character to the driving forces present in other cases of grain boundary migration, such as grain growth. Grain boundary properties under these conditions have, however, received comparatively little attention.

Here we present insights from atomistic models of grain boundaries between cold-worked and defect-free grains which begin to uncover trends in their static and dynamic properties under conditions of recrystallisation.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room7)

[SY-I7] Continuum Dislocation Dynamic Based Grain Fragmentation Modeling for Severe Plastic Deformation in FCC Metals

○Ali Al-Hadi I. Kobaissy[1], Georges Ayoub[2], Mu'Tasem Shehadeh[1] （1.Department of Mechanical Engineering, American University of Beirut, Lebanon, 2.Department of Industrial and Manufacturing Systems Engineering, University of Michigan-Dearborn, United States of America）

In this work, the mechanical response as well as the microstructural features of face-centered cubic (fcc) metals subjected to severe plastic deformation (SPD) are investigated. A multi-scale framework that couples crystal plasticity (CP) scheme with continuum dislocation dynamics (CDD) model is proposed to mimic the loading conditions during Equal Channel Angular Pressing (ECAP) processes. Several aspects of the deformation process have been considered including texture evolution, the evolution of statistically stored dislocations (SSDs) and geometrically necessary dislocations (GNDs), and the fragmentation of the grains and its effect on the overall mechanical response. The framework is applied to a reference volume element (RVE) in which the grains are distributed and assigned a position. Within the model, each grain is allowed to split into 1024 new smaller grains which subsequently lead to strain hardening and grain refinement. The latter is modeled by accounting for the grain-grain interaction, for which the concept of the GNDs is incorporated into the mean free path of the dislocations. GNDs are assumed to be induced by grain boundaries that restrict the free deformation of a grain and result in an increase of stresses leading to the grain size reduction. The grain refinement procedure is triggered when the misorientation threshold between subgrains is exceeded. The calibration of the model parameters is performed using torsion test of pure copper material. The simulations results of generated texture and grain size reduction are in very good agreement with experimental data available in the literature.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room7)

[SY-I7] Atomistic Investigation on Interaction of Stress-Assisted Grain Boundary Motion with Crack

○Mohammad Aramfard, Chuang Deng （Univ. Manitoba, Canada）

Stress-assisted grain boundary motion is a prominent phenomenon in crystalline materials. On the other hand, crack/voids are common features in physical materials, thus the interaction of a moving grain boundary mediated by stress with such features are important to study the microstructural evolution of crystalline materials under severe plastic deformation. In this work three major behaviors are studied using atomistic simulations when a stress-mediated moving grain boundary interacts with crack, i.e., crack healing, crack propagation and sub-grain formation. The underlying macromechanism is described using atomistic configurations for each case and the effect of loading type, i.e., monotonic or cyclic is described. It is shown that metastable phases are the main reason for crack heal-ability of grain boundaries. The effect of material type which is in terms of stacking fault energy is also explored.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room7)

[SY-I7] Effect of grain boundary structure on its Dynamic Response using Molecular Dynamics

Invited
○Saryu Fensin[1], Timothy Frolov[2] （1.Los Alamos National Lab, United States of America, 2.Lawrence Livermore National Laboratory, United States of America）

Grain boundaries (GBs) can play an important role in governing the mechanical behavior and damage evolution of a material during both quasistatic and dynamic loading. However, the general consensus of the shock physics community has been that minute details about the GB structure should not affect the response of a material to dynamic loading. In this paper, we present results of molecular-dynamics simulations investigating whether or not small changes in boundary structure are 'recognized' by the shock wave and can in turn affect the spall strength of a material. As a test case, we will study grain boundaries in both Copper and Tungsten with similar orientation relationships but varying local structures. Specifically, we propose to use grand-canonically optimized structures for grain boundaries that retain their ordered structure even at elevated temperatures.

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I8] Symposium I-8
Chair: Srikanth Patala(North Carolina State University, United States of America)
Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room7

[SY-I8] New Approaches for Understanding Nanocrystalline Mechanics: Physical Microstructures, Grain Boundary Descriptors and Deformation Mechanisms
○Garritt Tucker, Jacob Tavenner, Ankit Gupta （Colorado School of Mines, United States of America）

[SY-I8] **Grain Boundary Sliding: the best supporting role in ductile localization**
○Alexandre Dimanov[1], Jean Raphanel[1], Michel Bornert[2], Eva Héripré[3], Mathieu Bourcier[1], Ababacar Gaye[2], Alexandre El Sabbagh[1], Wolfgang Ludwig[4], Andrew King[5] （1.LMS, CNRS-UMR7649, Ecole Polytechnique, France, 2.Laboratoire Navier, CNRS-UMR8205, Ecole des Ponts, France, 3.MSSMAT, CNRS-UMR8579, Centrale-Supélec, France, 4.MATEIS, UMR5510, INSA-Lyon, France, 5.SOLEIL Synchrotron, Beam line Psiché, France）

[SY-I8] Polycrystal plasticity with anisotropic grain boundary energy described on the five-dimensional grain boundary space
○Nikhil Chandra Admal[1], Javier Segurado[2,1], Jaime Marian[1] （1.University of California Los Angeles, United States of America, 2.IMDEA, Spain）

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room7)

[SY-I8] New Approaches for Understanding Nanocrystalline Mechanics: Physical Microstructures, Grain Boundary Descriptors and Deformation Mechanisms

Invited

○Garritt Tucker, Jacob Tavenner, Ankit Gupta （Colorado School of Mines, United States of America）

Engineering interest in nanocrystalline (NC) materials has been founded on the potential to improve mechanical properties such as increased strength/hardness, while scientific interest stems from the alternative fundamental mechanisms that are operative. Compared to their coarser-grained counterparts, the influence of interfaces (i.e., grain boundaries (GB)) becomes more significant in NC materials. Current simulation techniques for understanding NC mechanics rely on non-physical microstructures, first-order grain boundary descriptors that poorly capture the complexity of interfacial structure-property relationships, and a lack of quantitative approaches that can accurately capture the specific contribution of different deformation mechanisms. In this study, we propose utilizing higher-order GB descriptors to improve interfacial understanding, while determining polycrystalline behavior through networks connecting bulk and boundary behaviors. We perform atomistic modeling (e.g., Molecular Dynamics) studies of both favored CSL and general high-angle GBs for analyzing empirical and structural descriptors from atomic-scale behavior at the interfaces. These descriptors then aid in our GB network modeling to understand larger-scale polycrystalline behavior by unraveling the complexity surrounding the competition/cooperation between different deformation mechanisms. The importance of choosing physically-based atomistic microstructures and proper equilibration techniques in such simulations are also discussed. Finally, by utilizing continuum-based kinematic metrics, which can resolve the individual contribution of various deformation mechanisms such as GB and dislocation-mediated deformation to the total strain in the material, we help to further unravel the complex microstructural deformation behavior in NC metals.

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room7)

[SY-I8] Grain Boundary Sliding: the best supporting role in ductile localization

○Alexandre Dimanov[1], Jean Raphanel[1], Michel Bornert[2], Eva Héripré[3], Mathieu Bourcier[1], Ababacar Gaye[2], Alexandre El Sabbagh[1], Wolfgang Ludwig[4], Andrew King[5] （1.LMS, CNRS-UMR7649, Ecole Polytechnique, France, 2.Laboratoire Navier, CNRS-UMR8205, Ecole des Ponts, France, 3.MSSMAT, CNRS-UMR8579, Centrale-Supélec, France, 4.MATEIS, UMR5510, INSA-Lyon, France, 5.SOLEIL Synchrotron, Beam line Psiché, France）

Viscoplastic deformation of polycrystalline materials conditions many aspects of our everyday life from industrial hot forming of metallic items and durability of engineered structures, to glacier flow or plate tectonics powered by convection of Earth's mantle rocks. Usually, polycrystalline viscoplastic deformation is largely based on crystal slip plasticity (CSP). However, grain boundary sliding (GBS) may become a dominant mechanism at high temperatures, small grain sizes and low strain rates. Both mechanisms are often considered to act in parallel and to contribute independently to the global behaviour. We considered different classes of polycrystalline materials, such as Silicates, NaCl and Aluminium, combining high temperature rheological investigations and micromechanical testing with *in situ* SEM multi-scale

observations. In the latter case, we performed full field strain measurements, based on digital image correlation (DIC). For NaCl we could perform micromechanical tests *in situ* synchrotron X-ray microtomography and obtain both 2D and 3D strain fields. We show that for all of the considered materials CSP and GBS are not independent, but co-operative. Depending on microstructure and loading conditions, each one may be either the dominant strain cumulative mechanism, or a secondary mechanism, allowing for accommodation of the local strain incompatibilities related to the previous one. Both are necessary to ensure macroscopically homogeneous flow. We show examples of minor but crucial contribution of GBS to ductile localization phenomena and strain propagation throughout the microstructure.

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room7)

[SY-I8] Polycrystal plasticity with anisotropic grain boundary energy described on the five-dimensional grain boundary space

○Nikhil Chandra Admal[1], Javier Segurado[2,1], Jaime Marian[1]　(1.University of California Los Angeles, United States of America, 2.IMDEA, Spain)

At high temperatures, grain boundaries are not static entities but can migrate in response to thermo-mechanical forces brought about by temperature, external stresses, and internal microstructure. This gives rise to a wide array of dynamic behavior, including recovery, recrystallization, grain growth, etc.

In this talk, we present a recently developed three-dimensional polycrystal plasticity model driven by a single energy functional that captures both grain boundary (GB) energy and bulk elastic energy in response to plastic deformation. The model represents any arbitrary grain boundary using geometrically necessary dislocations (GNDs), and the GB energy is constructed as a function of the GNDs. Moreover, in contrast to previous phase-field approaches for grain boundary evolution, our model's energy functional is described on the entire five-dimensional grain boundary space allowing the consideration of both misorientation and inclination in the grain boundary energy.

The model is parameterized using grain boundary energy data from atomistic simulations, after which it is used to simulate the microstructure evolution of polycrystalline samples. The framework is used first to simulate the recrystallization process in a three dimensional polycrystal without external loads. Finally, the deformation of polycrystals under external loads is simulated for a few selected cases.

Symposium | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[SY-G1] Symposium G-1

Chairs: Byeongchan Lee(KyungHee Univ., Korea), Keonwook Kang(Yonsei University, Korea)
Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room8

[SY-G1] A systematic method to develop a potential model for harsh environments

○Takuji Oda, Sehyeok Park, Woonghee Cho （Dept. of Nuclear Engineering, Seoul National Univ., Korea）

[SY-G1] Molecular dynamics study of the bulk cascades in W-Re alloy

○Hyunggyu Lee[1], Byeongchan Lee[2], Keonwook Kang[1] （1.yonsei university, Korea, 2.kyung hee university, Korea）

[SY-G1] Defect Energetics in W-Based Transition-Metal Ternary Systems

○Younggak Shin, Byeongchan Lee （KyungHee Univ., Korea）

[SY-G1] A numerical study of channel deformation and fracture in irradiated stainless steel single crystals

○Jean-Michel Scherer[1,2], Samuel Forest[2], Jacques Besson[2], Benoit Tanguy[1], Jérémy Hure[1] （1.DEN-Service d'Etudes des Matériaux Irradiés, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette cedex, France, France, 2.MINES ParisTech, PSL-Research University, Centre des matériaux, CNRS UMR 7633, 63-65 rue Henri Auguste DesbruèresBP 87 91003 Evry Cedex, France, France）

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room8)

[SY-G1] A systematic method to develop a potential model for harsh environments

Invited

○Takuji Oda, Sehyeok Park, Woonghee Cho （Dept. of Nuclear Engineering, Seoul National Univ., Korea）

Molecular dynamics (MD) calculation is an important computational method for materials science and engineering. To obtain meaningful results from MD simulations for harsh environments, one has to prepare a quality potential model that works appropriately not only in equilibrium states but also in non-equilibrium states. We have recently developed a systematic method to construct (i) two-body potentials [T. Oda, W.J. Weber, H. Tanigawa, Comp. Mater. Sci. 111 (2016) 53] and (ii) embedded-atom method (EAM) potentials [T. Oda, submitted]. In this method, potential functions are expanded with cosine/sine series in reference to energies, forces and stresses evaluated by first-principles calculations. In the present study, using this method, we aim to construct potential models of a metal (bcc-Fe) and a metal oxide (Li_2O) for radiation environments. For this aim, results of first-principles molecular dynamics calculations of several atomic collision events are included in the reference data. MD simulation results with the constructed potential models show a reasonable agreement with available experimental data on fundamental material properties and threshold displacement energies. It is indicated that the method can effectively construct a potential model for MD simulations of harsh environments.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room8)

[SY-G1] Molecular dynamics study of the bulk cascades in W-Re alloy

○Hyunggyu Lee[1], Byeongchan Lee[2], Keonwook Kang[1] （1.yonsei university, Korea, 2.kyung hee university, Korea）

Tungsten is widely used as a facing material, because it has a high thermal conductivity and low sputtering yield. However, under the neutron irradiation, pure tungsten transmutes into the Re and Os. This causes degradation of material properties due to the formation of defect clusters, such as precipitates, that caused by irradiation. Therefore, it is important to understand the formation mechanism of defect clusters for preventing the degradation of material properties. In this study, for knowing the formation mechanism of defect clusters, we conducted irradiation simulation of bulk W-Re alloy using molecular dynamics simulation. To describe the neutron irradiation, we choose the certain atom that is hit by neutron, which is called PKA (Primary Knock-on Atom) and shot the PKA with certain kinetic energy. We analyze the defects formation of bulk system as changing the initial energy of PKA.

Acknowledgement

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room8)

[SY-G1] Defect Energetics in W-Based Transition-Metal Ternary Systems

○Younggak Shin, Byeongchan Lee （KyungHee Univ., Korea）

W has been considered as a potential core element for plasma facing material of fusion reactors for ITER thanks to its outstanding high-temperature properties. However, studies so far on W and W-based binary alloys show precipitation and defect clustering under neutron irradiation. In this talk, we report the first principles calculations of the defect energetics in ternary W alloys. W-Ta-Re systems are chosen for extensive calculations on interstitial defect structures around solute atoms.

Overall, as in pure W or W binary alloys such as W-Re, the most preferable defect type is found to be the bridge interstitial, followed by <111> interstitials. With negative solute-solute binding energy, Ta and Re atoms prefer to make a solute pair in the system and the solute pair strongly attracts W self-interstitial atom, forming a solute-interstitial complex. The binding between a Ta-Re solute pair and a W self-interstitial atom can be stronger in this ternary alloy than in binary systems, and plays a role in slowing down the W interstitial diffusion as a primary dissociation barrier. The defect energetics in the alloys can be understood as the combined results of both strain-relief effect and electronic effect, but the former, which is related with atomic size of elements and local pressure felt by each atom in lattice, seems dominant.

To summarize, the defect complexes in W-Ta-Re alloys are expected to trap W self-interstitial atoms, preventing self-interstitial atoms from escaping to the surface or grain boundary. The reduction in the number of disappearing self-interstitial atoms increases the odds for Frenkel defects to annihilate, reducing residual void concentration and hence void formation. It is also expected that, at elevated temperature, the rise in configuration entropy increases the interaction energy between solute pair and self-interstitial atom, and hence further slows interstitial migration.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room8)

[SY-G1] A numerical study of channel deformation and fracture in irradiated stainless steel single crystals

○Jean-Michel Scherer[1,2], Samuel Forest[2], Jacques Besson[2], Benoit Tanguy[1], Jérémy Hure[1] （1.DEN-Service d'Etudes des Matériaux Irradiés, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette cedex, France, France, 2.MINES ParisTech, PSL-Research University, Centre des matériaux, CNRS UMR 7633, 63-65 rue Henri Auguste DesbruèresBP 87 91003 Evry Cedex, France, France）

Stainless steels are widely used as structural materials for nuclear core internals. Due to their proximity with the nuclear fuel, these materials are subjected to high level of irradiation doses. In the last decades, irradiation effects on structural materials' mechanical properties have been heavily investigated in order to ensure structures' reliability over nuclear plant lifetime. Irradiation induced defects - such as Frank dislocation loops and nanocavities - can lead to significant mechanical properties changes, as for example a significant hardening due to pinning of dislocations on defects. Under mechanical loading, gliding dislocations may incorporate sessile defects lying in their gliding plane, leaving behind a reduced defect density path. These zones, typically bands or channels of 10-100 nm width, beeing therefore softened by the "defects cleaning", may localize strain and lead to highly heterogeneous deformation at the grain scale. This process is called dislocation channelling. A peculiar fracture mode called channel fracture is oberved in

austenitic stainless steels irradiated at high temperature to high doses, leading to transgranular facets on fracture surfaces. It has been hypothesized [1] that channel fracture is due to nanovoids coalescence in dislocation channnels. Channel fracture is therefore assessed numerically in this study using a strain gradient crystal plasticity model that has been developped in order to take into account irradiation defect densities in the hardening/softening behaviour of the material and that has been implemented in a Finite Element solver [2]. Such model allows to regularize strain localization, and is used to model dislocation channelling. Single crystal porous unit-cells are subjected to simple shear, and the effect of void sizes and dislocation channels widths are systematically investigated. Numerical results are finally used to assess the hypothesis proposed in [1] regarding channel fracture in irradiated stainless steels.

[1] Margolin B. et al. (2016) The radiation swelling effect on fracture properties and fracture mechanisms of irradiated austenitic steels. Journal of Nuclear Materials
[2] Ling C. et al. (2017) Void growth and coalescence in triaxial stress fields in irradiated fcc single crystals. Journal of Nuclear Materials

Symposium | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[SY-G2] Symposium G-2

Chairs: Seunghwa Ryu(Korea Advanced Institute of Science and Technology, Korea), Keonwook Kang(Yonsei University, Korea)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8

[SY-G2] Multiscale modeling of strength enhancement of aluminium honeycombs under combined shear-compression at high strain rate

○Han Henri ZHAO[1], Bing Hou[2] (1.Ecole Normale Paris-Saclay, France, 2.School of aeronautics, NWPU, , China)

[SY-G2] Multiscale mechanical analysis of silicon and silicon dioxide as high capacity anode materials for lithium ion batteries.

○Janghyuk Moon[1], Kyeongjae Cho[2], Maenghyo Cho[3] (1.School of Energy System Engineering, Chung-Ang Univ., Korea, 2.Department of Materials Science and Engineering, University of Texas at Dallas, United States of America, 3.School of Mechanical &Aerospace Engineering, Seoul National University, Korea)

[SY-G2] Finite element analysis of the effect of interfacial bubbles on performance of epoxy coatings under the alternating hydrostatic pressure

○Li Liu (Institute of Metal Research, Chinese Academy of Sciences, China)

[SY-G2] Multiscale Modeling and Design of High-Strength and Low-Density 3D-Archecticured Metamaterial Systems

○Hussein M Zbib[1], Mehdi Hamid[1], Rahul Panat[2], Sadeq Saleh[2] (1.Washington State university, United States of America, 2.Carnegie Mellon University, United States of America)

[SY-G2] Multiscale-multiphysics simulations of metal nanotips under high electric field

○Mihkel Veske[1], Andreas Kyritsakis[1], Kyrre Ness Sjobak[2], Vahur Zadin[3], Flyura Djurabekova[1] (1.Helsinki Institute of Physics, University of Helsinki, Finland, 2.Department of Physics, University of Oslo, Norway, 3.Institute of Technology, University of Tartu, Estonia)

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8)

[SY-G2] Multiscale modeling of strength enhancement of aluminium honeycombs under combined shear-compression at high strain rate

○Han Henri ZHAO[1], Bing Hou[2] (1.Ecole Normale Paris-Saclay, France, 2.School of aeronautics, NWPU, , China)

Aluminum honeycombs are widely used as sandwich cores in the protective component in transport industry. For example, they are involved in the bird strike shielding as well as in the crashworthiness design, etc. Under impact loading, testing results showed a significant enhancement of the out-of-plane crushing strength of honeycombs with respect to the quasi-static case, which cannot be explained by the rate sensitivity of aluminum alloy.

This paper firstly presents the quasi-static and impact testing results for a series of aluminium honeycombs of different cell sizes (3003 and 5052 alloys). A significantly different strength enhancement of 3003 honeycombs is found from the 5052 ones. In order to understand and model this strength enhancement, a comprehensive numerical investigation with rate insensitive constitutive laws is performed to reproduce the experimental results for different cell size/wall thickness/base materials. In fact, due to the lateral inertia effect under impact buckling, larger strain under impact loading than quasi-static case in the element nears intersectional line is observed. Different ratios of the strain hardening stress over the yield stress of the 3003 alloy from the 5052 alloy lead to the different honeycomb strength enhancements. Finally, aluminum 5052 and 3003 honeycombs are studied under combined shear-compression loading. It was focused on the interaction between the additional shear loading and the lateral inertia effect under the impact loading. It was found that the expansion of the crush envelopes from the quasi-static loading to the dynamic loading was almost homogeneous for the two honeycombs.

Hou B., Zhao H., Pattofatto S., Liu J.G., Li Y.L., 2012, Inertia effects on the progressive crushing of aluminium honeycombs under impact loading, Int. J. Solids &Struct.,, 49 (19-20), 2754-2762.
Hou B., Pattofatto S., Li Y. L., Zhao H., 2011, Impact behavior of honeycombs under combined shear-compression, Part II Analysis, Int. J. Solids &Struct.. 48, 698-705

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8)

[SY-G2] Multiscale mechanical analysis of silicon and silicon dioxide as high capacity anode materials for lithium ion batteries.

○Janghyuk Moon[1], Kyeongjae Cho[2], Maenghyo Cho[3] (1.School of Energy System Engineering, Chung-Ang Univ., Korea, 2.Department of Materials Science and Engineering, University of Texas at Dallas, United States of America, 3.School of Mechanical &Aerospace Engineering, Seoul National University, Korea)

The mechanical issues on high capacity electrode materials, such as silicon, tin, and silicon oxide, prevents their usage for lithium ion batteries. So, the oxides (i.e. silicon dioxide) are the prevalent materials used for a high-expected capacity and strong mechanical stability during cycles. Although tremendous efforts have devoted to the study of the electro-chemo-mechanical behaviors of high-capacity electrode materials, the mechanical behavior of amorphous SiO_2 during electro-chemical reaction remains largely unknown. Here we

systematically investigate the inelastic stress evolution, the electronic structure and the mechanical deformation of lithiated silicon dioxide through first-principles computation and finite element method. The structural and thermodynamics analysis was performed to predict electrochemistry characteristics Si and Si-O system. The mechanical strength and brittle behavior of SiO2 due to strong Si-O bonds are also compared with Si. Although both Si and SiO2 experience mechanical softening during lithiation, the clearly distinguishable relaxation kinetic of SiO$_2$ inducing deviatoric inelastic strains due to mechanical constraints is found by density functional theory calculation. These results would provide fundamental perspectives on the chemo-mechanical behavior of silicon and silicon oxide electrode for the practical use.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8)

[SY-G2] Finite element analysis of the effect of interfacial bubbles on performance of epoxy coatings under the alternating hydrostatic pressure

$^{\circ}$Li Liu　(Institute of Metal Research, Chinese Academy of Sciences, China)

Coatings suffer dramatic deterioration and premature damage in the deep-sea environment, in sharp contrast to the good protective performance in typical marine environments. Hydrostatic pressure (HP), which varies with ocean depth, has pronounced impact on coating performance when compared with other factors, such as oxygen level and pH value. The idea that loss of wet adhesion is the first step towards coating failure seems to be raising some controversy, with some researchers suggesting that the loss of adhesion results from the pressure relief process in the experiment rather than from hydrostatic pressure itself. AHP decreased the protective properties of coatings more rapidly than HP via a "push-and-pull" effect, which promotes bubbles formation at the interface between coatings and base metal.

Compared to other simulation methods, the finite element method (FEM) is capable of providing a multi-physical field to solve complex engineering problems more effectively. The interface is most susceptible to corrosion and the coating failure can be affirmed when the corrosion products are visible on there.

In this study, we attempt to develop a model of the growth of a bubble and the change of the stress distribution at the coating/substrate interface under AHP by means of FEM. The results show that the impacts of alternating hydrostatic pressure and hydrostatic pressure on the interface were compared with a precondition of bubbles inducing the coating failure.

1. Hydrostatic pressure cannot mechanically destroy the coating/metal interface because it acts as a compressive stress on the dry bubbles. If the bubbles turn into wet, the pressure loaded on the bubble will disappear.

2. Alternating hydrostatic pressure can provide tensile stress on the wet bubbles during every immersion period, so it accelerates disbonding of the coating.

3. The maximum stress on the bottom of wet bubbles is able to be minimized to less than the stable adhesion value if the lag time is large enough. In this case, alternating hydrostatic pressure cannot accelerate disbonding any more. The lag time will be different if the period of alternating pressure is changed. Thus, the lag time of a coating should be considered when it is designed to serve under alternating hydrostatic pressure.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8)

[SY-G2] Multiscale Modeling and Design of High-Strength and Low-Density 3D-Archecticured Metamaterial Systems

○Hussein M Zbib[1], Mehdi Hamid[1], Rahul Panat[2], Sadeq Saleh[2] （1.Washington State university, United States of America, 2.Carnegie Mellon University, United States of America）

Designing high energy-efficiency structural materials with superior mechanical properties is a key challenge for scientists and engineer. Among these properties, strength versus mass density and strength versus ductility are amongst the most important factors that affect component design, and thus structure weight. Ideal structural materials are the ones that may retain high strength with low mass density and excellent ductility. However, current state-of-the-art materials have a drastic tradeoff between these properties. In this work, a multiscale modeling approach is developed and used to design a new class of high-strength-ductility material system. It is shown that by integrating the effects of nanoparticle, nanolaminate and gradient structure on strength and ductility, it is possible to design and manufacture 3D-architectured lightweight metamaterial systems. The system is made of interconnected microscale metallic ligaments reinforced by nanolaminate metallic layers and have superior mechanical properties (strength-density, strength-ductility) compared to their bulk counterparts.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8)

[SY-G2] Multiscale-multiphysics simulations of metal nanotips under high electric field

○Mihkel Veske[1], Andreas Kyritsakis[1], Kyrre Ness Sjobak[2], Vahur Zadin[3], Flyura Djurabekova[1] （1.Helsinki Institute of Physics, University of Helsinki, Finland, 2.Department of Physics, University of Oslo, Norway, 3.Institute of Technology, University of Tartu, Estonia）

We propose a method for efficiently coupling the finite element method with atomistic simulations like molecular dynamics or kinetic Monte Carlo. Our method enables to dynamically build an unstructured mesh with optimized density that follows the geometry defined by atomistic data. On this mesh, multiphysics problems can be solved to obtain distribution of physical quantities of interest, which can then be fed back to the atomistic system. The simulation flow is optimized to maximize computational efficiency while maintaining good accuracy.

We use this method to simulate the evolution of nanostructures under high electric field. By solving Poisson equation, we obtain the 3D distribution of electric field around the nanostructure. Using the field, we calculate electron emission currents, surface and space charge and electrostatic forces for surface atoms. By

taking Joule and Nottingham heating into account and solving 3D heat equation, we also obtain atomistic velocity perturbation.

Our method has shown remarkable overlapping with an analytical solution and has proved to be efficient and robust enough to simulate large-scale thermal runaway processes. Using those simulations, we demonstrated for the first time the disintegration of Cu nanotip in extreme field conditions. This process is widely believed to lead to the formation of plasma and cause vacuum arcing in high gradient structures.

Symposium | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[SY-G3] Symposium G-3

Chairs: Seunghwa Ryu(Korea Advanced Institute of Science and Technology, Korea), Keonwook Kang(Yonsei University, Korea)
Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8

[SY-G3] Simulations on severely transient FSI problems associated with shock compression of matters in extreme conditions

○Jai-ick Yoh （Seoul National University, Korea）

[SY-G3] **Modeling and simulation of shock waves in solids using branched Hugoniots**

Jae-Wan Lee[1], Jimin Choi[1], Keonwook Kang[1], Soonho Song[1], ○Won-Suk Ohm[1], Jung Su Park[2]
（1.Yonsei University, Korea, 2.Agency for Defense Development, Korea）

[SY-G3] Branched Hugoniot curve of aluminum in strong shock using molecular dynamics

○Jimin Choi[1], Sanghyuk Yoo[1], Soonho Song[1], Jung Su Park[2], Keonwook Kang[1] （1.Yonsei Univ., Korea, 2.Agency for Defense Development, Korea）

[SY-G3] **Shear relaxation behind the shock front in <1 1 0> molybdenum**

○Roman Kositski[1], Dominik Steinberger[2], Stefan Sandfeld[2], Dan Mordehai[1] （1.Department of Mechanical Engineering, Technion - Israel Institute of Technology, 32000 Haifa, Israel, 2.Chair of Micromechanical Materials Modelling (MiMM), Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, 09599 Freiberg, Germany）

[SY-G3] **Hypervelocity shock behavior of graphene-metal nanocomposites via molecular dynamics simulations**

○Stefano Signetti, Seunghwa Ryu （Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea）

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8)

[SY-G3] Simulations on severely transient FSI problems associated with shock compression of matters in extreme conditions

Invited

○Jai-ick Yoh （Seoul National University, Korea）

Some special numerical techniques are desired when simulating the behavior of matters in extreme conditions, and in particular, the chemical-thermal energy release from the combustion of explosives and propellants must be carefully addressed when capturing the high strain rate deformation of metals and polymeric binders interacting with the energetic elements of the system. In this talk, selective research accomplishments associated with modeling of both energetic and inert matters exposed to high pressure conditions are discussed. Models are developed for addressing the problems of shock-induced ignition and multi-scale hot spot initiation of metalized energetic components from the shock compression system. To do so, one needs to adapt a stable interface tracking algorithm for severely transient fluid-structure interaction problems. We have developed a multi-material hydrodynamic shock physics code with a hybrid particle level set method for simulating the shock induced chemical reaction of energetic materials and volumetric deformation of metals. The experimental measurements are obtained to validate the simulated results presented in this talk.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8)

[SY-G3] Modeling and simulation of shock waves in solids using branched Hugoniots

Jae-Wan Lee[1], Jimin Choi[1], Keonwook Kang[1], Soonho Song[1], ○Won-Suk Ohm[1], Jung Su Park[2] （1.Yonsei University, Korea, 2.Agency for Defense Development, Korea）

Shock compression is an effective means of probing the mechanical and thermodynamic properties of solids. The majority of shock compression studies to date have reported principal Hugoniot curves, for which the material ahead of the shock is conveniently chosen to be in the quiescent state (P = 0 and u = 0). However, studies of branched Hugoniots (that emanate from non-quiescent states) are relatively rare, although branched Hugoniots are equally important for accurate description of shock wave physics involving interaction. In this talk, we discuss a sophisticated modeling scheme for shock hydrodynamics, accompanied by a full deck of principal and branched Hugoniots obtained with molecular dynamics computations. The system is a single-crystalline aluminum impacted at velocities ranging from 0.1 to 3.0 km/s, as described in the companion paper. Simulations show that branched Hugoniots should be used for accuracy in predictions, especially when there are material boundaries causing reflection and interaction of shocks.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8)

[SY-G3] Branched Hugoniot curve of aluminum in strong shock using molecular dynamics

○Jimin Choi[1], Sanghyuk Yoo[1], Soonho Song[1], Jung Su Park[2], Keonwook Kang[1] (1.Yonsei Univ., Korea, 2.Agency for Defense Development, Korea)

Two different embedded-atom method(EAM) potentials were used in single crystalline FCC Al : WKG (J.M. Winey, Alison Kubota, and Y.M. Gupta), and FWYD (Qin-Na Fan, Chong-Yu Wang, Tao Yu, Jun-Ping Du). A 300k single crystalline Al system is inflicted planar shock at an adiabatic condition of 0.1 to 3.0 km/s. Pressure, volume and temperature profiles are obtained after shock as impact velocity. We extract the principle Hugoniot curve in averaged value of profiles. Branch points are selected on the principle Hugoniot curve. We made an isentropic equilibrium system that approximates branch points. The isentropic equilibrium system is inflicted planar shock to impact at an adiabatic condition of 0.1 to 3.0 km/s to obtain the branched Hugoniot curve. It is observed that either stacking fault formation or phase transformation from FCC to HCP or FCC to BCC occurs depending on the potential model. This study shows how the branched Hugoniot curve of single crystalline aluminum differs from the principle Hugoniot curve in strong shock. In addition, by analyzing the differences according to potential models, we show that the potential model must be carefully selected in the strong shock simulation.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8)

[SY-G3] Shear relaxation behind the shock front in <1 1 0> molybdenum

○Roman Kositski[1], Dominik Steinberger[2], Stefan Sandfeld[2], Dan Mordehai[1] (1.Department of Mechanical Engineering, Technion - Israel Institute of Technology, 32000 Haifa, Israel, 2.Chair of Micromechanical Materials Modelling (MiMM), Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, 09599 Freiberg, Germany)

In this work we study shock-induced plasticity in Mo single crystals, using a method to relate information of dislocations from the atomic to the continuum scale [1]. We use molecular dynamics (MD) simulations to simulate the shock propagation along the <110> crystal orientation. Shock waves with compressive axial stresses of about 120 GPa are simulated. These stresses induce homogeneous nucleation of dislocations but barely lead to a phase transition. Using the Dislocation Extraction Algorithm (DXA) and the newly developed Discrete to Continuum (D2C) technique, the atomistic information is turned into continuous dislocation fields. In conjunction, we extract from the MD simulations thermo-dynamical macroscopic quantities such as macroscopic strain, density, temperature and stress tensor during the propagation of the shock wave. Correlating the stress evolution and the evolution of the continuous dislocation fields, we analyze the attenuation of the sharp elastic jump at the front of the shock wave and the plastic deformation behind it. Analyzing the MD simulations, we show that the initially an elastic precursor wave overshoots the dislocation nucleation stress, after which dislocations on a specific group of slip planes (which we denote as out-of-plane) are nucleated, slightly lagging behind the elastic front. As dislocations are nucleated in the out-of-plane direction, the resolved shear stress on these planes is relaxed, but the principal lateral stresses increase. This leads to an increase in the shear stresses on a plane parallel to the shock wave (denoted as in-plane), resulting in an additional retarded front of dislocation nucleation on planes parallel to the shock front. Finally, the two-stage process of plasticity results in close to isotropic stress state. Interestingly, the DXA-D2C analysis shows that non-zero contributions in the Kroener-Nye tensor appear only in the first stage of plasticity, right behind the shock front. The MD simulation results are employed to calculate the dislocation densities on specific slip planes and the plastic deformation behind the shock, bridging the gap between the information on the atomic scale and the continuum level.

[1] Kositski, et al. Computational Materials Science 149 (2018): 125-133.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8)

[SY-G3] Hypervelocity shock behavior of graphene-metal nanocomposites via molecular dynamics simulations

○Stefano Signetti, Seunghwa Ryu （Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea）

Graphene and other 2D materials with superior mechanical properties have been widely proposed as effective reinforcement for stronger and tougher nanocomposites [1] to realize structures capable to sustain extreme mechanical conditions, such impact loads. However current studies are limited to constitutive properties in the quasi-static regime [1] or to the impact properties of stand-alone 2D materials armors [2] without considering the behavior of the resulting nanocomposite under real hypervelocity shock conditions, where second order effect occur, such as elastic-plastic shock wave propagation or induced phase transformation. We present a molecular dynamics (MD) simulation study on shock behavior of graphene-reinforced single crystal copper (Cu), investigating the role of graphitic inclusion on the shock Hugoniot of such nanocomposites. Our results give insights of the failure behavior of graphene-metal nanocomposite under hypervelocity shock load and the consequent implications to their engineering applications.

References

[1] Y. Kim, J. Lee, M. Yeom, J. Shin, H. Kim, Y. Cui, J.W. Kysar, J. Hone, Y. Jung, S. Jeon, S. Han. Strengthening effect of single-atomic-layer graphene in metal-graphene nanolayered composites. *Nature Communications* 4:2114, 2013.
[2] S. Signetti, S. Taioli, N.M. Pugno. 2D Materials Armors Showing Superior Impact Strength of Few Layers. *ACS Applied Materials &Interfaces* 8:40820-40830, 2017.

[SY-G4] Symposium G-4

Chairs: Keonwook Kang(Yonsei University, Korea), Byeongchan Lee(KyungHee Univ., Korea)
Wed. Oct 31, 2018 4:00 PM - 4:45 PM Room8

[SY-G4] Effect of surface and internal defects on the mechanical properties of metallic glasses

Sunghwan Kim, ○Seunghwa Ryu （Dept. of Mechanical Engineering, Korea Advanced Institute of Science and Technology, Korea）

[SY-G4] Weighted Voronoi Tessellation for metallic glasses by molecular dynamics and powder packing by discrete element method

○Junyoung Park[1], Jaehee Lyu[1], Shibutani Yoji[2] （1.Dept. of Mechanical Design Engineering, Kumoh National Institute of Technology, Korea, 2.Dept. of Mechanical Engineering, Osaka University, Japan）

[SY-G4] Potential of lineal-path function as a characterization parameter related to material properties

○Tong-Seok Han, JI-SU KIM （Yonsei University, Korea）

(Wed. Oct 31, 2018 4:00 PM - 4:45 PM Room8)

[SY-G4] Effect of surface and internal defects on the mechanical properties of metallic glasses

Sunghwan Kim, ○Seunghwa Ryu （Dept. of Mechanical Engineering, Korea Advanced Institute of Science and Technology, Korea）

Despite the significance of surface effects on the deformation behaviors of small-scale metallic glasses, systematic investigations on surface states are lacking. In this work, by employing atomistic simulations, we characterize the distributions of local inhomogeneity near surfaces created by casting and cutting, along with internal distributions in pristine and irradiated bulk specimens, and investigate the effects of inhomogeneity on the mechanical properties. The cast surface shows enhanced yield strength and degrees of shear localization, while the cut surface shows the opposite effects, although the fraction of vibrational soft spots, known to indicate low-energy barriers for local rearrangement, is high near both surfaces. Correspondingly, plastic deformation is initiated near the cut surface, but far from the cast surface. We reveal that improved local orientational symmetry promotes strengthening in cast surfaces and originates from the effectively lower quenching rate due to faster diffusion near the surface. However, a significant correlation among vibrational soft spots, local symmetries, and the degree of shear localization is found for the pristine and irradiated bulk materials. Our findings reveal the sensitivity of the surface state to the surface preparation methods, and indicate that particular care must be taken when studying metallic glasses containing free surfaces.

(Wed. Oct 31, 2018 4:00 PM - 4:45 PM Room8)

[SY-G4] Weighted Voronoi Tessellation for metallic glasses by molecular dynamics and powder packing by discrete element method

○Junyoung Park[1], Jaehee Lyu[1], Shibutani Yoji[2] （1.Dept. of Mechanical Design Engineering, Kumoh National Institute of Technology, Korea, 2.Dept. of Mechanical Engineering, Osaka University, Japan）

Voronoi tessellation technique, or also called as Voronoi analysis, has been quite widely adopted to describe the internal structure of materials from molecular level such as short-range order of icosahedra on metallic glasses to centimeter-order powder level such as occupied volume on powder packing. Especially, Voronoi tessellation technique is applied to the investigations by molecular dynamics or discrete element method. In the ordinary Voronoi tessellation technique, a face is placed halfway between equal-sized atoms or particles. However, as the size of particles or atoms in single material are not same, bisection cannot depict the exact plane to represent a convex polyhedron including an atom or a particle. Moreover, packed particles in an vessel usually has a Gaussian particle size distribution for natural powders and a Rosin-Rammler particle size distribution for pulverized powders. It is not just a problem for size distribution. It makes a huge difference on estimation of occupied volume and number of faces by atoms or particles. Therefore, we suggest an alternative way, Radical Plane Method, to solve these problems in this paper. It shows that the error of results could reach up to 60% differences.

(Wed. Oct 31, 2018 4:00 PM - 4:45 PM Room8)

[SY-G4] Potential of lineal-path function as a characterization parameter related to material properties

○Tong-Seok Han, JI-SU KIM （Yonsei University, Korea）

The hydrated cement paste has complex microstructures. The pore and solid phase distribution characteristics within microstructures affect the material responses significantly. Material microstructure and its responses have been correlated with porosity [1]. However, porosity might not be sufficient to describe the complex microstructures. In this study, the relation between microstructure characteristics and material properties is investigated using a statistical method. To extract the microstructural characteristics of cement paste, micro-CT images are used. Pore and solid phase are separated from micro-CT images using the Powers' model. A lineal-path function [2], one of the low-order probability functions, is selected for estimating the microstructure characteristics. Particularly, the area of lineal-path function [3] is used as a quantitative parameter related to the material property in this study. Virtual specimens obtained from synchrotron micro-CT are used to evaluate material mechanical properties. The phase field fracture model is applied to evaluate stiffness and strength of cement paste with complex microstructures. From this study, it is concluded that the area of lineal-path function has a potential to be an alternative parameter for correlating material characteristics and properties.

[1] C. Miehe, M. Hofacker, F. Welschinger, A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits, Comput. Meth. Appl. Mech. Eng. 199 (2010) 2765-2778.
[2] B. Lu, S. Torquato, Lineal-path function for random heterogeneous materials, Phys. Rev. A 45 (1992) 922-929.
[3] T. S. Han, X. Zhang, J. S. Kim, S. Y. Chung, J. H. Lim, C. Linder, Area of lineal-path function for describing the pore microstructures of cement paste and their relations to the mechanical properties simulated from μ-CT microstructures. Cem. Concr. Compos. 89 (2018) 1-17.

[SY-H3] Symposium H-3

Chair: Hansohl Cho(Los Alamos National Laboratory, United States of America)
Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room9

[SY-H3] Polydomain liquid crystal elastomers1

○Kaushik Bhattacharya （California Institute of Technology, United States of America）

[SY-H3] **Mechanical behavior of hydrated polymers at nanoscale: from elasticity to rupture.**

○William Goncalves[1], Takuya Mabuchi[2], Takashi Tokumasu[1] （1.Institute of Fluid Science, Tohoku University, Sendai, Miyagi 980-8577, Japan, 2.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Sendai, Miyagi 980-8577, Japan）

[SY-H3] Structural properties of mixtures of stars polymers and long chains

○Emanuele Locatelli[1], Daniele Parisi[2,3], Maria Merola[2], Domenico Truzzolillo[4], Mario Gauthier[5], Christos N. Likos[1], Dimitris Vlassopoulos[2,3] （1.Faculty of Physics, University of Vienna, Austria, 2.Institute of Electronic Structure and Laser, FORTH, Greece, 3.Department of Materials Science and Technology, University of Crete, Greece, 4.Laboratoire Charles Coulomb, UMR 5221 CNRS - Universitè de Montpellier, France, 5.Faculty of Science, University of Waterloo, Canada）

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room9)

[SY-H3] Polydomain liquid crystal elastomers1

Invited

○Kaushik Bhattacharya （California Institute of Technology, United States of America）

Liquid crystal elastomers are rubbery solids with liquid crystal mesogens incorporated into their main chains. They display an isotropic to nematic phase transformation accompanied by a large spontaneous deformation. Depending on how these liquid crystal elastomers are synthesized, they can either be a mono domain (uniform liquid crystal order) or polydomain (nonuniform liquid crystal order). This talk will describe various phenomena and modeling questions related to the effective behavior of polydomain liquid crystal elastomers1

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room9)

[SY-H3] Mechanical behavior of hydrated polymers at nanoscale: from elasticity to rupture.

○William Goncalves[1], Takuya Mabuchi[2], Takashi Tokumasu[1] （1.Institute of Fluid Science, Tohoku University, Sendai, Miyagi 980-8577, Japan, 2.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Sendai, Miyagi 980-8577, Japan）

Because of their emissions free of carbon dioxyde, polymer electrolyte fuel cells (PEFCs) are of great interest for energy production respectful of the environment. The transport of charges between the electrodes of the fuel cell is insured by a hydrated polymer membrane such as perfluorosulfonic acid (PFSA) membrane. The durability of the fuel cell is still limited by the chemical and mechanical degradation of the polymer membrane after cycles of utilization. This work focuses on the study of the mechanical behavior of PFSA membrane at nanoscale. The understanding of the relation between structure and mechanical properties is the key point to improve the resistance of the membrane against mechanical degradation.

Molecular Dynamics (MD) simulations are performed using a Coarse-Grained model to generate samples of PFSA membranes. The results obtained from structural characterization are compared with data from previous atomistic models and experiments. After validation of the nanostructures, mechanical tests are performed on the hydrated polymer membrane. With an increasing level of hydration, the results for elastic properties are in good agreement with experimental values and a similar trend as experiments is observed for early plastic behavior. The computation of the local mechanical properties of the samples allows to discuss the void nucleation and the influence of water content on the rupture behavior.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room9)

[SY-H3] Structural properties of mixtures of stars polymers and long chains

○Emanuele Locatelli[1], Daniele Parisi[2,3], Maria Merola[2], Domenico Truzzolillo[4], Mario Gauthier[5], Christos N. Likos[1], Dimitris Vlassopoulos[2,3] （1.Faculty of Physics, University of Vienna, Austria, 2.Institute of Electronic Structure and Laser, FORTH, Greece, 3.Department of Materials Science and Technology, University of Crete,

Greece, 4.Laboratoire Charles Coulomb, UMR 5221 CNRS - Universitè de Montpellier, France, 5.Faculty of Science, University of Waterloo, Canada）

We employ a novel coarse-graining approach[6], to study star-chain mixtures[1-4], in the limit of long chains. The coarse-grained approach is based on the calculation of the effective interaction between a star polymer and a short chain of length N_c =10 at infinite dilution. A multi-blob-like approach is then employed to coarse-grain chains of arbitrary length N_c . We study mixtures of star polymer and linear chains in the protein limit, i.e. when $q = R_h^c / R_h^s > 1$. We find that the addition of linear chains makes the star fluid more structured, confirming experimental observation obtained through rheological measurements.

[1] E. Stiakakis, et al. Physical Review Letters, (2002).
[2] E. Stiakakis, et al. Europhysics Letters, (2005).
[3] M. Camargo and C.N. Likos. Physical Review Letters, (2010).
[4] B. Lonetti, et al. Physical Review Letter, (2011).
[5] C. Pierleoni, B. Capone, and J.P. Hansen. Journal of Chemical Physics, (2007).
[6] Locatelli, B.Capone and C.N. Likos. Journal of Chemical Physics (2016)

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H4] Symposium H-4

Chair: Meredith Silberstein(Cornell University, United States of America)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room9

[SY-H4] Enhanced Dissipation Behavior of Main-Chain LCE Networks

○Thao D Nguyen （Johns Hopkins University, United States of America）

[SY-H4] Thermo-mechanically coupled model for large strain of ultra-high molecular weight semi-crystalline polymers

○Chrystelle A. Bernard[1], Tiana Deplancke[4], Olivier Lame[4], Kazuhiro Ogawa[3], Jean-Yves Cavaillé[2] （1.Frontier Research Institute for Interdisciplinary Sciences (FRIS), Tohoku Univ., Japan, 2.Engineering Science Lyon Tohoku joint lab for Materials under Extreme Conditions (ELyTMaX) UMI3757, Tohoku Univ., Japan, 3.Fracture and Reliability Research Institute (FRI), Tohoku Univ., Japan, 4.Materials Engineering and Science (MATEIS), CNRS, INSA-Lyon, UMR5510 Univ. de Lyon, France）

[SY-H4] Design principles for high modulus and toughness of assembled hairy nanoparticles

Nitin Krishnamurthy Hansoge, Tianyu Huang, Robert Sinko, Wenjie Xia, Wei Chen, ○Sinan Keten （Northwestern University, United States of America）

[SY-H4] Effect of Chain Alignment on Entanglements, Diffusion and Polymer Weld Strength

Marco Galvani, Thomas C O'Connor, ○Mark Owen Robbins （Dept. Physics and Astronomy, Johns Hopkins Univ., United States of America）

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room9)

[SY-H4] Enhanced Dissipation Behavior of Main-Chain LCE Networks
Invited
○Thao D Nguyen （Johns Hopkins University, United States of America）

Liquid-crystalline elastomers (LCEs) are soft stimuli-responsive materials that exhibit remarkable mechanical and optical properties. LCEs consist of stiff mesogens, bound in a network of flexible polymer chains, which can self-organize into crystalline order while retaining liquid-like properties. The directional ordering of the mesogens changes in response to external stimuli and the director coupling between the mesogens and network chains brings about unusual behaviors. These include large reversible actuation in response to temperature or light and soft-elasticity. LCEs also exhibit enhanced dissipation behaviors, including a high *tan delta* 0.5-1.0 for wide range of frequencies and temperatures, spanning the glass and nematic transition temperatures, and large hysteresis in the stress response that increases with the strain rate [1]. We hypothesize that the enhanced dissipation behavior arises from the relative motions of the mesogens within the network and set out to measure the effect of mesogen ordering and network orientation on the enhanced dissipation behavior of LCEs. Experiments were performed to measure the rate-dependent hysteresis and frequency dependent dynamic properties for main-chain LCEs in the nematic state with different network structures, including an unoriented and macroscopically isotropic polydomain as well as monodomains with different degrees of mesogens and chain alignment. Oriented monodomains with an aligned or unaligned network can be synthesized by applying a second-stage crosslinking or exchangeable bond reaction to a stretched LCE sample. In this presentation, I will briefly describe the experimental methods, then compare the dissipative behavior of the different network structures, and discuss how the results will be applied to develop a rate-dependent constitutive model for the main-chain LCE networks.

[1] A. Azoug, V. Vasconcellos, J. Dooling, M. Saed, C. M. Yakacki and T. D. Nguyen (2016) *Polymer* 98:165-171.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room9)

[SY-H4] Thermo-mechanically coupled model for large strain of ultra-high molecular weight semi-crystalline polymers
○Chrystelle A. Bernard[1], Tiana Deplancke[4], Olivier Lame[4], Kazuhiro Ogawa[3], Jean-Yves Cavaillé[2] （1.Frontier Research Institute for Interdisciplinary Sciences (FRIS), Tohoku Univ., Japan, 2.Engineering Science Lyon Tohoku joint lab for Materials under Extreme Conditions (ELyTMaX) UMI3757, Tohoku Univ., Japan, 3.Fracture and Reliability Research Institute (FRI), Tohoku Univ., Japan, 4.Materials Engineering and Science (MATEIS), CNRS, INSA-Lyon, UMR5510 Univ. de Lyon, France）

Polymers are largely used in everyday life; however, their large strain behavior is still not well understood because of the complexity of the mechanisms involved in their deformation. To improve the current knowledge on these materials, extensive experimental and theoretical researches have been performed leading to development of constitutive numerical models to predict their large strain behavior. Most of models based on polymer physics have been developed for amorphous polymers. The few ones predicting the mechanical behavior of semi-crystalline polymers do not consider the important evolution of microstructure occurring during the plasticity. This is especially true for ultra-high molecular weight semi-crystalline (UHMWSC) polymers. Because their microstructure exhibits very long macromolecular chains, one

chain belongs at the same time at the crystal network and macromolecular network. During the plastic deformation of the polymers, fibrillation process occurs leading to the progressive collapse of the crystalline network and inducing strong variations in the material mechanical properties. Thus, to accurately predict the mechanical behavior of UHMWSC polymers, the mechanical coupling between crystallites and fibrils and its evolution during the deformation has to be taken into account. From the expression of the mechanical coupling for the elastic modulus given by Humbert et al. [1] (non-parallel/non-series configuration), Deplancke et al. [2] developed a one-dimensional model for the prediction of the mechanical behavior of Ultra High Molecular Weight PolyEthylene (UHMWPE). However, to extend its possible range of applications, transformation into a three-dimensional model is needed. Therefore, we have developed a 3D model which take into account the evolutive mechanical coupling, between crystals and fibrils, as a function of the deformation. The model is based on series configuration with consideration of the crystal ratio in the definition of the deformation gradients. Good agreement is found between the experimental results and 3D numerical predictions during loading and unloading.

[1] Humbert et al., *Polymer* **52** (2011) 4899-4909

[2] Deplancke et al., on going

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room9)

[SY-H4] Design principles for high modulus and toughness of assembled hairy nanoparticles

Nitin Krishnamurthy Hansoge, Tianyu Huang, Robert Sinko, Wenjie Xia, Wei Chen, $^{\bigcirc}$Sinan Keten
（Northwestern University, United States of America）

Matrix-free polymer-grafted nanocrystals, called assembled hairy nanoparticles (aHNPs), can significantly enhance the thermomechanical performance of nanocomposites by overcoming nanoparticle dispersion challenges and achieving stronger interfacial interactions through grafted polymer chains. However, effective strategies to improve both the mechanical stiffness and toughness of aHNPs is lacking given the general conflicting nature of these two properties and the large number of molecular parameters involved in design of aHNPs. Here, we propose a computational framework that combines multi-response Gaussian process metamodeling and coarse-grained molecular dynamics simulations to establish design strategies for achieving optimal mechanical properties of aHNPs within a parametric space. Taking poly(methyl methacrylate) grafted to high-aspect ratio cellulose nanocrystals as a model nanocomposite, our multi-objective design optimization framework reveals that the polymer chain length and grafting density are the main influencing factors governing the mechanical properties of aHNPs, in comparison to the nanoparticle size and the polymer-nanoparticle interfacial interactions. In particular, the Pareto frontier marking the upper-bound of mechanical properties within the design parameter space can be achieved when the weight percentage of nanoparticle is above around 60% and the grafted chains exceed the critical length scale governing transition into the semi-dilute brush regime. We show that theoretical scaling relationships derived from the Daoud-Cotton model capture the dependence of the critical length scale on graft density and nanoparticle size. Our established modeling framework provides valuable insights into the mechanical behavior of these hairy nanoparticle assemblies at the molecular level and allows us to establish guidelines for nanocomposite design.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room9)

[SY-H4] Effect of Chain Alignment on Entanglements, Diffusion and Polymer Weld Strength

Marco Galvani, Thomas C O'Connor, ○Mark Owen Robbins （Dept. Physics and Astronomy, Johns Hopkins Univ., United States of America）

Extrusion in fused filament fabrication is typically fast enough to produce significant chain alignment that may change the weld strength of 3D printed objects in several ways. Some studies suggest that alignment may enhance interdiffusion because of the entropic force driving chains towards unaligned conformations or by reducing entanglement density. Alignment of strong backbone bonds along the interface may also change the mechanical properties of material near the joint. As part of a multiscale study of 3D printing, we have used molecular dynamics simulations of a generic polymer model to examine the effect of alignment on the dynamics of welding and evolution of weld strength. Entropy drives chain retraction in the tube, but this does not speed interdiffusion since the tubes are aligned along the interface. There is also no indication of accelerated interdiffusion due to entanglement loss. The ambiguities in recent real space methods for identifying entanglements will be discussed. Alignment does reduce the strength of bulk material adjacent to the weld. At intermediate times this greatly enhances weld strength by moving failure away from the interface. The dependence of the bulk strength on alignment is presented for different thermal histories.

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H5] Symposium H-5

Chair: Alexey Lyulin(Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands)
Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room9

[SY-H5] **Microstructural Effects in the Dynamic Response of Random 3D Structural Polymeric Foams**
○Axinte Ionita, Brittany Branch, Brian M. Patterson, Brad E. Clements, Dana M. Dattelbaum, Alexander H. Mueller （Los Alamos National Laboratory, United States of America）

[SY-H5] **Monte Carlo simulation predicting generation and growth of spherulites in thermoplastic polymer**
○Ryota Osawa[1], Yoshiteru Aoyagi[2] （1.Dept. of Mechanical Engineering, Tohoku Univ., Japan, 2.Tohoku Univ., Japan）

[SY-H5] **Determination of mechanical properties of polymers from coarse grained molecular dynamics simulations: a few case studies**
○Sumit Basu （Indian Institute of Technology Kanpur, India）

[SY-H5] **Modulating Elastomer Strength and Toughness with Metal Ligand Cross-linking**
○Meredith Silberstein Silberstein, Yuval Vidavsky, Suwon Bae （Cornell University, United States of America）

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room9)

[SY-H5] Microstructural Effects in the Dynamic Response of Random 3D Structural Polymeric Foams

○Axinte Ionita, Brittany Branch, Brian M. Patterson, Brad E. Clements, Dana M. Dattelbaum, Alexander H. Mueller （Los Alamos National Laboratory, United States of America）

Polymeric foams materials can have various applications in engineering. We consider in this work the effect of the foam microstructure in the homogenized response of a random 3D structural polymeric foam under high dynamic mechanical loading conditions (shock). In the analysis, the microstructure of the foam is extracted from 3D computed micro-tomography. The mechanical response of the solid part of the foam is described in terms of deviatoric and pressure response. Using Direct Numerical Simulations (DNS), Finite Element Method (FEM) and the concepts of Micromechanics the average foam response to shock is determined. The results are compared with the 1D-shock equations for the homogenized case to determine the effect of fluctuating fields of physical quantities due to the randomness of the foam microstructure.

LA-UR-18-22612

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room9)

[SY-H5] Monte Carlo simulation predicting generation and growth of spherulites in thermoplastic polymer

○Ryota Osawa[1], Yoshiteru Aoyagi[2] (1.Dept. of Mechanical Engineering, Tohoku Univ., Japan, 2.Tohoku Univ., Japan）

Crystalline thermoplastic polymers have a complicated hierarchical structure consisting of lamellae of amorphous phases with a random coil structure and crystalline phases in which molecular chains are regularly arranged. The lamellae grow radially repetition of secondary nucleation on a surface of growing lamellae and spherulite structures are generated. Peculiar mechanical characteristics of the crystalline thermoplastic polymers, such as nonlinear elasticity, strain softening after yielding, propagation of necking, and orientation rehardening cannot be seen in the case of metals. Mechanical properties of crystalline thermoplastic polymers depend on the complicated microstructures, and the microstructures varies depending on molding conditions. A theoretical model predicting the microstructure and reproducing the mechanical properties are expected in the field of industrial CAE to enhance formability and reliability of the crystalline thermoplastic polymers. Phenomenological models on macroscopic crystallinity or crystallization rate are popular in terms of industrial availability. Such models cannot investigate effects of sizes, shapes, and distribution of spherulites. In this study, we construct a model expressing generation of spherulite structures for prediction of microstructures of crystalline thermoplastic polymers depending on thermal conditions. A spherulite growth are represented by initial nucleation in an amorphous phase and secondary nucleation on surfaces of spherulites. Rates of the both nucleation are identified by experimental observations of spherulites growth under different thermal conditions. Monte Carlo simulations are performed using the constructed method to reproduce the generation and growth of spherulites in an amorphous phase. In addition, we evaluate effects of crystallization temperature on the nucleation rate and the growth rate by comparison of experiment and analysis results.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room9)

[SY-H5] Determination of mechanical properties of polymers from coarse grained molecular dynamics simulations: a few case studies

○Sumit Basu （Indian Institute of Technology Kanpur, India）

Polymers, by virtue of being synthetic, microscopically tailorable and light materials, are finding uses in challenging new technological situations. These new applications, involving high temperatures, harsh environments, impact, sustained dead loading and others, often demand changes in the macromolecular architecture. The ability to predict the effects of an architectural alteration on the ultimate mechanical behaviour of a bulk polymer is therefore, useful. Coarse grained molecular dynamics provide a route to conducting large and long simulations to establish structure property relationships in these materials. However, a wide variety of coarse graining methodologies exist and their suitability for obtaining mechanical properties needs to be systematically established before they can become effective predictive tools. In this talk, we will focus on our experience with coarse grained molecular dynamics simulations on long chained and crosslinked polymers. In particular, we will discuss, coarse graining strategies that rely on Boltzmann inversion based techniques for calibrating bonded interactions, and a variety of heuristic techniques targetting specific physical properties for the non-bonded. We will highlight the problems associated with simultaneously targetting multiple end properties like density, total energy and atomic virial. Moreover, the mismatch in time scales between detailed atomistic and coarse grained simulations and their influence on the rate dependent behaviour of properties like the glass transition temperature and uniaxial stress-strain response will also be discussed. Finally, we will demonstrate a few case studies on polystyrene and a group of crosslinked polyimides to show that coarse grained molecular dynamics simulations of polymers have good predictive capability and sometimes can provide useful insights into material behaviour.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room9)

[SY-H5] Modulating Elastomer Strength and Toughness with Metal Ligand Cross-linking

○Meredith Silberstein Silberstein, Yuval Vidavsky, Suwon Bae （Cornell University, United States of America）

Non-covalent cross-linking interactions such as metal ligands can be used to tailor stiffness and structure of linear polymers while enabling interesting features like self-healing, energy dissipation, and extended stretching capability. Here we present a novel system of copper(II) carboxylate bonds used to crosslink a low Tg acrylic backbone. These crosslinks behave in a covalent manner to form novel materials with increased stiffness, strength, and dissolution resistance, and decreased ductility. It was found that substitution of the copper cation with different ligands imparts a dynamic nature to the crosslinks, thereby enabling dissolution and regeneration of the initial linear polymer. These ligands also strongly influence behavior in the solid-state polymer, increasing ductility with minimal stiffness and strength reduction, and enabling self-healing behavior. The polymer was characterized under monotonic uniaxial tensile loading at different temperatures and strain rates. This experimentally observed mechanical behavior is then considered in the context of topological and mechanochemical elastomer models. The mechanochemical model highlights how modulation of the dynamic cross-link strength within an otherwise linear elastomer can modulate bulk mechanical behavior.

[SY-H6] Symposium H-6

Chair: Alexey Lyulin(Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands)

Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9

[SY-H6] Coarse-Grained Molecular Dynamics Simulation of Filled Rubber under Cyclic Tensile Deformation

○Takashi Kojima, Masataka Koishi （The Yokohama Rubber Co.,Ltd., Japan）

[SY-H6] Modelling of Influence of Fatigue Damage on Oxygen Diffusion in Rubbers

○Jan Heczko, Radek Kottner （NTIS - New Technologies for the Information Society, Faculty of Applied Sciences, University of West Bohemia, Czech Republic）

[SY-H6] On the modeling and calculation of tensile properties of real rubber using molecular dynamics simulation

○Osamu HIno （TOYO TIRE&RUBBER CO.,LTD., Japan）

[SY-H6] A molecular dynamics study of dissolution of covalent adaptable networks in organic solvent

○Yaguang Sun[1], Hua Yang[2], Yafang Guo[1] （1.Dept. of Mechanics, Beijing Jiaotong Univ., China, 2.State Key Lab. for Geomechanics and Deep Underground Engineering, China Univ. of Mining and Tech., China）

[SY-H6] A minimal micromechanical model for the viscoelasticity in biophysical filamentous networks

Arjan E. Boerma[1], Patrick R. Onck[1], ○Erik Van der Giessen[1], Stefanos Papanikolaou[2] （1.Univ. of Groningen, Netherlands, 2.West Virginia Univ., United States of America）

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9)

[SY-H6] Coarse-Grained Molecular Dynamics Simulation of Filled Rubber under Cyclic Tensile Deformation

○Takashi Kojima, Masataka Koishi （The Yokohama Rubber Co.,Ltd., Japan）

Filler morphology, radius, and strength of the filler-polymer interaction impact the physical properties of filled rubber. It is crucial to understand relationships between them so as to improve tire performances. Four large-scale coarse-grained molecular dynamics models were created. The first model is a reference model in which filler particles are distributed in a lattice pattern. The second model is an aggregated model including a non-homogenous filler distribution. The third model is a small particle size model in which small particles are distributed with identical morphology and volume fraction with the reference model. The forth model is a weak interaction model. The polymer-filler interaction is weaker than the reference model, even though the morphology and the particle size match the reference model.

Comparing stress-strain curves, we confirmed that effects of them which are observed in experimental results; filler aggregates, small particles, and strong interaction make modulus and hysteresis greater, were reproduced qualitatively. Measuring a polymer density distribution and a change of polymer chains bridging fillers, it was found that an increase of polymer density around fillers induced by the polymer-filler attractive interaction grows the modulus of the polymer phase and irreversible changes of polymer chains cause hysteresis. We determined that these changes observed in all models are fundamental mechanisms of filled rubber. Comparing the stress-strain curves of the reference model and the aggregated model, we found that the differences are attributed to filler stress. Fillers are to be contacted with another filler particle during deformation and filler stress grows when fillers are aggregated. Comparing the reference model and the weak interaction model, we found that the number and force per a bond of extended chains in the reference model, which are main sources of polymer stress, are greater than the weak interaction model, even though length of the extended chains are much the same. These differences of polymer stress make modulus and hysteresis greater.
Last, a significant increase of the number of extended chains grows polymer stress, when fillers are small and the volume fraction of filler is identical with the reference model. Thus the modulus and hysteresis become greater.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9)

[SY-H6] Modelling of Influence of Fatigue Damage on Oxygen Diffusion in Rubbers

○Jan Heczko, Radek Kottner （NTIS - New Technologies for the Information Society, Faculty of Applied Sciences, University of West Bohemia, Czech Republic）

Rubbers are frequently used in vibration isolation, e.g. as the material for engine mounts or tram wheel suspension segments. These parts are subjected to periodical mechanical loading and to the effects of the environment, such as temperature or chemical reactions. Depending on the nature of the structure changes induced by the environment, physical or chemical ageing may be distinguished (see e.g. [1]). Chemical ageing is governed by the consumption of oxygen, which in turn depends on its transport by diffusion.

Both damage and ageing lead to changes in mechanical properties, each of the phenomena, however, takes

place at a different length scale. This contribution is focused on the influence of fatigue damage on the diffusion of oxygen. The central assumption is that the formation and growth of microcracks influence the paths of the gas molecules, which manifest itself as the coefficient of diffusivity on the macroscopic scale. We present various examples of crack geometries and the resulting oxygen flux and concentration computed by the finite element method (FEM). These results will be further used to derive a phenomenological model of coupled fatigue damage and diffusion-limited oxidation (DLO). This model will be an extension of an existing model [2], in which, however, no explicit relation for the coupling between fatigue damage and diffusivity is considered.

[1] Herzig, A. , Johlitz, M. and Lion, A. Consumption and diffusion of oxygen during the thermoxidative ageing process of elastomers. *Mat.-wiss. u. Werkstofftech*, 47: 376-387, 2016.
[2] Heczko, J., Kottner, R. Modelling of ageing and fatigue under large strains. In *Computational Mechanics - EXTENDED ABSTRACTS*, 2017.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9)

[SY-H6] On the modeling and calculation of tensile properties of real rubber using molecular dynamics simulation

○Osamu HIno （TOYO TIRE&RUBBER CO.,LTD., Japan）

A molecular dynamics approach to calculate general tensile properties of real rubber is developed to alleviate lengthy experimental procedures for the determination of the strain energy function of the rubber material. In this presentation, first, the general framework for the calculation of tensile properties of rubber using molecular dynamics simulation will be illustrated. The overview on the molecular modeling for the real rubber is followed and some pilot calculations are performed to obtain the tensile properties for carbon black filled styrene-butadiene rubbers.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9)

[SY-H6] A molecular dynamics study of dissolution of covalent adaptable networks in organic solvent

○Yaguang Sun[1], Hua Yang[2], Yafang Guo[1] （1.Dept. of Mechanics, Beijing Jiaotong Univ., China, 2.State Key Lab. for Geomechanics and Deep Underground Engineering, China Univ. of Mining and Tech., China）

Thermosets have outstanding mechanical strength and solvent resistance due to their permanently cross-linked networks. They cannot flow upon heating and cannot be reshaped and recycled. The recently developed reversible networks provide opportunities to recycle thermoset polymers. For example, the covalent adaptable networks (CANs; also known as vitrimers) can rearrange their network topology through reversible bond exchange reactions (BERs). It was recently reported that CANs can be dissolved in solvents. At high temperature, small solvent molecules can break long polymer chains into short segments via BERs. In this study, molecular dynamics simulations are used to investigate the dissolution of an epoxy CAN in alcohol solvents due to the transesterification type BER. The diffusion of solvent molecules and the decomposition of epoxy networks are analyzed. It is found that the dissolution proceeds in a surface erosion mode, which is consistent with experimental observations.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9)

[SY-H6] A minimal micromechanical model for the viscoelasticity in biophysical filamentous networks

Arjan E. Boerma[1], Patrick R. Onck[1], $^{\bigcirc}$Erik Van der Giessen[1], Stefanos Papanikolaou[2]　(1.Univ. of Groningen, Netherlands, 2.West Virginia Univ., United States of America)

The static elastic behaviour of biophysical networks comprising cross-linked semi-flexible filaments is well characterised due to extensive theoretical, computational and experimental studies of in-vitro materials. The dynamic response of these networks, however, still holds several mysteries, including the peculiar variation of the loss modulus with frequency, $G''(\omega)$. For example, entropic effects can explain the increase of G'' with frequency at high frequencies, but not the minimum in $G''(\omega)$ at intermediate frequencies. The latter feature has been suggested to be governed by the cross-linker dynamics, but the experimental trends are yet to be predicted by theory in a phenomenologically consistent manner. Here, we present a minimal micromechanical description, consisting of two semi-flexible filaments coupled by cross-linkers, whose dynamics is described through a Grand Canonical Monte Carlo scheme.

[SY-B1] Symposium B-1

Chair: Lorenzo Malerba(CIEMAT, Energy, Environment and Technology Research Centre, Spain)
Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10

[SY-B1] Thermal stability of carbon-vacancy complexes in iron alloys and steels
　　　　○Milan J Konstantinovic, Lorenzo Malerba （Belgian nuclear institute, SCK.CEN, Belgium）

[SY-B1] Computational study of phosphorous migration to grain-boundary in alpha-iron
　　　　○Ken-ichi Ebihara, Tomoaki Suzudo （Center for Computational Science &e-Systems, Japan Atomic Energy Agency, Japan）

[SY-B1] **Properties of interstitials in concentrated Fe-Cr alloys from first principles**
　　　　○Marcin Roland Zemla[1], Jan Stanislaw Wrobel[1], Marek Muzyk[1], Tomasz Wejrzanowski[1], Duc Nguyen-Manh[2], Sergei L. Dudarev[2], Luca Messina[3], Par Olsson[3], Christophe Domain[4] （1.Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland, 2.CCFE, Culham Centre for Fusion Energy, Abingdon, Oxon OX14 3DB, UK, 3.KTH Royal Institute of Technology, Nuclear Engineering, 106 91 Stockholm, Sweden, 4.Dé partement Matériaux et Mécanique des Composants, EDF-R&D, Les Renardières, F-77250 Moret sur Loing, France）

[SY-B1] **Defect production in cascade overlap with defect clusters in iron and tungsten**
　　　　○Jesper Byggmastar[1], Fredric Granberg[1], Andrea E Sand[1], Kai Nordlund[1] （1. Department of Physics, University of Helsinki, Finland）

[SY-B1] Multiscale modelling of radiation damage evolution in Fe and Fe-based alloys
　　　　○Fredric Granberg[1], Haixuan Xu[2], Kai Nordlund[1] （1.Department of Physics, University of Helsinki, Finland, 2.Department of Materials Science and Engineering, University of Tennessee, United States of America）

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10)

[SY-B1] Thermal stability of carbon-vacancy complexes in iron alloys and steels

○Milan J Konstantinovic, Lorenzo Malerba （Belgian nuclear institute, SCK.CEN, Belgium）

Many industrially important alloys and steels are intentionally processed and explored, as metastable microstructures comprising a supersaturation of crystal defects in various forms of aggregation. Even though it is well understood that this microstructural complexity governs the material performance, the defects composition, thermal stability, how they are distributed and in which concentrations are not yet resolved experimentally. Hardened ferritic steels are important example where the lattice defects play deterministic role in their deformation behavior..

While it is long-known that carbon atoms dispersed in the matrix of iron and steels have an influence on the type of defects produced, it is only recently that atomistic simulations have clearly and quantitatively revealed that carbon atoms bind very strongly to vacancies, giving rise to the formation of a whole fauna of carbon-vacancy (mCnV) complexes. These complexes may act as traps for other defects, which suggests that hardening in iron and its alloys will be the consequence of the interaction of dislocations with complex defects formed by not only point defects but also carbon atoms. In this context, the formation of mCnV clusters is the triggering mechanisms for the growth of other complex defects.
In this study, the focus is given on the examination of relaxation processes which occur in the internal friction spectra of a variety of iron alloys and steels with different carbon concentrations, and out-of-equilibrium vacancy concentrations, achieved either by fast cooling (quenching) or plastic deformation. The relaxation peaks are analyzed on the basis of the Debye relaxation model and their activation energies and integrated intensities are determined. By comparing the results with theoretical calculation, positron annihilation spectroscopy results, and magnetic after effect measurements, the observed relaxation processes are assigned to the dissolution of carbon-vacancy (mCnV) clusters [1]. Dissolution energies and relaxation strengths (concentrations) of various mCnV clusters are found to be in the correct energy range according to density functional calculations.

[1] M. J. Konstantinović and L. Malerba, Phys. Rev. Mat. **1,** 053602 (2017).

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10)

[SY-B1] Computational study of phosphorous migration to grain-boundary in alpha-iron

○Ken-ichi Ebihara, Tomoaki Suzudo （Center for Computational Science &e-Systems, Japan Atomic Energy Agency, Japan）

Phosphorus(P) causes Grain-boundary(GB) embrittlement that is considered as one factor of ductile-brittle transition in reactor pressure vessel steels. While the prediction of GB P segregation is desired, the detailed process of P segregation to GB is still unclear. We studied the process of P segregation to GB by simulating the migration of a mixed interstitial dumbbell, an octahedral interstitial P atom and a P-vacancy complex using a molecular dynamics method. As a result, it was found that the P atom of them becomes a substitutional atom before they reach the GB. The self-interstitial atom (SIA) or vacancy of them was absorbed by the GB. This phenomenon was also confirmed partially by first-principles calculations. In

addition, it was found that the P atom left behind approaches the GB by successively interacting with an SIA or a vacancy coming to its nearest neighbor site. We think that the conventional understanding of GB P segregation should be revised.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10)

[SY-B1] Properties of interstitials in concentrated Fe-Cr alloys from first principles

○Marcin Roland Zemla[1], Jan Stanislaw Wrobel[1], Marek Muzyk[1], Tomasz Wejrzanowski[1], Duc Nguyen-Manh[2], Sergei L. Dudarev[2], Luca Messina[3], Par Olsson[3], Christophe Domain[4] （1.Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland, 2.CCFE, Culham Centre for Fusion Energy, Abingdon, Oxon OX14 3DB, UK, 3.KTH Royal Institute of Technology, Nuclear Engineering, 106 91 Stockholm, Sweden, 4.Département Matériaux et Mécanique des Composants, EDF-R&D, Les Renardières, F-77250 Moret sur Loing, France）

Point defects, for example self-interstitials and vacancies, play an important part in controlling properties of materials and their kinetic evolution. As a consequence, proper understanding and modelling of materials properties require precise knowledge of point defect behaviour and their characteristics, in particular their formation and migration energies. In magnetic alloys such as FeCr, the investigation of point defects is complicated, because their properties strongly depend on various parameters such as Cr composition, alloy short-range ordering and the defect local environment [1-3].

In this work, we have investigated properties of dumbbell-type defects in FeCr with a large dataset of density functional theory calculations, for Cr concentrations ranging from low to approx. 35%. Analysis shows that properties of self-interstitial and interstitial (IA) defects in concentrated bcc FeCr alloys fluctuate significantly as functions of the above parameters. These fluctuations are observed to a lesser or greater extent for the lattice parameter, chemical potentials, bulk moduli, relaxation volumes, magnetic moments, and migration energies of dumbbells. We conclude that the formation energy of dumbbells depends on the Cr content and also on the number of Cr atoms in the local environment of a defect. For each chemical composition the average migration energies of Cr IA defects (Cr-Cr, Cr-Fe dumbbells) moving to the first nearest-neighbour (1NN) position, are significantly smaller than those of Fe-Fe exchanging with the 1NN Fe atom. The relaxation volumes of dumbbells increase in the ordered structure and decrease in the disordered one with the increase of number of Cr atoms in the local environment of a defect. The trends exhibited by the mean values of the various properties have been observed and analysed, and the most stable directions of Fe-Fe, Fe-Cr and Cr-Cr dumbbells have been determined. Moreover, the energy of elastic interaction between such defects are quantitatively estimated using the suitably parametrized dipole tensors of the defects.

[1] D. Costa, G. Adjanor, C.S. Becquart, et al., J. Nucl. Mater. 452 (2014) 425-433

[2] D. Nguyen-Manh, M.Y. Lavrentiev, S.L. Dudarev, C. R. Physique 9 (2008) 379-388

[3] D. Nguyen-Manh, M.Y. Lavrentiev, M. Muzyk et al., J Mater Sci (2012) 47: 7385

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10)

[SY-B1] Defect production in cascade overlap with defect clusters in iron and tungsten

○Jesper Byggmastar[1], Fredric Granberg[1], Andrea E Sand[1], Kai Nordlund[1] （1. Department of Physics, University of Helsinki, Finland）

During the lifetime of a typical reactor, the radiation damage in the wall materials will reach high damage doses. Collision cascades initiated by subsequent irradiation will therefore become increasingly likely to overlap with pre-existing atomistic damage, such as dislocation loops, voids, and other defect structures. We have therefore carried out a large number of molecular dynamics simulations using well-established interatomic potentials, to build a database for the defect production in collision cascades overlapping with pre-existing defect clusters in both iron and tungsten. We primarily study cascades overlapping with dislocation loops of different size. Cascade overlap on other defect clusters leads to similar results. We find that cascades overlapping with pre-existing interstitial clusters result in a significant reduction in the number of new point defects. The overlap effect on vacancy clusters is weaker. By running cascades on different-sized clusters, with different cascade energies and at different temperatures, we obtain a database that can be used to fit a simple analytical model for the defect production bias due to the overlap effects. The data and the fitted analytical model can be transferred to larger-scale simulation methods, such as Monte Carlo techniques, to model the radiation damage accumulation at longer length and time scales.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10)

[SY-B1] Multiscale modelling of radiation damage evolution in Fe and Fe-based alloys

○Fredric Granberg[1], Haixuan Xu[2], Kai Nordlund[1] （1.Department of Physics, University of Helsinki, Finland, 2.Department of Materials Science and Engineering, University of Tennessee, United States of America）

In order to predict the behaviour of materials used in places where radiation is present, many aspects must be considered. The macroscopic effects like swelling and cracking, are a product of defect evolution starting at atomistic level. The energetic ion will, on the atomic level, transmit energy to lattice atoms, which will start collision cascades in the material. To be able to predict what the irradiation will do to the material, we must start on this level. The problem arises from that there is no single method that can accurately simulate everything from single atoms or electrons up to macroscopic parts that builds up the construction. To tackle this problem, a combination of two or more methods can be used consecutively, to be able to extend the time and/or length scale of the simulation. In this study, we focus on extending the time scale, to be able to predict the evolution of irradiation induced defects.

To study the irradiation effect in Fe and Fe-based alloys we utilize Molecular Dynamics (MD), to simulate the primary damage production on an atomistic level. The simulations are carried out by giving a recoil energy to a random atom in the simulation box. These simulations are very accurate to study the movement of all atoms, but are limited to nanoscale simulation boxes and times on the pico- or nanosecond time scale. The length scale is sufficient to accurately simulate the defect production, however the time scale is not sufficient for a long term evolution of the system. This long term evolution is needed to obtain comparable results with experiments and to compare with materials in use in these kinds of environments. To remedy the time scale problem, we utilize Kinetic Monte Carlo (KMC), to obtain longer time scales. A special version of KMC, Self-Evolving Atomistic KMC (SEAKMC), is used as no predefined and pre-calculated barriers are needed. This on-

the-fly method is perfect for cases where the defects produced can have many different complicated structures. In these cases, it would be impossible to predict their structure beforehand and calculate all the barriers. A combination of MD and SEAKMC is used to both accurately predict the produced primary damage (with MD) as well as its evolution (with SEAKMC), before a second cascade will hit the same region, as in experimental cases where intensive irradiation is present.

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B2] Symposium B-2

Chair: Davide Pizzocri(Politecnico di Milano, Italy)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room10

[SY-B2] Atomic scale calculations of nuclear fuel properties to sustain multiscale modeling of fuel behavior

○Emeric Bourasseau, Marjorie Bertolus, Michel Freyss, Gérald Jomard, Ibrahim Cheik Njifon, Martin-Stéphane Talla Noutack, Cyrille Takoukam Takoundjou （CEA/DEN/DEC, Centre CEA de Cadarache, France）

[SY-B2] Influence of vibrational entropy on the concentrations of uranium vacancies in UO_2

○Jean-Paul Crocombette[1], Fabien Bruneval[1], Aurélien Soulié[1], Mihai-Cosmin Marinica[1], Samuel Murphy[2] （1.CEA Saclay, France, 2.Lancaster University, UK）

[SY-B2] **Modelling of defect and rare gas transport properties in UO_2 from the atomic to the grain scale**

○Marjorie Bertolus, Michel Freyss, Emerson Vathonne, Emeric Bourasseau, Serge Maillard, Gérald Jomard （CEA, DEN, Département d'Etude des Combustibles, Centre de Cadarache, 13108 Saint-Paul-lez-Durance, France）

[SY-B2] **Intragranular bubble impact on nuclear fuel thermomechanical properties**

Fabienne Ribeiro[1], Mehdi Colbert[1], ○Jack Arayro[1], Guy Tréglia[2] （1.Institut de Radioprotection et de Sûreté Nucléaire/PSN-RES/SEMIA/LPTM, France, France, 2.Centre Interdisciplinaire de Nanoscience de Marseille, CNRS, France, France）

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room10)

[SY-B2] Atomic scale calculations of nuclear fuel properties to sustain multiscale modeling of fuel behavior

Invited

○Emeric Bourasseau, Marjorie Bertolus, Michel Freyss, Gérald Jomard, Ibrahim Cheik Njifon, Martin-Stéphane Talla Noutack, Cyrille Takoukam Takoundjou （CEA/DEN/DEC, Centre CEA de Cadarache, France）

Until recently, simulations of the fuel behavior during normal or accidental operation in nuclear reactor were based on rather empirical laws built from numerous experimental observations. Nowadays, simulation codes try to render the underlying physics, and are used to understand the measurements performed during irradiations or post-irradiation experiments. Thus, the fuel modelling and the laws used to predict its behavior must be improved by fundamental researches and feed by results from separate effects experiments. In support to these experiments, multi-scale modelling is an important tool, which aim is to understand the phenomena occurring at the microscopic scale to improve the modelling of the material at the macroscopic scale.

In this presentation, we will show our recent works concerning atomic scale simulations used to improve the knowledge of nuclear fuel properties before and during irradiation. Three points will be emphasized. First, we will present ab initio calculations of point defects in MOX fuels, and how they can be used to determine the elementary mechanisms of atomic diffusion in the irradiated fuel. Then, we will show a study of the energetic and structural properties of grain boundaries in UO_2 using classical molecular dynamics. In particular, an interesting correlation observed between cleavage energy and disorientation angle will be shown. And finally, we will present the results of the determination of thermodynamic properties of $(U,Pu)O_2$ through molecular Monte Carlo method. This method appears to be particularly relevant to explore the various cationic configurations available in mixed oxide.

For each examples, we will try to underline the link with experimental works, and to show how our results are included in simulations at higher scales.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room10)

[SY-B2] Influence of vibrational entropy on the concentrations of uranium vacancies in UO_2

○Jean-Paul Crocombette[1], Fabien Bruneval[1], Aurélien Soulié[1], Mihai-Cosmin Marinica[1], Samuel Murphy[2] （1.CEA Saclay, France, 2.Lancaster University, UK）

The wide deviations of the composition of UO_2 around its nominal composition are accommodated by point defects or clusters of oxygen interstitials. The formation energies of these defects have been the subject of many studies DFT calculations. In the high temperature understoichiometric regime, atomistic calculations and experiment agree on the fact that oxygen vacancies are the dominant defect. At the opposite for the overstoichiometric material the formation energies predict uranium vacancies to dominate over oxygen interstitials. This contradicts experimental facts which show that oxygen interstitials, either isolated or clustered are accommodating the overstoichiometry in UO_{2+x}. This so-called "uranium vacancy problem" has been noticed for many years [1] and has resisted the various calculations improvements, either methodological (e.g. use of DFT+U) or numerical (e.g. calculations made on bigger boxes).

Considering the vibrational entropy of the defects enables to solve this problem. We have combined ab initio formation energies of point defects and oxygen clusters in UO_2 [2] with harmonic entropies calculated with a many body empirical potential with charge equilibration [3]. Including the vibrational contribution to the free energy of defects de-stabilizes the uranium vacancies compared to the oxygen defects. The latter are then predicted to be dominant at high temperatures or large overstoichiometry in agreement with experiments. However our calculations exhibit a composition and temperature domain where uranium vacancies may in fact be the majority defect in UO_{2+x}. Some experimental observations (dilatometry, positron annihilation spectroscopy and uranium diffusion measurements) tend to confirm this prediction.

[1] J.P. Crocombette, *et al.*, Phys. Rev. B **64**, 104107 (2001).
[2] F. Bruneval, *et al.*, Phys. Rev. Materials **2**, 023801 (2018).
[3] A. Soulié, *et al.*, Acta Mater. **150**, 248 (2018).

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room10)

[SY-B2] Modelling of defect and rare gas transport properties in UO_2 from the atomic to the grain scale

○Marjorie Bertolus, Michel Freyss, Emerson Vathonne, Emeric Bourasseau, Serge Maillard, Gérald Jomard （CEA, DEN, Département d'Etude des Combustibles, Centre de Cadarache, 13108 Saint-Paul-lez-Durance, France）

One of the challenges for the next generation of nuclear reactors is to increase significantly the efficiency in designing and qualifying innovative fuels. One way of doing this is to develop a more physically-based description of nuclear fuels to enhance the predictive capability of fuel behaviour simulation. This should enable a better selection of promising fuel systems and a reduction of the effort necessary for the design of new fuels. Basic research approaches combining multiscale modelling and separate effect experiments can bring significant insight into key phenomena involved in the evolution of nuclear fuels during their reactor life.

We will describe the multiscale modelling approach developed from the atomic to the mesoscopic scale to investigate the transport properties of defects and rare gases in nuclear fuels. We will show examples of the results obtained at atomic scale on uranium dioxide concerning the data necessary for the mesoscale models and for the interpretation of separate experiments on fuels. We will also present the application of mesoscale models, in particular cluster dynamics.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room10)

[SY-B2] Intragranular bubble impact on nuclear fuel thermomechanical properties

Fabienne Ribeiro[1], Mehdi Colbert[1], ○Jack Arayro[1], Guy Tréglia[2] （1.Institut de Radioprotection et de Sûreté Nucléaire/PSN-RES/SEMIA/LPTM, France, France, 2.Centre Interdisciplinaire de Nanoscience de Marseille, CNRS, France, France）

UO2 is used as a standard fuel in pressurized water reactors. During fission reactions bubbles of xenon are generated. The presence of these bubbles modifies the thermo-mechanical properties of the fuel. The need to characterize these effects led to an extensive work both from experimental and theoretical points of view. Our contribution belongs to the later type.

First, the variation of the thermomechanical properties of UO2 versus porosity is studied through atomistic simulations with semi-empirical potentials. A good agreement is found between the elastic properties calculated in the present simulations, and those coming from micro-mechanical modelling and experimental ones. Concerning thermal properties, an analytical model taking into account the nanoporosities is derived. This study emphasizes the importance of bubble surface effects of intragranular bubbles on the thermomechanical behavior of the matrix.

Second, to clarify this effect, we study simplified systems of xenon on UO2 surfaces. We first determine the surface relative stability according to their orientations and then to their polarities, by combining thermostatistical relaxation and analytic formulations within a simple electrostatic model. The main result is that, whereas the (111) surface appears stable with only minor reorganization, the polar (100) one is only stabilized through drastic rearrangement of the surface region. Xenon adsorption on these relaxed surfaces is then realized through Grand Canonical Monte Carlo simulation.

Finally, the pressure inside the Xenon and in the UO2 matrix is investigated. For the Xenon, we show that whatever its cristallographic structure, the pressure increases with the density, but not with the temperature for a fixed density. In the latter case, we present stress profiles through the UO2 matrix before and after xenon adsorption. The next step will be to introduce these results in a micromechanical model in order to derive a thermomechanical behavior law for the porous UO2.

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B3] Symposium B-3

Chair: Kazuto Arakawa(Shimane University, Japan)
Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10

[SY-B3] Formation of radiation-induced Re and Os precipitation in W and its effects on mechanical properties

○Guang-Hong Lu, Yu-Hao Li, Hong-Bo Zhou （Beihang University, China）

[SY-B3] Elastic fields and interaction between self-interstitial atom defects in bcc metals.

○Sergei L Dudarev, Pui-Wai Ma （UK Atomic Energy Authority, UK）

[SY-B3] Molecular dynamics simulation study of the interaction of Re with interstitial defects in tungsten bulk

Yangchun Chen[1], Jingzhong Fang[1], Ning Gao[2], Hong-Bo Zhou[3], Wangyu Hu[4], Fei Gao[4,5], ○Huiqiu Deng[1,4] （1.School of Physics and Electronics, Hunan University, China, 2.Institute of Modern Physics, Chinese Academy of Sciences, China, 3.Department of Physics, Beihang University, China, 4.College of Materials Science and Engineering, Hunan University, China, 5.Department of Nuclear Engineering and Radiological Science, University of Michigan, United States of America）

[SY-B3] Hydrogen super-saturated layers in plasma loaded tungsten: a global model combining Density Functional Theory data, Thermodynamic and Kinetic models

○Yves Ferro, Etienne Hodille （Aix-Marseille University, France）

[SY-B3] Mobility of small vacancy and interstitial prismatic dislocation loops in BCC tungsten

○Jan Fikar[1], Roman Gröger[1], Robin Schäublin[2] （1.Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic, Switzerland, 2.Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, Switzerland）

(Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10)

[SY-B3] Formation of radiation-induced Re and Os precipitation in W and its effects on mechanical properties

Invited

○Guang-Hong Lu, Yu-Hao Li, Hong-Bo Zhou （Beihang University, China）

Tungsten (W) is one of the most promising candidates for plasma facing materials in future fusion reactors. Rhenium (Re) and Osmium (Os) are not only the typical alloying elements but also the main productions of transmutation in W. More importantly, Re and Os will aggregate and precipitate under high energy radiation, which substantially enhance the radiation hardening and embrittlement, leading to the great concerns for the life-limiting of W. So far, the formation mechanism of Re/Os-rich clusters in W as well as its influences on the mechanical properties remains to be fully elucidated.

We have investigated the interaction between Re/Os and defects in W using a first-principles method in combination with thermodynamic models in order to explore the precipitating mechanism of Re/Os under irradiation. It is found that the presence of defects can significantly reduce the total nucleation free energy change of Re/Os, and thus facilitate the nucleation of Re/Os in W. Kinetically, self-interstitial atom is shown to be easily trapped by substitutional Re/Os, and form W-Re/Os mixed dumbbell. Such W-Re/Os dumbbell combining with the substitutional Re/Os atom will transfer to high stable Re/Os-Re/Os dumbbell, which can serve as a trapping centre for subsequent W-Re/Os dumbbells, leading to the growth of Re/Os-rich clusters. Consequently, an interstitial-mediated migration and aggregation mechanism for Re and Os precipitation has been proposed.

To shed light on the effects of transmutation elements on the mechanical properties, we further have investigated the influences of Re on the motion of 1/2 screw dislocation in W. It is found that the influence of Re on the dislocation motion is directly related to the distribution of Re in W. For the state of Re dispersed distribution, the addition of Re will reduce the generalized stacking fault energy (GSFE) for both 1/2{112} and 1/2{110}, and improve the ductility. However, the influence of Re clusters (for the state of Re aggregation) on the dislocation motion is significantly different from that of dispersed Re. The presence of Re clusters will substantially increase the Peierls stress and energy, inhibiting the dislocation mobility. This will significantly exacerbate the irradiation hardening, and thus degrade the mechanical properties of W.

(Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10)

[SY-B3] Elastic fields and interaction between self-interstitial atom defects in bcc metals.

○Sergei L Dudarev, Pui-Wai Ma （UK Atomic Energy Authority, UK）

Strongly anisotropic self-interstitial defect configurations form spontaneously in body-centred cubic metals, like sodium or tungsten, if an extra atom is inserted in the crystal lattice and the resulting structure is relaxed into the lowest energy configuration. The equilibrium structure and modes of Brownian motion of individual SIA defects in body-centred transition metals are now well established. Yet, there is still no regular approach to modelling evolution of ensembles of such defects that would include the treatment of elastic interaction between them. The difficulty appears fundamental, illustrating the lack of a suitable mathematical formalism, linking the discrete atomistic representation of nano-scale defects with continuum elasticity. We derive an analytical expression for the dipole tensor of a dislocation loop, valid in the isotropic and anisotropic

elasticity approximations, and explore it in the limit of infinitely small loop size. We discover that the prediction for the dipole tensor of a point defect that does not agree with numerical calculations even for defects in tungsten, a material that is well described by isotropic elasticity theory. We then derive an analytical formula for the dipole tensor of a defect using a two-parameter tensor form, which shows that in addition to a pure prismatic dislocation loop character, the elastic field of a SIA defect contains a significant dilatation component. We evaluate the energy of interaction between SIA defects, and between a SIA defect and a dilatation centre, e.g. a vacancy cluster. To illustrate applications of the new formalism, we compute the energy of interaction between SIA defects ordered as a periodic simple cubic super-lattice, encountered in a DFT calculation. Surprisingly, we find that the energy minimum of such a periodic configuration corresponds to the orientation of the directional unit vector of the defect collinear with a 111 direction.

(Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10)

[SY-B3] Molecular dynamics simulation study of the interaction of Re with interstitial defects in tungsten bulk

Yangchun Chen[1], Jingzhong Fang[1], Ning Gao[2], Hong-Bo Zhou[3], Wangyu Hu[4], Fei Gao[4,5], ○Huiqiu Deng[1,4]
 （1.School of Physics and Electronics, Hunan University, China, 2.Institute of Modern Physics, Chinese Academy of Sciences, China, 3.Department of Physics, Beihang University, China, 4.College of Materials Science and Engineering, Hunan University, China, 5.Department of Nuclear Engineering and Radiological Science, University of Michigan, United States of America）

Tungsten (W) and W-based alloys have been considered as promising candidates for plasma-facing materials (PFMs) in future fusion reactors. However, the neutrons generated in fusion reactions result in not only the cascade damage but also the transmutation products (mainly Re and Os) in W bulk. The irradiation defects and transmutation products will have a serious effect on the service behaviors of W PFMs under the condition of fusion irradiation. With molecular dynamics simulations and W-Re potentials developed recently in our group, we have systematically investigated the interaction between Re atom/cluster and interstitial defects in W bulk. It is found that: (1) the self-interstitial atoms (SIAs) and interstitial Re atoms are energetically favorable to align along <111> direction in the form of W-W and Re-W dumbbell/crowdion, respectively; (2) the SIA clusters and 1/2<111> interstitial dislocation loops can undergo fast migration along <111> direction and their migration barriers (< 0.1 eV) are nearly independent of defect size; (3) Re atoms inhibit the migration and growth of SIA clusters, due to their strong attractions; (4) newly formed Re-Re dumbbells and Re-W mixed dumbbell clusters are thermally stable and immobile, which can serve as the trapping center for subsequent Re-W mixed dumbbell, leading to the growth of Re clusters in W. The present work is helpful for understanding the interaction of Re with interstitial defects and dislocation loops and the initial nucleation mechanism of Re atoms in bulk W, and the results can also be used to supply more accurate inputs for larger-scale simulations such as object kinetic Monte Carlo simulations.

(Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10)

[SY-B3] Hydrogen super-saturated layers in plasma loaded tungsten: a global model combining Density Functional Theory data, Thermodynamic and Kinetic models

○Yves Ferro, Etienne Hodille （Aix-Marseille University, France）

In this work, we combined Density Functional Theory data, a Thermodynamic and a kinetic model to build a global model enabling to determine the total concentration of hydrogen implanted in the sub-surface of tungsten exposed to a hydrogen flux. This is achieved given a flux of hydrogen, a temperature of implantation, and the energy of the incoming hydrogen ions. This model is built step by step; an equilibrium with a molecular hydrogen gas phase is first considered and the resulting solubility is compared with experimental results. A kinetic model is subsequently used to determine a chemical potential for hydrogen in the sub-surface of tungsten. Combining both these models, two regimes are then established in which hydrogen is trapped at interstitial sites or in vacancies. The existence of these two regimes are driven by the temperature of implantation; above a temperature of implantation is the *interstitial* regime, below is the *vacancy* regime in which super-saturated layers are formed. A simple analytical and easy to use expression is work-out for the transition temperature, which allows to plot a diagram of existence of the super-saturated layer depending on the implantation temperature, the incident energy and the flux of the hydrogen ions.

(Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10)

[SY-B3] Mobility of small vacancy and interstitial prismatic dislocation loops in BCC tungsten

○Jan Fikar[1], Roman Gröger[1], Robin Schäublin[2] （1.Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic, Switzerland, 2.Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, Switzerland）

Vacancies and self interstitials produced in collision cascades often form clusters, which can further collapse into prismatic dislocation loops. In BCC metals dislocation loops with Burgers vectors 1/2 and are observed and they can be either vacancy or interstitial type. These dislocation loops usually move easily in the direction of the Burgers vector. The mobility of prismatic dislocation loops is studied by molecular dynamics. The small dislocation loops under 100 defects seem to behave more like point defect clusters and the mobility of vacancy loops is substantially lower than the one of interstitial loops. Similar effect is observed in formation energies, where the small vacancy loops have higher formation energies than the corresponding interstitial loops. At larger sizes the dislocation loops seem to behave as perfect dislocations and there is no difference between vacancy and interstitials loops mobilities and formation energies.

[SY-B4] Symposium B-4

Chair: Gary S Was(University of Michigan, United States of America)

Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room10

[SY-B4] **Kinetics of Precipitation in Fe-Cr and Fe-Cr-C alloys under Irradiation**

○Frederic Soisson （CEA Saclay, France）

[SY-B4] **The complex problem of the experimental validation of atomistic and microstructural evolution models**

○Lorenzo Malerba （CIEMAT, Energy, Environment and Technology Research Centre, Spain）

[SY-B4] Physically based prediction of radiation hardening: application to steels and model alloys

○Ghiath Monnet （EDF - R&D, MMC, France）

[SY-B4] **Oxygen diffusion in bcc Fe under the influence of foreign atoms and vacancies**

○Xiaoshuang Wang, Matthias Posselt, Jürgen Faßbender （Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany）

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room10)

[SY-B4] Kinetics of Precipitation in Fe-Cr and Fe-Cr-C alloys under Irradiation

Invited
○Frederic Soisson （CEA Saclay, France）

In ferritic steels, the precipitation of the Cr-rich α' phase leads to a degradation of mechanical properties. Below 400°C, the precipitation is usually too slow to be a real concern, but it can be significantly accelerated by irradiation, due to an increase in point defect concentrations. Irradiation also produces a ballistic mixing between Fe and Cr atoms, and therefore prevent the nucleation of α' precipitates or the dissolution of existing ones.

We present a multiscale approach which models these contradictory effects by taking into account the different mechanisms of atomic transport taking place under irradiation: the creation of vacancies and self-interstitials and the ballistic mixing within displacement cascades, the thermally activated diffusion of point defects, and their elimination at sinks or by mutual recombination. The method combines DFT calculations (which provide the fundamental information on thermodynamics and point defects properties), atomistic Kinetic Monte Carlo Simulations (to model the diffusion of point defects and the α' precipitation), and Cluster Dynamics (to model the evolution of the sink density under irradiation). The simulations show that the acceleration of the α' precipitation occurs under irradiation at low or moderate dose rates, but that ballistic dissolution becomes dominant under ion irradiation at high dose rates -- due to a large density of sinks that limits the point defect supersaturation.

The results of the simulations are compared with recent experimental studies. The same multiscale approach is used to model the diffusion of carbon atoms in Fe-Cr alloys and their strong interaction with point defects. We will consider their possible effect on Fe and Cr diffusion, and on the kinetics of α' precipitation under irradiation.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room10)

[SY-B4] The complex problem of the experimental validation of atomistic and microstructural evolution models

○Lorenzo Malerba （ CIEMAT, Energy, Environment and Technology Research Centre, Spain）

The development of physical models for the description of the behaviour of materials under certain conditions goes hands-in-hands with the use of advanced experimental characterization techniques. The experiments provide data and reveal phenomena that the models are expected to predict and explain. The exchange of information between models and experiments is therefore continuous and goes in two directions: models may predict results that need to be verified experimentally and experiments observe processes that the models are expected to reproduce and explain in terms of physical laws and mechanisms. This continuous interplay is often denoted as "experimental validation" of models. While this definition is somewhat restrictive, the validation of models is a discipline in itself that requires first of all the performance of experiments that may be long and expensive, and need to be carefully designed. In addition, the comparison between the results of the models, in particular computer simulations, and the observations from characterization techniques is not always straightforward, because both the experimental and the simulation

outcomes need to be properly treated.

In this presentation these problems will be discussed taking the example of the comparison between models that describe the microstructural evolution of iron alloys under irradiation and the results of microstructural characterization techniques such as positron annihilation, small angle neutron scattering, atom probe and transmission electron microscopy.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room10)

[SY-B4] Physically based prediction of radiation hardening: application to steels and model alloys

○Ghiath Monnet （EDF - R&D, MMC, France）

Based on a multiscale modeling framework, it is shown that radiation hardening can be rationalized in several industrial materials and model alloys. Microstructure features of the as-received materials are first considered for the assessment of the yield stress prior to irradiation. The later can be decomposed into two contributions: short-range stresses induced by local obstacles (such as forest dislocations, precipitates, etc.) and long-range stresses resulting from sub-grain dislocation walls and grain boundaries. Introducing radiation defects as local obstacles, the same methodology can be employed to predict the yield stress of the irradiated materials. The considered radiation defects are solute clusters (SCs) and Dislocations Loops (DLs). SCs are assumed to be spherical coherent precipitates that can be sheared by dislocations with a given shear resistance, computed from atomistic simulations. This resistance is used in Dislocations Dynamics (DD) simulations to compute hardening induced by SCs. The sizes and densities implemented in DD simulations are those given by experiment (TEM, APT, SANS etc.). The contribution of DLs is computed from DD simulations. Upon interaction with mobile dislocations, small DLs are absorbed leading to strong pinning and high hardening level, while large DLs experience classical dislocation-dislocation interactions (junction, annihilation, etc.). The yield stress of the irradiated materials is predicted using the constitutive equations of radiation hardening induced by SCs and DLs.

Several FeCr, FeMnNi model alloys and some RPV steels are considered for the validation of the model. It is shown that local obstacles (present before irradiation) may have a significant effect on radiation effects on the mechanical properties: radiation hardening is not independent of the initial yield stress. With almost no adjustable parameters, the predicted increase in the yield stress is found in close agreement with experiment.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room10)

[SY-B4] Oxygen diffusion in bcc Fe under the influence of foreign atoms and vacancies

○Xiaoshuang Wang, Matthias Posselt, Jürgen Faßbender （Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany）

A multiscale approach including Density Functional Theory (DFT) and Atomistic Kinetic Monte Carlo (AKMC) simulations is applied to investigate the diffusion of oxygen in bcc Fe under the influence of substitutional

foreign atoms or solutes (Al, Si, P, S, Ti, Cr, Mn, Ni, Y, Mo, W) and vacancies. The solutes can be assumed to be immobile since their diffusion coefficient is much smaller than that of oxygen. On the other hand, the vacancy mobility must be considered in the calculations because it is comparable to that of oxygen. The most stable state of oxygen in pure bcc Fe is the octahedral interstitial configuration. Recently, jumps of oxygen in pure bcc Fe, between first-, second-, and third-neighbor octahedral interstitial sites were investigated by DFT. It was found that the first-neighbor jump is most relevant. The second-neighbor jump consists of two consecutive first-neighbor jumps whereas the barrier of the third-neighbor jump is too high to be significant for the diffusion process. In this work DFT is used to determine the modified migration barriers in the presence of solutes. It is found that Si, P, Ni, Mo and W have some effect on the migration barriers of oxygen and their interaction with O is mainly repulsive. Al, Cr and Mn have a significant influence on the barriers and they exhibit strong attractive interactions with O. The most important modification of the barriers is found for S, Ti, and Y where deep attractive states exist. The barriers for oxygen jumps near a vacancy and barriers for vacancy jumps in the environment of oxygen are also calculated by DFT. Based on the migration barriers obtained by DFT, AKMC simulations on a rigid lattice are employed to determine the diffusion coefficient of oxygen in a dilute iron alloy containing different substitutional foreign atoms. It is found that Si, P, Ni, Mo, and W have almost no influence on the diffusivity of O. The presence of Al, Cr, Mn, S, Ti, and Y causes a significant reduction of the mobility of oxygen. Another version of the AKMC code is applied to investigate the mutual influence of oxygen and vacancy diffusion as well as the migration of the oxygen-vacancy pair.

[PO-A2] Poster Session 2

Symposium A
Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-01] Multiscale model of solid state amorphization during processing of pharmaceutical materials

Chunyu Li[1], Yifei Zeng[1], Lorena Alzate-Vargas[1], Pilsun Yoo[1], Rachel Frocino[2], Jeff Brum[2], Peilin Liao[1], Marisol Koslowski[1], ○Alejandro Strachan[1]　(1.Purdue University, United States of America, 2.GlaxoSmithKline, Analytical Sciences and Development, United States of America)

[P2-02] FTMP-based Modeling and Simulations of HCP Mg Single Crystal

○Takahiro Kitano, Tadashi Hasebe　(Dept. of Mechanical Engineering, Kobe Univ., Japan)

[P2-03] Nonlinear elasticity on Riemannian manifold and its application to general surface development

○Yuto Horikawa[1], Ryuichi Tarumi[2], Yoji Shibutani[1]　(1.Dept. of Mechanical Engineering, Osaka Univ., Japan, 2.Grad. Sch. of Engineering Science, Osaka Univ., Japan)

[P2-04] The challenge of achieving quantitative phase field models for microstructure evolution in irradiated solids - the case of voids

○Anter El-Azab　(Purdue University, United States of America)

[P2-05] A Molecular-Dynamics Study of Surface Tension: From Alloy Droplets to Bubbles in Molten Alloy

○Xiangming Ma, Hongtao Liang, Yang Yang　(East China Normal Univercity, China)

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-01] Multiscale model of solid state amorphization during processing of pharmaceutical materials

Chunyu Li[1], Yifei Zeng[1], Lorena Alzate-Vargas[1], Pilsun Yoo[1], Rachel Frocino[2], Jeff Brum[2], Peilin Liao[1], Marisol Koslowski[1], ○Alejandro Strachan[1]　(1.Purdue University, United States of America, 2.GlaxoSmithKline, Analytical Sciences and Development, United States of America)

Processing of active pharmaceutical ingredients and excipients to reduce and control particle size involve milling and micronization which result in severe plastic deformation and fracture. The increase in free energy of the crystal during deformation can result in polymorphic transformations and amorphization and affect the physical properties of the product, including bioavailability.

In order to predict how materials properties and processing conditions affect plastic deformation and phase transitions in pharmaceutical materials we developed a multiscale model that combines electronic structure using density functional theory, large-scale molecular dynamics simulations and a phase field modeling. At the finer scale, we use DFT to predict elastic constants of the crystals and amorphous systems of interest and validate the force fields used with MD. MD simulations provide insight into the process of amorphization and enables the characterization of the difference in enthalpy between the crystal and amorphous phase and their interfacial energy, critical to describe the nucleation and growth of the amorphous phase. Finally, the materials properties from DFT and MD calculations are used to inform a phase field model that describes, self-consistently, plastic deformation, including the nucleation of crystal defects informed by dislocation dynamics, with phase transformations.

Using the multiscale model, we investigate the effect of deformation, shear, impact and particle surface roughness on the evolution of the crystallite size and the nucleation and growth of an amorphous phase in molecular crystals of interest for pharmaceutical applications.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-02] FTMP-based Modeling and Simulations of HCP Mg Single Crystal

○Takahiro Kitano, Tadashi Hasebe　(Dept. of Mechanical Engineering, Kobe Univ., Japan)

Extended usages of Mg and Mg alloys have been widely promoted to date, attempting to make the best use of their attractive properties, such as light weight, high specific strength, superior recyclability and excellent bio-compatibility. Modeling attempts of Mg and Mg alloys, however, often meet difficulty in the treatments of the complex plasticity, mainly stem from their highly anisotropic slip systems and intricate activities of twinning. The present study aims at enhancing the feasibility of the recently-proposed model for deformation twinning based on FTMP (Field Theory of Multiscale Plasticity) toward extended applications to HCP Mg single crystal. The major updates of the model are two fold: one is the extension to efficient 3D simulations by introducing special computational schemes, while the other is to apply modified lattice rotation based on the rotational part of the incompatibility tensor. The twinning model with the modified lattice rotation is introduced in the hardening law in the FTMP-based crystalline plasticity framework, and is further implemented into a finite element code accommodated with the above new scheme. Deformation analyses are performed based on 2D/3D FEM for pure single crystal magnesium with HCP (hexagonal close-packed) structure, and critical comparisons are made with experimental data obtained under plain-strain

compression in multiple orientations by Kelly and Hosford, particularly, with those exhibiting the unique stress-strain responses induced by deformation twinning, i.e., orientations A, E and F. Natural expression of twin-induced lattice rotation is attempted by introducing a modification based on the pure rotation part of the incompatibility tensor, spontaneously evolved during deformation. The modification is shown to allow autonomic transitions between slip and twinning modes, e.g., from twin-dominant stress response to that carried by slip, as in the orientations E and F by Kelly-Hosford.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-03] Nonlinear elasticity on Riemannian manifold and its application to general surface development

○Yuto Horikawa[1], Ryuichi Tarumi[2], Yoji Shibutani[1]   (1.Dept. of Mechanical Engineering, Osaka Univ., Japan, 2.Grad. Sch. of Engineering Science, Osaka Univ., Japan）

This study aims to develop a theoretical framework to construct a three-dimensional curved surface from pieces of an elastic sheet which is embedded in two-dimensional Euclidean space. Our formulation is based on the standard nonlinear elasticity within the framework of differential geometry. We first introduce the Riemannian manifolds which equip the metrics, g[0] and g[t], for reference and current configurations. The strain energy density is defined as a quadratic form of Green strain tensor under the assumption that elastic medium is isotropic in the reference configuration g[0]. Then, the surface development problem ends up with a variational problem such that to find an embedding mapping which minimizes the strain energy functional. We solve the variational problem numerically using the isogeometric analysis (IGA). To this end, we first derive a weak form equilibrium equation from the first variation of the functional. The embedding mapping is approximated by a linear combination of non-uniform rational B-spline (NURBS) functions with the coefficients ξ. Consequently, the equilibrium equation yields a system of nonlinear algebraic equations for ξ and which is solved iteratively around a linearized solution by the Newton method. It should be noted here that present method consider in-plane deformation of the elastic sheet exclusively. It implies that two-dimensional isometric deformation, such as out-of-plane bending deformation, produces no strain energy in the medium. In this regards, present method is a fair generalization of conventional surface development method which is frequently used in the paper craft such as origami. Numerical analysis for a one-dimensional system demonstrates that present method converges to an exact solution within a sufficient accuracy.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-04] The challenge of achieving quantitative phase field models for microstructure evolution in irradiated solids - the case of voids

○Anter El-Azab   (Purdue University, United States of America）

We present a thermodynamics-consistent formalism of a phase field model of void growth in irradiated solids, along with its sharp interface counterpart. Asymptotic matching of the two models was performed to yield all phase field model parameters in terms of real materials properties. In this presentation, the results of a first quantitative simulations of void growth driven by irradiation using our phase field approach will be reported. This work was performed in collaboration with Srujan Rokkam, Thomas Hochrainer, and Karim Ahmed.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-05] A Molecular-Dynamics Study of Surface Tension: From Alloy Droplets to Bubbles in Molten Alloy

○Xiangming Ma, Hongtao Liang, Yang Yang （East China Normal Univercity, China）

We present a substantial atomistic simulation study of the equilibrium surface tension for liquid-state binary alloy systems. Four types of spherical surface/interfaces are investigated: liquid Pb droplet embedded in bulk liquid Al, liquid Al droplet in bulk liquid Pb, a bubble in liquid state Pb-Bi eutectic (LBE) and a LBE droplet. The surface tension for these non-planar surfaces are calculated based on the calculation of the local pressure tensor in spherical coordinates. Several thermodynamics property (droplet size, temperature, capillary pressure, mutual miscibilities) dependencies of surface tension are obtained. Our results provide useful input data for the mesoscale simulations of the selective laser melting, advanced welding and bubble formation in nuclear coolants.

[PO-B2] Poster Session 2

Symposium B

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-06] Effects of rhenium on the mechanical behavior of irradiated tungsten: a molecular dynamics study using neural-network potential

○Ryo KOBAYASHI （Nagoya Institute of Technology (NITech), Japan）

[P2-07] Diffusion behavior and temperature dependence of hydrogen in tungsten and molybdenum under isotropic strain state

○QuanFu Han[1], Yue-Lin Liu[2], Ying Zhang[1], Guang-Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

[P2-08] Diffusion of Point Defects on Tungsten Surface

Jiannan Hao[1], ○Shuo Jin[1], Haixuan Xu[2], Xiaolin Shu[1], Guanghong Lu[1] （1.School of Physics and Nuclear Energy Engineering, Beihang University, China, 2.Department of Material Science and Engineering, The University of Tennessee, Knoxville, United States of America）

[P2-09] Influence of anisotropic strain and temperature on hydrogen dissolution in tungsten

○Ying zhang[1], Quan Fu Han[1], Yue lin Liu[2], Guang Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

[P2-10] Screw dislocation-interstitial solute coevolution in W-O alloys using atomistically-informed kinetic Monte Carlo simulations

○Yue Zhao[1], Lucile Dezerald[3], Jaime Marian[1,2] （1.Dept. of Materials Science and Engineering, University of California, Los Angeles, United States of America, 2.Dept. of Mechanical Engineering, University of California, Los Angeles, United States of America, 3.Institut Jean Lamour, University of Lorraine, France）

[P2-11] Kinetic Monte-Carlo Simulations of Radiation Damage in W(Re,Os) Alloys

○Matthew James Lloyd[1,2], David Armstrong[1], Enrique Martinez Saez[3], Duc Nguyen-Manh[2] （1.Department of Materials, University of Oxford, UK, 2.Culham Centre for Fusion Energy, UK, 3.Los Alamos National Laboratory, United States of America）

[P2-13] Dynamics of Magnetism in Neutron Irradiated Iron-Chromium Steels

○Jacob B. J. Chapman, Pui-Wai Ma, Sergei L. Dudarev （Culham Centre for Fusion Energy (CCFE), UK）

[P2-14] Atomistic insights into the grain boundaries interaction with radiation-induced point defects in bcc Fe-Cr alloys

○Marcin Roland Zemla, Jan Stanislaw Wrobel, Tomasz Wejrzanowski （Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland）

[P2-15] Production and Process of Cascade Development in Irradiated Pure α-Zr from Molecular Dynamics Simulations

○Rongjian Pan[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Bang Wen[1], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3] （1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine）

[P2-16] Microstructure evolution of cascade annealing in irradiated pure α-Zr from molecular dynamics simulations

○Bang Wen[1], Rongjian Pan[1], Wei Zhang[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3]　(1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine)

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-06] Effects of rhenium on the mechanical behavior of irradiated tungsten: a molecular dynamics study using neural-network potential

○Ryo KOBAYASHI （Nagoya Institute of Technology (NITech), Japan）

Tungsten (W) is considered as a promising candidate for the plasma facing wall material at divertor in nuclear fusion reactors. In order to assess the lifetime of the divertor for safe operation of the nuclear fusion reactors, mechanical response to the irradiation of high energy neutrons and helium atoms should be precisely understood from atomistic scale. Under the irradiation of high energy neutrons, not only defects are formed but also transmutation occurs, which will produce a few percent of rhenium (Re) concentration within several-year operation of nuclear fusion reactor. Thus the effect of solute Re atoms on the mechanical behavior of host material, W, should be taken into account, such as recovering rate after cascading damage, H/D/T retention, He bubble formation, or dislcation mobility. In this study, we create a neural-network (NN) potential for quarternary system, W-Re-H-He, combined to an EAM potential for W-Re binary system. It is known that machine-learning (ML) potentials such as NN can well reproduce DFT energies of wide variety of atomic configurations, but it requires big data to learn a lot of free parameters and it is usually much slower than the classical potentials such as EAM. By combining the NN with EAM potentials, we can construct a potential with smaller number of referece data and make it much faster than fully NN potential. The properties of the potential and the effect of Re on the recovering rate after cascading damage, He bubble formation/growth rate, and dislocation punching will be discussed.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-07] Diffusion behavior and temperature dependence of hydrogen in tungsten and molybdenum under isotropic strain state

○QuanFu Han[1], Yue-Lin Liu[2], Ying Zhang[1], Guang-Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

The interaction between hydrogen and metal exhibits a great scientific and technological importance so that it has a direct impact on the design and operation of metallic materials. Here, we have carried out first-principles calculations to investigate interstitial hydrogen diffusion behaviors in tungsten and molybdenum by considering double effects of temperature and strain. The temperature and strain effects are reflected by the vibration Helmholtz free energy in the quasi-harmonic approximation and isotropic loading, respectively. The hydrogen diffusion is analyzed through two nearest neighbor tetrahedral sites. At a ground state (0-K) condition, the hydrogen diffusion activation energy can increase and decrease notably with rising compressive and tensile strain, respectively. While at each compressive/tensile strain case, the hydrogen diffusion activation energy depends distinctly on the temperature and increases with rising temperature. This is mainly originated from the contribution of vibration Helmholtz free energy induced by the larger vibration frequency of hydrogen in two metals. With the increasing temperature, the hydrogen diffusivity is shown to be dependent on the compressive/tensile strain alteration. The present study demonstrates a remarkable influence of "temperature and strain" on the hydrogen diffusion behaviors in tungsten and molybdenum.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-08] Diffusion of Point Defects on Tungsten Surface

Jiannan Hao[1], °Shuo Jin[1], Haixuan Xu[2], Xiaolin Shu[1], Guanghong Lu[1]   (1.School of Physics and Nuclear Energy Engineering, Beihang University, China, 2.Department of Material Science and Engineering, The University of Tennessee, Knoxville, United States of America)

Hydrogen (H) / helium (He) retention in tungsten (W) and can significantly reduce the thermal conductivity and sputtering threshold of W, and at the same time, continuous bombardment with 14.1 MeV neutron can introduce Frenkel defects (composed of self-interstitial atoms (SIAs) and vacancies), which lead to a high concentration of W impurity. The surface deformation and blisters are observed experimentally in W, in which the surface morphology is relevant to the plasma fluence and surface directions [1-2]. The near-surface atomistic configuration is changed via diffusion of frenkel defects which is driven by heat and/or bubble loop punching process. Therefore, revealing the evolution mechanism of point defects on the W surfaces under H/He irradiation is crucial for W application in future fusion reactors.

We employ the first-principles and molecular dynamics simulation to calculate the energy barriers of single adatom (AD) and vacancy (VA) diffusion on the W (100), (110) and (111) surface. The diffusion paths of defects is determined by the dimmer method built in the SEAKMC code [3]. At least three diffusion paths with high energy barriers are found for both AD and VA on the (100) surface. However, only one path with low energy barrier of both AD and VA on the (110) surface are dominated throughout the diffusion process. Moreover, the diffusion of AD and VA on the (111) surface is investigated, in which the formation energies of different surface defects are biased. Nonetheless, the symmetry of the (111) surface will break spontaneously at the certain temperature and concentration of impurity through the thermodynamic calculation, and the morphology is in good agreement with the SEM images [1]. The work will help to understand the early stage of surface morphology evolution under irradiations or in the annealing process.

Keywords: tungsten, point defects, diffusion, surface

References

[1] H. Y. Xu, Y. B. Zhang, Y. Yuan, B. Q. Fu, A. Godfrey, G. De Temmerman, W. Liu, and X. Huang, J. Nucl. Mater. 443, 452 (2013).

[2] F. W. Meyer, H. Hijazi, M. E. Bannister, K. A. Unocic, L. M. Garrison, and C. M. Parish, Phys. Scr. T167, 14019 (2016).

[3] H. Xu, Y. N. Osetsky, and R. E. Stoller, J. Phys. Condens. Matter 24, 375402 (2012).

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-09] Influence of anisotropic strain and temperature on hydrogen

dissolution in tungsten

○Ying zhang[1], Quan Fu Han[1], Yue lin Liu[2], Guang Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

Tungsten (W) is an alternative candidate for a plasma facing material in the future fusion reactor due to its high melting point, high thermal conductivity and low plasma sputtering yield. The solubility of hydrogen in tungsten is a basic and crucial factor to influence the formation of hydrogen bubbles. In this work, we have investigated the effects of anisotropic strain and temperature on the dissolution of H in tungsten via the first-principles calculation in combination with thermodynamic models. The temperature and strain effects are reflected by the vibration Helmholtz free energy in the quasi-harmonic approximation and uniaxial/biaxial strain loading, respectively. It is found that the solubility of hydrogen can be enhanced by both compressive and tensile anisotropic strain, independent with of the sign of strain. This is different from the influence of isotropic strain, where the solubility of hydrogen in tungsten responds to the isotropic strain monotonically. Besides, the difference of the dissolution energy between hydrogen dissolves in tetrahedral and octahedral site constantly changes in the anisotropic strain range of -4%-4%. Further, under same anisotropic strain condition, the solution energy of hydrogen in tungsten increases with the increasing of the temperature from 300-1800 K, which can be mainly contributed to the vibration Helmholtz free energy. Our finding suggests that the local anisotropic strain and temperature can significantly influence the dissolution of hydrogen in tungsten, which may play a key role on hydrogen bubble formation.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-10] Screw dislocation-interstitial solute coevolution in W-O alloys using atomistically-informed kinetic Monte Carlo simulations

○Yue Zhao[1], Lucile Dezerald[3], Jaime Marian[1,2]   (1.Dept. of Materials Science and Engineering, University of California, Los Angeles, United States of America, 2.Dept. of Mechanical Engineering, University of California, Los Angeles, United States of America, 3.Institut Jean Lamour, University of Lorraine, France）

The interaction of interstitial impurities with in-grown dislocations in metals can lead to various processes, including solute solution hardening and/or dynamic strain aging. The coevolution of solutes and dislocations occurs on length and time scales that are very challenging to resolve experimentally. The interaction of interstitial solutes with dislocation segments is highly local, however, and models must be capable of resolving the fine details of the interaction if we are to gain any understanding from the process. Here we develop a kinetic Monte Carlo model of dislocation motion in the presence of diffusing solutes. We focus on the W-O solid solution, such that the subject of our study is screw dislocations, as they control plastic flow at low temperatures in body-centered cubic metals and alloys. Solute diffusion is affected by dislocation strain fields, which we study via the elastic dipole tensor using electronic structure calculations. As well, we calculate binding energies of O atoms to screw dislocation cores, and discuss the joint structures formed, the implications of the calculated energetics, and show the effect on the dislocation velocity of solute diffusion at several temperatures.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-11] Kinetic Monte-Carlo Simulations of Radiation Damage in W(Re,Os) Alloys

○Matthew James Lloyd[1,2], David Armstrong[1], Enrique Martinez Saez[3], Duc Nguyen-Manh[2]　(1.Department of Materials, University of Oxford, UK, 2.Culham Centre for Fusion Energy, UK, 3.Los Alamos National Laboratory, United States of America)

The realisation of fusion energy is dependant on the development of high performance materials that can withstand the extreme conditions that they will be subjected to. The plasma facing components of a fusion reactor will experience a combination of high thermal loading (~10MWm^{-2}) and an intense flux of both 14MeV neutrons and high energy He/H ions (~5-20dpa/yr), meaning they will have to operate at very high temperatures (~1300 K). Tungsten is currently the leading candidate material due to its high melting temperature (~3695K); good thermal conductivity (~150Wm^{-1}K^{-1}) and resistance to sputtering (Eth=200eV). But at such a high neutron flux, transmutation of W in a fusion reactor is significant, resulting in several at.% Re, Os and Ta over the lifetime of the reactor. Precipitation of Re and Os has been observed well below their solubility limit in W, resulting in embrittlement, hardening, and a reduction in thermal conductivity.

The research presented examines irradiated W-(Re,Os,Ta) alloy systems, using a combination of DFT parametrised, multicomponent atomistic kinetic Monte-Carlo (AKMC) modelling, and high resolution nanoscale characterisation techniques such as atom probe tomography (APT). The role of interstitial defects in W-Re and W-Os is thought to play an important role in precipitation, because of the low rotation energy of the W-Re/W-Os mixed dumbbell. This enables the 3D transport of solute atoms, that would otherwise be confined to the <111> direction. We present a multicomponent kinetic Monte Carlo model, incorporating both vacancy and interstitial defects, and solute concentration dependant interactions. The predictions made by our model are supported by APT data of W-Re and W-Os alloys irradiated at high temperature, using W ions.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-13] Dynamics of Magnetism in Neutron Irradiated Iron-Chromium Steels

○Jacob B. J. Chapman, Pui-Wai Ma, Sergei L. Dudarev　(Culham Centre for Fusion Energy (CCFE), UK)

Ferritic-martensitic (F/M) steels, with a high chromium content, are critical materials for magnetic confinement fusion technology due to high temperature stability and corrosion resistance, facilitating the thermal efficiency necessary for fusion power plant operation. To predict the evolution of the steel microstructure and mechanical properties when subjected to sustained high doses of radiation at elevated temperatures, we must understand how radiation damage affects magnetic properties of the materials, which strongly influence phase stability and chromium solubility.

We investigate the effect of neutron irradiation on the magnetic properties of F/M steel alloys, relating experimentally observed [1] concentrations, radii and number densities of Cr precipitates within a Fe-Cr matrix to the dynamics and degradation/enhancement of magnetism across a broad range of temperatures. The Curie temperature is shown to vary, strongly dependent upon microstructure, increasing significantly with Cr precipitation observed at high doses and ageing times. These large-scale non-collinear calculations are performed using a method implementing magnetic cluster expansion (MCE), parameterised using a

database of DFT-generated observables [2], with spin-dynamics (SD) incorporating both transverse and longitudinal spin fluctuations [3]. SD simulations provide valuable insight into the ageing of alloys under realistic magnetic confinement conditions to inform material choices and construction strategy for fusion power plant design.

[1] E.R.Reese *et al.*, JNM **500**, 192 (2018); [2] M.Y.Lavrentiev *et al.*, JAP **109**, 07E123 (201); [3] P.-W.Ma *et al.* , PRB **81**, 184202 (2017)

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-14] Atomistic insights into the grain boundaries interaction with radiation-induced point defects in bcc Fe-Cr alloys

○Marcin Roland Zemla, Jan Stanislaw Wrobel, Tomasz Wejrzanowski （Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland）

Grain boundaries (GBs) are an immanent components of crystal structure of the structural materials, such as e.g. Fe-Cr steels. Moreover, they have considerable influence on the materials properties, especially on the mechanical one. As a consequence of that, is necessary to investigate effect of radiation-induced defects on the GBs in order to a deeper understanding of the radiation damage.

In current study, we investigated characteristics of bcc-Fe and Fe-Cr based tilt GBs interacting with point defects such as vacancy, self-interstitial (SIA, dumbbell-type), and interstitial atoms (He impurities). Several tilt GBs with the rotation axis along [100] and [110] directions were modelled with He impurities, vacancy, and SIA in Fe-Cr. Molecular dynamics (MD) simulations using the interatomic Fe-Cr-He embedded atom model potential were conducted, for twelve GBs, in order to investigate GBs energies, He segregation energies, and the weakening effect of He impurity for several Cr and He concentrations. Furthermore, spin-polarized density functional theory (DFT) calculations focused at two GBs, $\Sigma 3(111)$ and $\Sigma 5(210)$, allowed to deeper insights into GBs properties. For example, the DFT results show that the presence of He significantly influences the magnetic properties of the system in the relatively distant neighbourhood [1]. The fluctuation of magnetic moments, chemical potentials, formation and migration energies of point defects were studied as a function of distance from GB's plane. Representative structures of GBs, with Cr content ranging 6-10%, generated using DFT-based Monte Carlo simulations [2] were used to analyse how parameters, such as alloy short-range ordering or local environment, effects on defects properties.

[1]. M. R. Zemla, J. S. Wrobel, T. Wejrzanowski, D. Nguyen-Manh, K. J. Kurzydlowski, Nuclear Instruments and Methods in Physics Research Section B Beam Interactions with Materials and Atoms 393:118 (2017).

[2]. J.S. Wrobel, D. Nguyen-Manh, M.Y. Lavrentiev, M. Muzyk, S.L. Dudarev, Physical Review B 91 (024108) 2015.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-15] Production and Process of Cascade Development in Irradiated Pure α-Zr from Molecular Dynamics Simulations

○Rongjian Pan[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Bang Wen[1], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3]　(1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine)

The formation and development of cascade in pure α-Zr crystals at sample temperatures T=300K and T=500K, energy of 2, 6 and 10 keV and initially driving directions and of primary knock atoms (PKA) are investigated by molecular dynamics. The simulation results show that when crystals temperature is T=300K and 500K and initial direction of motion for PKA is the cascades volume is greater than for the initial direction at same all other parameters. The largest size of cascade is found after 0.4 ps, which regardless of crystal temperature, energy and initial direction of primary knock-on atom (PKA). The formation of crowdions is caused by channeling during cascade development.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-16] Microstructure evolution of cascade annealing in irradiated pure α-Zr from molecular dynamics simulations

○Bang Wen[1], Rongjian Pan[1], Wei Zhang[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3]　(1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine)

The microstructure evolution of cascade annealing in α-Zr crystals at T=300K, 400K, and 500 K for energy of 2, 6 and 10 keV with initially driving directions <0001> and <01-10> of primary knocked atoms (PKA) are investigated by using molecular dynamics simulations. The results show that the relaxation time (τ_r) of cascades can play a role of an effective parameter for describing radiation damages during molecular dynamics simulations. of cascade with the larger surface area but with the same volume is much smaller, which promotes faster recombination of defects during cascade annealing. Energy is a crucial factor in the formation of cascade displacements of atoms and appearing of defects compared with temperature and direction of movement for initially knocking atoms.

Poster Session | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[PO-C2] Poster Session 2
Symposium C
Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-18] Prediction of Biaxial Tensile Deformation Behavior of Aluminum Alloy Sheets using Crystal Plasticity Finite Element Method and Machine Learning
○Kota Koenuma[1], Akinori Yamanaka[1], Ikumu Watanabe[2], Toshihiko Kuwabara[1]　(1.Tokyo University of Agriculture and Technology, Japan, 2.National Institute of Materials Science, Japan）

[P2-19] MobiDiC: A 3-D Dislocation Dynamics Simulation
○Ronan MADEC[1], Laurent COLOMBET[1], Ladislas KUBIN[2]　(1.CEA, DAM, DIF, France, 2.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay, France）

[P2-20] Temperature dependence of fatigue crack growth in Ti-6Al-4V
○Bhargavi Rani Anne, Masaki Tanka, Tatsuya Morikawa　(Dept. of Materials Science and Engineering, Kyushu University, Japan）

[P2-21] Parametric model of discrete dislocation dynamics based on mathematical theory of moving curves
○Miroslav Kolar, Jan Kratochvíl, Petr Pauš, Michal Beneš　(Czech Technical University in Prague, Czech Republic）

[P2-22] On Visualization of Multiscale Information Transfer/Exchange Processes via FTMP-based Duality Diagram Representation Scheme
○Takuya Takagi, Tadashi Hasebe　(Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P2-23] Rotational Field Evolutions based on Field Theory of Multiscale Plasticity (FTMP)
○Tadashi Hasebe[1], Yasutaka Matsubara[2]　(1.Kobe Univ., Japan, 2.Graduate School of Kobe Univ., Japan）

[P2-24] A 2D MESOSCALE STUDY OF DISLOCATIONS, CRACKS AND MARTENSITIC PHASE TRANSFORMATIONS
○Rachel Derby, Michael Budnitzki, Stefan Sandfeld　(TU Bergakademie Freiberg, Germany）

[P2-25] Effects of Stress Distribution on the Plastic Deformation of Metallic Glasses under Different Geometries
○Chih-Jen Yeh[1], Hsuan-Teh Hu[1], Chang-Wei Huang[2], Yu-Chieh Lo[3]　(1.National Cheng Kung University, Taiwan, 2.Chung Yuan Christian University, Taiwan, 3.National Chiao Tung University, Taiwan）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-18] Prediction of Biaxial Tensile Deformation Behavior of Aluminum Alloy Sheets using Crystal Plasticity Finite Element Method and Machine Learning

○Kota Koenuma[1], Akinori Yamanaka[1], Ikumu Watanabe[2], Toshihiko Kuwabara[1]　(1.Tokyo University of Agriculture and Technology, Japan, 2.National Institute of Materials Science, Japan)

Aluminum alloy sheets are used for automotive body parts to reduce the weight of automotive. However, because the formability of aluminum alloy sheets is much lower than that of steel sheets, the plastic deformation behavior of aluminum alloy sheets during plastic forming processes has been predicted by sheet metal forming simulations based on the finite element method. In order to predict the plastic deformation behavior of an aluminum alloy sheet subjected to a biaxial stress state in a sheet metal forming process, we proposed the numerical biaxial tensile test (NBT) methodology using the crystal plasticity finite element method (CPFEM) and the mathematical homogenization method. The NBT method has been already applied to predict the contour of equal plastic work of a 5000-series aluminum alloy sheet. The results demonstrated that the contour of equal plastic work (the yield locus) calculated by the NBT method shows a good agreement with that measured by the experimental biaxial tensile test using a cruciform specimen. Unfortunately, because we need to perform multiple NBTs to calculate the contour of equal plastic work, the disadvantage of the NBT method is its high computational cost. In this study, in order to predict the biaxial tensile deformation behavior of aluminum alloy sheets more efficiently, we propose a new numerical material testing methodology by combining the NBT method with machine learning methods. The deformation behavior of aluminum alloy sheets predicted by the proposed method is verified by experimental multi-axitial material tests.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-19] MobiDiC: A 3-D Dislocation Dynamics Simulation

○Ronan MADEC[1], Laurent COLOMBET[1], Ladislas KUBIN[2]　(1.CEA, DAM, DIF, France, 2.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay, France)

In 3D lattice-based dislocation dynamics (DD) codes, dislocation segments are discretized on an underlying lattice in which they move by discrete jumps. The first version of such codes goes by the name of microMegas and dates back to the beginning of the 1990s [1]. It makes use of a line model in which dislocations are discretized in their slip planes into a succession of straight segments with edge and screw characters. Two more sophisticated versions of the initial code are currently in use, Tridis, which retains the 'screw-edge' line model [2] and an evolved version of microMegas with two additional mixed line directions [3].

MobiDiC (for 'Mobile Dislocation Colony') derives from this last version of microMegas and is devoted to mass mesoscopic simulations involving a large number of perfect dislocations. It is designed to overcome some limitations of the parent code in order to provide an improved and efficient framework for DD simulations that can further evolve.

The specificities of this code will be presented, in particular the ability to handle complex crystallographic structures and dislocation reactions. Indeed, MobiDiC is considerably more flexible than other lattice-based

DD codes because there is no limitation to the number of vectors per slip system. In addition a semi-nodal approach is used. For instance, the movements of segments connected to a high connectivity node, like triple nodes of a junction, are coordinated to move the node with the adequate degree of freedom.

Examples of applications will be given as well as results obtained with OpenMP and hybrid parallelisms using many-core processors.

[1] L. P. Kubin, G. Canova, M. Condat, B. Devincre, V. Pontikis and Y. Bréchet, Solid State Phenomena., 23-24, 455 (1992).
[2] M. Verdier, M. Fivel and I. Groma, Model. Simul. Mater. Sci. Eng. 6, 755-770 (1998).
[3] B. Devincre, R. Madec, G. Monnet, S. Quereau, R. Gatti, L. Kubin, Modeling crystal plasticity with dislocation dynamics simulations: the 'microMegas' code, in Mechanics of Nano-Objects, O. Thomas, A. Ponchet, S. Forest, (Eds.), Presses des Mines, Paris 2011, pp. 81-89.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-20] Temperature dependence of fatigue crack growth in Ti-6Al-4V

○Bhargavi Rani Anne, Masaki Tanka, Tatsuya Morikawa （Dept. of Materials Science and Engineering, Kyushu University, Japan）

Fatigue properties of dual phase (α+ß and primary α) Ti-6Al-4V were studied with respect to the range of temperatures and stress intensity range. Fatigue tests were conducted with both high and low stress intensity ranges in the temperature range between room temperature and 550K. Micro crack propagation was observed. Crack growth rate (da/dN) was measured where a is a crack length and N is a number of cycles, changing temperature. It was found that da/dN was increased with temperature. It is assumed that da/dN is the Arrhenius type of equation as it shows temperature dependence. Activation energy calculations were attained from Arrhenius plot between the logarithm of da/dN and the reciprocal of temperature. The dependence of activation energy on stress intensity range was also obtained, which provides the information on the dislocation mobility controlling the fatigue crack growth. The comparison of fatigue crack growth rate with the temperature dependence of dislocation motion was also studied in detail.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-21] Parametric model of discrete dislocation dynamics based on mathematical theory of moving curves

○Miroslav Kolar, Jan Kratochvíl, Petr Pauš, Michal Beneš （Czech Technical University in Prague, Czech Republic）

In this contribution we present the comprehensive model of discrete dislocation dynamics based on the mathematical theory of moving curves. The purpose of our model is the precise and mathematically rigorous description of the dynamics of dislocations, which are represented as smooth curves evolving in their respective slip planes.

Dislocations are described by parametric curves and their motion is governed by the curvature driven flow.

The parametric model is coupled with the model of tagential velocity for increased stability, and with algorithms for topological changes which allow modeling of complex effects as merging, splitting, self-replication or interaction with obstacles.
The numerical algorithm is based on the flowing finite volume method.

We present qualitative and quantitative results of our numerical simulations. We demonstrate the capabilities of our model in the predicting of dipole formation and consequent estimation of the endurance limit, in the modeling of several interacting dislocations, and in the application of our method on complex scenarios involving moving dislocations interactiong with several obstacles.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-22] On Visualization of Multiscale Information Transfer/Exchange Processes via FTMP-based Duality Diagram Representation Scheme

○Takuya Takagi, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

It may safely be said that one of the critical issues about multiscale polycrystalline plasticity modeling are ultimately consolidated into those about "information transfer and exchange" concurrently taking place among plural scales of spontaneously evolving kinds. In tackling these, we make an attempt here to introduce the duality diagram-based scheme of FTMP into multi-grained models under tension, where FTMP stands for Field Theory of Multiscale Plasticity. The model used is composed of systematic combinations of representative crystallographic orientations, i.e., three multi-slip [100], [110] and [111], and two single-slip [123] and [125]. Strongly orientation-dependent intragranular substructure evolutions, successfully reproduced solely via FTMP-based finite element analyses, result in distinct overall deformation/fracture modes, including, e.g., local instability-induced brittle-like fracture modes. Corresponding duality diagrams, i.e., the spatial trace of the incompatibility tensor versus fluctuation of the elastic strain energy, are drawn and are compared with their rate versions. Found first is a similarity between the two diagrams, i.e., the normal and their rate forms, when they are constructed via grain-wise net sum basis, without taking the absolute values as we have done so far. Phase space diagrams are newly introduced both for the incompatibility and strain energy fluctuation to further examine those similarities in general. Demonstrated thereby is the models yielding "in-phase" responses roughly correspond to the cases that exhibit relatively stable and ductile deformation/fracture modes. The phase shifts, on the other hand, are shown to be closely related to instability outset, based on which the construction of a possible measure of the "degree" of instability is also attempted.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-23] Rotational Field Evolutions based on Field Theory of Multiscale Plasticity (FTMP)

○Tadashi Hasebe[1], Yasutaka Matsubara[2] （1.Kobe Univ., Japan, 2.Graduate School of Kobe Univ., Japan）

FTMP-based modeling and simulations have revealed its prominent descriptive capability of deformation-induced evolving inhomogeneities, e.g., band-like dislocation substructures, which are generally accompanied by misorientation across them. Three representative cases are examined in detail, i.e., (a)spontaneously evolved dislocation substructures, (b)eigenstrain-driven misorientation development for modeling lath martensite block structures, and (c)alternative degrees of freedom-driven lattice rotations enriched by incompatibility-based modified spin. For (a), we discuss deformation-induced spontaneous evolution of misoriented dislocation substructures, comparing dislocation density contours for BCC and FCC models, while, for (b), comparison is made of the eigenstrain-driven misoriented lath block structures among three incompatibility conditions, where screw dislocation networks are commonly evolved, yielding twisted lath boundaries. For (c), we examine emerging "kink-like" patterns associated with tensile twining assisted by incompatibility-based modification of rotation, comparing component-wise contributions of incompatibility tensor on evolving rotation fields with "kink-like" morphology for Mg single crystal under c-axis tension. In addition to these, "crystallization-like" patterns evolved in single crystal sample are extensively examined, where initially-prescribed laminated misorientation distributions and/or hardening moduli are introduced to the model used in (c).

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-24] A 2D MESOSCALE STUDY OF DISLOCATIONS, CRACKS AND MARTENSITIC PHASE TRANSFORMATIONS

○Rachel Derby, Michael Budnitzki, Stefan Sandfeld　(TU Bergakademie Freiberg, Germany)

TRIP-Steels are of commercial interest due to their exceptional strength. This is a result of the microstructure; a matrix of both austenite and martensite that when plastically strained, exhibits strain hardening behavior. Plastic deformation arises from the presence of dislocations and the martensitic phase transformations (MT) that take place inside the metal. To understand the macroscopic properties of TRIP-Steels, it is necessary to understand the underlying dynamics occurring at the mesoscale.

Most models do not take into account the interactions between martensitic phase transformations and dislocations, and therefore are missing the impact that these two phenomena exert on each other. While MD simulations can resolve both phenomena naturally, they are prohibitively expensive for larger crystal sizes or time scales. On the contrary, continuum models cannot resolve the motion of dislocations inside the material.

We combine dislocation dynamics and martensitic phase transformations to study the interplay between the two phenomena. For the dislocation problem we use a continuum dislocation dynamics (CDD) model, allowing us to reduce computational cost and increase the system size. CDD is coupled with a Phase Field approach, which we use to model martensitic phase transformations. This allows us to study how dislocation motion can be influenced in the presence of an MT. Additionally, simple crack geometries can also be modeled as special dislocation configurations, which helps to understand how cracks and voids may trigger or inhibit MT.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-25] Effects of Stress Distribution on the Plastic Deformation of Metallic Glasses under Different Geometries

○Chih-Jen Yeh[1], Hsuan-Teh Hu[1], Chang-Wei Huang[2], Yu-Chieh Lo[3]　(1.National Cheng Kung University, Taiwan, 2.Chung Yuan Christian University, Taiwan, 3.National Chiao Tung University, Taiwan）

Metallic glasses (MGs) generally have diverse mechanical properties, such as high strength and poor ductility. The deformation behaviors of MGs, to a large extent, depend on the ambient conditions. For example, the deformation of MGs is homogenous at high temperature and low stress. On the other hand, the deformation of MGs is inhomogeneous at low temperature and high stress. However, the inhomogeneous deformation further causes the shear band which is an accumulation of local plastic deformation. The formation of shear band always leads to a catastrophic failure with the increasing plastic deformation. In order to study the generation of shear band, a multiscale model which considers the microscopic shear transformation in macroscopic deformation is inevitable. In this paper, a mesoscale model combines the finite element method and the kinetic Monte Carlo method is used to investigate the properties of the metallic glasses. More mechanical properties and deformation behaviors of the MGs can be explored through the proposed model. In addition, the geometries of pores in composite MGs are investigated. Stress concentration and redistribution due to the different shapes and sizes of pores in composite MGs are discussed. These results can improve the design of the MGs and prevent MGs from catastrophic failure.

Poster Session | D. Data-Driven and Physics-Informed Materials Discovery and Design

[PO-D2] Poster Session 2
Symposium D
Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-26] Generalized nano-thermodynamic model for predicting size-dependent surface segregation in multi-metal alloy nanoparticles from smaller particles

○Abhijit Chatterjee （Dept. of Chemical Engg., Indian Institute of Technology Bombay, India）

[P2-27] Development of thermodynamic database of Nd-Fe-B-based permanent magnet alloys

○Jiang Wang, Lei Xu, Kaicheng Yang, Qingrong Yao, Guanghui Rao, Huaiying Zhou （School of Material Science and Engineering, Guilin University of Electronic Technology, China）

[P2-28] Design of proteins and biopolymers: role of directional interactions and of water.

○Valentino Bianco[1], Ivan Coluzza[2] （1.University of Vienna, Austria, 2.CIC biomaGUNE, center for cooperative research in biomaterials, Spain）

[P2-29] Aquatic pollutant removal by adsorption in zeolite structures: An experimental and molecular simulation study

○Mate Erdos[1], Nan Jiang[2], Sebastian G. J. Heijman[2], Othonas A. Moultos[1] （1.Process &Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Netherlands, 2.Department of Water Management, Faculty of Civil Engineering and Geosciences, Delft University of Technology, Netherlands）

[P2-30] Optimizing elastic moduli of the silicate glasses through high-throughput atomistic modeling and machine learning techniques

Yong-Jie Hu[1], Ge Zhao[2], Tyler Del Rose[1], ○Liang Qi[1] （1.Dept. of Materials Science and Engineering, University of Michigan, United States of America, 2.Department of Statistics, Pennsylvania State University, United States of America）

[P2-31] High pressure phase transition and structural stability of transition metal compounds

○Fanyan Meng[1], Wandong Xing[1,2], Rong Yu[2] （1.Dept. of Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-32] Development of artificial neural network model for prediction of electronic density of states in atomistic systems

○Atsushi Kubo, Yoshitaka Umeno （Institute of Industrial Science, the University of Tokyo, Japan）

[P2-33] Development of First-principles Platform Technology for Energy Research

○Kanghoon Yim[1], Chan-Woo Lee[1], Jehyun Lee[1], Incheol Jeong[2], Yong Youn[3], Seungwu Han[3] （1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Dept. of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science &Technology, Korea, 3.Seoul National University, Korea）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-26] Generalized nano-thermodynamic model for predicting size-dependent surface segregation in multi-metal alloy nanoparticles from smaller particles

○Abhijit Chatterjee （Dept. of Chemical Engg., Indian Institute of Technology Bombay, India）

Multi-metal alloy nanoparticles (NPs) offer new avenues for exploration and design of nanoscale-properties, e.g., catalytic, electronic and optical, by virtue of their tunable composition. Unfortunately, a method that can aid such exploration by accurately predicting the size-, shape- and composition-dependent elemental distribution associated with nanomaterials is crucially missing. A nano-thermodynamic model based on distribution coefficients Δ is introduced to fill this gap. Δ is employed to predict surface segregation in NPs as a function of the NP size and composition. Interestingly, we find Δ to be independent of size for NPs beyond 2 nm. This key finding motivates the construction of thermodynamic tables for distribution coefficients using segregation observed with one or more NP sizes. The tables can enable accurate prediction of phase diagrams for nanomaterials across a wide-range of sizes. Key concepts of this new theory are demonstrated with Au-Pt-Pd, Ag-Au-Pd and Ni-Pt-Pd, which are found to exhibit complex size-dependent segregation behavior for 2-6 nm NPs and relatively weaker size-dependence beyond 6 nm. Numerically well-converged values of Δ are calculated for small NPs using Monte Carlo simulations in the canonical ensemble. Simulations are based on an embedded atom method (EAM) potential for metal alloys.
[1] S Divi, A Chatterjee, RSC Advances 8, 10409, 2018.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-27] Development of thermodynamic database of Nd-Fe-B-based permanent magnet alloys

○Jiang Wang, Lei Xu, Kaicheng Yang, Qingrong Yao, Guanghui Rao, Huaiying Zhou （School of Material Science and Engineering, Guilin University of Electronic Technology, China）

Nd-Fe-B permanent magnets with excellent magnetic properties have been used in the industrial applications including medical apparatus and instruments, electrical machinery, aerospace, permanent magnet motor and wind power. In order to fully balance the application of rare-earth resource in magnetic materials and reduce the costs, it is a promise way to introduce high abundant rare earth (RE) metals (e.g. La, Ce, Y) into Nd-Fe-B permanent magnets [1-3]. Phase diagrams and thermodynamic information of the RE-Fe-B alloys are necessary to understand the effect of the abundant rare earth metals on phase formation, microstructure and magnetic properties of Nd-Fe-B permanent magnets.

In this work, the RE-Fe, RE-B and Fe-B sub-binary systems were reviewed firstly in the published literature. After that, the RE-Fe-B (RE=La, Ce, Pr, Nd) ternary systems were assessed using CALPHAD method on the basis of thermodynamic data and phase equilibria data, which is fundamental to obtain the thermodynamic database of multi-component RE-Fe-B alloy systems. The calculated results including liquid projects, isothermal sections and vertical sections as well as the solidification path of some alloys were compared with the experimental results using the thermodynamic database obtained. The thermodynamic database of the Nd-Fe-B-based permanent magnet alloy systems with high abundant rare earth elements is developed finally, which is necessary to design alloy composition and heat treatments of novel Nd-Fe-B permanent magnets

with good magnetic properties and low costs.

References

[1] X.J. Cao, L. Chen, S. Guo, J.H. Di, G.F. Ding, R.J. Chen, A.R. Yan, K.Z. Chen, Aip Adv. 8 (2018) 056222.
[2] L. Liu, H. Sepehri-Amin, T. Ohkubo, M. Yano, A. Kato, T. Shoji, K. Hono, J. Alloy. Comp. 666 (2016) 432-439.
[3] J.Y. Jin, T.Y. Ma, M. Yan, Y.J. Zhang, B.X. Peng, Y.S. Liu, F.H. Cao, J. Alloy. Comp. 735 (2018) 2225-2235.

Acknowledgements

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-28] Design of proteins and biopolymers: role of directional interactions and of water.

○Valentino Bianco[1], Ivan Coluzza[2]   (1.University of Vienna, Austria, 2.CIC biomaGUNE, center for cooperative research in biomaterials, Spain)

The design of a (bio-)polymer is a rational scheme allowing to transfer the one-dimensional information contained in the polymer sequence into the three-dimensional information contained in the polymer folded conformation.
Proteins are an example of designable heteropolymers able to fold in unique target structures. The stability of the native conformation depends on the protein sequence and on the thermodynamic conditions of temperature and pressure.
In our work we use a multiscale approach to investigate how the geometry of the polymer backbone and the properties of the surrounding water affect the selection and the stability of proteins and, more in general, of artificial heteropolymers.
We find that the key actors are: i) the directional interactions along the backbone and ii) the hydrophilic/hydrophobic composition of the surface and core of the folded structure.

References:

V. Bianco, G. Franzese, C. Dellago, I. Coluzza, Phys. Rev. X 7, 021047, 2017.
V. Bianco, N. Pagès-Gelabert, I. Coluzza, G. Franzese, J. Mol. Liq. 245, 129, 2017.
C. Cardelli, V. Bianco, L. Rovigatti, F. Nerattini, L. Tubiana, C. Dellago, I. Coluzza, Sci. Rep. 7, 4986, 2017.
V. Bianco, G. Franzese, Phys. Rev. Lett. 115, 108101, 2015.
V. Bianco, S. Iskrov, G. Franzese, J. Biol. Phys. 38, 27, 2012.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-29] Aquatic pollutant removal by adsorption in zeolite structures: An experimental and molecular simulation study

○Mate Erdos[1], Nan Jiang[2], Sebastian G. J. Heijman[2], Othonas A. Moultos[1]　(1.Process &Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Netherlands, 2.Department of Water Management, Faculty of Civil Engineering and Geosciences, Delft University of Technology, Netherlands)

Water contamination with micropollutants poses a serious threat to public health and the ecosystem. Technologies based on adsorption are widely used to remove micropollutants (inorganic and organic) from wastewater. Zeolites show a promising potential as adsorbents in these applications. Zeolites are crystalline, microporous aluminosilicates with well-defined 3-dimensional structure, composed of tetrahedral SiO_4 and AlO_4 clusters connected to each other by shared oxygen atoms. To compensate the charge imbalance caused by the aluminum content of the framework, exchangeable cations (usually alkali and alkaline earth cations) are located in the cavities of the structure. By removing the aluminum content of the framework the hydrophobicity of the zeolite can be increased, providing favorable adsorption characteristic to organic molecules. In this study, the effect of aluminium content of zeolite structures for aquatic pollutant removal are investigated. To that end, molecular simulations using Monte Carlo method are performed. In comparison with experimental methods, these simulation techniques can provide fundamental understanding of the nano scale behavior of the system which is crucial for designing new materials.
In this study, two types of zeolites (FAU, BEA) with different aquatic pollutants (2,4,6-trichlorophenol, triclosan) are investigated experimentally and with simulations. The simulated and experimentally measured results show qualitative agreement. To obtain insights into the adsorption mechanisms, radial distribution functions, and the distribution of adsorbates are calculated for each structure. The preferred adsorption sites and configuration of adsorbates (e.g., pi-pi stacking, H-bonding) are identified for each adsorbates and structures. Based on the simulation and experimental results the relationship of aluminium content and adsorption affinity can be determined and the performance of the different zeolites can be evaluated.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-30] Optimizing elastic moduli of the silicate glasses through high-throughput atomistic modeling and machine learning techniques

Yong-Jie Hu[1], Ge Zhao[2], Tyler Del Rose[1], ○Liang Qi[1]　(1.Dept. of Materials Science and Engineering, University of Michigan, United States of America, 2.Department of Statistics, Pennsylvania State University, United States of America)

Chemical design of the silicate glass with high elastic moduli is of great interest. However, it is difficult to find a universal expression to predict the elastic moduli according to the glass composition before synthesis since the elastic moduli are a complex function of several material properties at different length scales. This work presents a computational framework to efficiently predict the elastic moduli of the silicate glass across a multicomponent compositional design space, including 11 types of additive oxides, by integrations of high-throughput molecular dynamic (MD) calculations and machine learning (ML) techniques. Our newly developed ML model can predict the elastic moduli for k-nary silicate glass systems, using the learning datasets generated from MD calculations for only binary and ternary systems. The usefulness of our model is

illustrated by identifying the most relevant materials descriptors that determine the elastic moduli and screening for the silicate glasses with high stiffness.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-31] High pressure phase transition and structural stability of transition metal compounds

○Fanyan Meng[1], Wandong Xing[1,2], Rong Yu[2]　(1.Dept. of Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China)

The lattice, charge, spin and other degrees of freedom in transition metal compounds couple to one another, giving these materials rich physics and properties. The extreme conditions of high pressure and high temperature provide a new way to create new structures that do not exist at ambient pressure, which has become an important way for the discovery of novel transition metal compounds. In recent years, important progress has been made in the theoretical prediction and high pressure synthesis of new structures. First, this work suggests a lot of new materials to be investigated by changing stoichiometry in phase diagrams. Taking the V-C binary system as an example, here we report the first-principles prediction of a new type of vanadium carbide, V_5C_3, which has an unprecedented stoichiometry in the V-C system. It is demonstrated that the new phase is mechanically stable, and is energetically favorable than known phases under high pressures. We believe that this work opens a door to materials design by changing stoichiometry. And the relationship between the crystal structure, electronic structure and physical properties are discussed. Secondly, the phase transition under high pressure will be analyzed to understand the structural stability of materials at high temperatures and high pressures, providing important theoretical basis for optimizing high-pressure synthesis conditions.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-32] Development of artificial neural network model for prediction of electronic density of states in atomistic systems

○Atsushi Kubo, Yoshitaka Umeno　(Institute of Industrial Science, the University of Tokyo, Japan)

Recently, the artificial neural network (ANN) model has been intensively applied to interatomic potentials for atomistic simulations. ANN-based potential functions possess basic characteristics; i.e., (1) they do not have any physical background besides the least geometrical conditions, e.g., physical quantity conservation against any coordinate transformation; (2) theoretically they can mimic any continuous functions. These features make ANN potentials applicable to complex atomistic systems, where various crystal structures and phases are relevant.

Since an ANN potential can be simply regarded as a mapping from atomistic structure to a real number, it is found that the application of ANNs does not have to be limited only for prediction of potential energy; i.e., ANNs are applicable to prediction of other physical quantities or material properties of the atomistic systems, e.g., electronic density of states (DoS), magnetic moment, etc. However, to the best of our knowledge, there has been no attempt to apply ANNs to prediction of physical quantities beside potential energy in atomistic systems. It will be of great impact if we can evaluate physical quantities such as electric or magnetic properties in huge atomistic structures using ANNs with the accuracy of the first-principles calculation.

In this study, we developed an ANN model to predict the DoS, as an exemplified case of prediction of general physical quantities in atomistic systems with ANNs. The ANN was optimized to reproduce the DoS in various crystal structures of silicon-carbon system that was obtained by first-principles calculations based on the density functional theory.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-33] Development of First-principles Platform Technology for Energy Research

○Kanghoon Yim[1], Chan-Woo Lee[1], Jehyun Lee[1], Incheol Jeong[2], Yong Youn[3], Seungwu Han[3] (1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Dept. of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science &Technology, Korea, 3.Seoul National University, Korea)

As future energy technologies such as high-capacity energy storage and renewable energy applications require exceptional functionalities of host materials, the importance of employing a novel material is getting bigger and bigger. However, discovering a new superior material is very hard to success though it requires large costs and manpower. Recently, many researchers attempt to use an informatics technology such as machine learning in materials screening to overcome the realistic limitations of conventional trial and error method. The key to successive research using informatics technology largely depends on the quantity and quality of the considered database rather than technical details of informatics model. Since property data from experiments are usually sparse or biased to favorable materials in industry, it is hard to obtain a practical database for the informatics research. In that point of view, first-principles calculation is an excellent tool for generating systematic and reliable data of materials properties. However, first-principles calculation itself also requires considerable computational resources and many practical properties are hard to obtain by simple calculations. Therefore, a decent automation of first-principles calculation can do a significant role to establish a successive database. In this talk, I'll introduce the first-principles platform of Korea Institute of Energy Research aiming at providing a practical computing platform for various researchers with different backgrounds. After introducing the importance of well-defined automation procedure in former materials design studies such finding novel high-k dielectrics and p-type transparent oxides, I'll introduce the automated platform technology for surface-adsorption reactions which have great importance in most energy applications.

Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E2] Poster Session 2

Symposium E

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-34] Dynamics of a solidification front made by invasion of fluid with a different temperature

○So Kitsunezaki, Chika Yamanaka （Nara Women's Univ., Japan）

[P2-35] Strengthening through solid solution in $W_{1-x}Ta_xB$ system

○Iijuan Iiu[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-36] Desiccation crack patterns based on phase-field modeling and their statistical properties

○Shin-ichi Ito[1], Satoshi Yukawa[2] （1.The Univ. of Tokyo, Japan, 2.Osaka Univ., Japan）

[P2-37] Ce-terminated (111) surface of CeO_2

○YaNan Zhao[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-39] Numerical analysis of elasto-plastic behavior of metallic architectured materials

○Filip Siska[1], Ivo Dlouhy[1], Jan Cizek[2], Hanus Seiner[3] （1.Institute of Physics of Materials, Czech Academy of Sciences, Czech Republic, 2.Institute of Materials Science and Engineering, Brno University of Technology, Czech Republic, 3.Institute of Thermomechanics, Czech Academy of Sciences, Czech Republic）

[P2-40] Automatic analysis and numerical prediction of flow stress curves for aluminium alloys

○Evgeniya Kabliman, Johannes Kronsteiner, Ana-Helena Kolody （Light Metals Technologies Ranshofen, Center fo Low-Emission Transport, Austrian Institute of Technology, Austria）

[P2-41] Comparison of different alkali activated mortars with hemp fibres response during fracture test by acoustic emission method

Libor Topolar[1], ○Hana Simonova[1], Barbara Kucharczykova[1], Zbynek Kersner[1], Jelena Dragas[2], Ivan Ignjatovic[2], Miroslav Komljenovic[3], Violeta Nikolic[3] （1.Brno University of Technology, Faculty of Civil Engineering, Czech Republic, 2.University of Belgrade, Faculty of Civil Engineering, Serbia, 3.University of Belgrade, Institute for Multidisciplinary Research, Serbia）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-34] Dynamics of a solidification front made by invasion of fluid with a different temperature

○So Kitsunezaki, Chika Yamanaka （Nara Women's Univ., Japan）

When fluid flows into another hotter or colder fluid, solidification often occurs in narrow regions at the vicinity of the interface. Such interfaces exhibit peculiar patterns in the growth process because of accompanying solidification fronts. Similar phenomena are observed in soft membranes created by chemical reactions of two fluid, as reported by H.~Wagatsuma et al.(Physical Review E, 2017). In geological scales, we could also see examples of such phenomena in pillow lava and growth of a volcanic island.
We carried out experiments by pouring ice-cold water into paraffin melt in a Hele-Shaw cell and found that solidification of paraffin causes fingering patterns with large meandering. The melting temperature of paraffin we used is about 56-58 degrees C, but the rheological measurements indicated that paraffin behaves as a soft viscoelastic material under the temperature. We infer that precipitous increase of the viscosity of paraffin is mainly responsible for large meandering of fingering growth.
A simple two-dimensional mathematical model is considered to find an interface dynamics in such phenomena theoretically. Although a standard method of the center-manifold reduction can not be used for solidification fronts growing in time, we develop a similar systematic method to derive the equations of interface motion.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-35] Strengthening through solid solution in $W_{1-x}Ta_xB$ system

○lijuan liu[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

The elastic properties, electronic structures and the energy barriers in slip processes of $W_{1-x}Ta_xB$ system have been studied using first-principles calculations. It was found that the (110) plane is the easiest slip plane in tungsten monoboride. By substituting tungsten with tantalum, slipping on the (110) plane can be hindered through dislocation pinning, resulting in the increase of overall hardness of tungsten monoboride Strengthening of the easiest planes is an effective approach to creating new hard materials in more metallic materials.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-36] Desiccation crack patterns based on phase-field modeling and their statistical properties

○Shin-ichi Ito[1], Satoshi Yukawa[2] （1.The Univ. of Tokyo, Japan, 2.Osaka Univ., Japan）

We investigate morphological properties on desiccation crack patterns through numerical simulations of a phase-field (PF) model. Since our PF model does not require any assumptions related to crack nucleations and numerical lattice configurations, we can investigate the pattern formations that purely depend on material/external parameters. Our PF model showed us various pattern formations depending on a drying

speed and material constants. We discovered, in particular, the difference of the drying speed provides a significantly qualitative difference in the pattern formations. Cellular patterns resulting from sequential fragmentations of straight cracks can be observed when using a slow drying speed, while random network patterns resulting from connections of micro cracks that appear simultaneously can be observed when using a rapid drying speed. We quantify the difference of the pattern formations statistically, and explain the origin of the difference on the basis of a simple continuum theory of a thin layer of viscoelastic material.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-37] Ce-terminated (111) surface of CeO$_2$

○YaNan Zhao[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] (1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China)

Surface structure and properties of ceria are closely related to the applications of ceria in catalysis. Here, the atomic structures of the (111) surface of CeO$_2$ nanoparticles have been studied combining aberration-corrected transmission electron microscopy and first-principles calculations. Besides the oxygen termination that have reported extensively previously, the cerium termination has also been revealed by direct atomic imaging, which can be viewed as the simultaneous loss of surface and subsurface oxygen. The stabilization mechanism, electronic structure and magnetism of the surface, and the behavior of oxygen vacancies have been discussed.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-39] Numerical analysis of elasto-plastic behavior of metallic architectured materials

○Filip Siska[1], Ivo Dlouhy[1], Jan Cizek[2], Hanus Seiner[3] (1.Institute of Physics of Materials, Czech Academy of Sciences, Czech Republic, 2.Institute of Materials Science and Engineering, Brno University of Technology, Czech Republic, 3.Institute of Thermomechanics, Czech Academy of Sciences, Czech Republic）

Architectured materials is a class of materials that is characteristic by the ordering of constituents in specific geometrical manner. Such geometry provides an extra degree of freedom which allows reaching combinations of properties that cannot be obtained by standard materials. Metallic architectured materials are especially attractive because metals are important structural materials and adding internal architecture can enhance their performance in particular applications.
Our study is focused on a numerical investigation of an elasto-plastic response of different planar architectured patterns under the basic types of loading (tension-compression, bending). These patterns are made by different combinations of basic metals (for example: Al, Fe, Ti). The objective is to find the relation between the geometry and the resulting properties like stiffness, strength, hardening, ductility, buckling resistance. These relations will help to find optimal internal structure geometries for given materials combinations and loadings. The results from FE simulations will be further used for the production of the real structures using cold spray technology which is very well suited for a fabrication of structures and materials made of metals with different mechanical and physical properties.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-40] Automatic analysis and numerical prediction of flow stress curves for aluminium alloys

○Evgeniya Kabliman, Johannes Kronsteiner, Ana-Helena Kolody （Light Metals Technologies Ranshofen, Center fo Low-Emission Transport, Austrian Institute of Technology, Austria）

In present work, we develop a toolkit for automatic analysis of experimental flow stress curves as well for their numerical prediction by a combined approach of physics based and data driven modelling. By using a single environment it is possible to filter measured raw data, account for temperature increase during a deformation process, extract the mechanical properties such as yield and ultimate strength, obtain the processing maps for the optimization of deformation conditions, as well as to predict the flow stress curves by using a dislocation density based model in combination with algorithms of machine learning. It is possible to account for processes such as work hardening and recovery due to spontaneous annihilation of dislocations and their climb. For testing purposes we choose a conventional AA6082 alloy and perform a series of hot compression tests by using a deformation and quenching dilatometer DIL805A/D of TA Instruments. In order to choose the most suitable algorithm of machine learning, different approaches found in literature for the prediction of flow stress curves are compared. A modified version of a flow stress model is formulated and implemented into a finite element framework, as a result.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-41] Comparison of different alkali activated mortars with hemp fibres response during fracture test by acoustic emission method

Libor Topolar[1], ○Hana Simonova[1], Barbara Kucharczykova[1], Zbynek Kersner[1], Jelena Dragas[2], Ivan Ignjatovic[2], Miroslav Komljenovic[3], Violeta Nikolic[3] （1.Brno University of Technology, Faculty of Civil Engineering, Czech Republic, 2.University of Belgrade, Faculty of Civil Engineering, Serbia, 3.University of Belgrade, Institute for Multidisciplinary Research, Serbia）

In last decades, natural fibres are increasingly used as reinforcements for the production of low-cost composites in civil engineering. The benefits of natural fibers include non-abrasive nature, high specific properties, and biodegradability. However, their disadvantages are the bad moisture absorption, poor wettability and large scattering in mechanical properties. The aim of this paper is contribute to the better understanding of mechanical behaviour and failure modes of alkali activated materials reinforced by hemp fibers. Two different mortars based on alkali activated fly ash and slag were investigated. The paper includes the results of acoustic emission measurement captured during the three-point bending fracture test of specimens made of mentioned composites. Acoustic emission method is proving useful for the capability of real-time monitoring of materials over the whole volume and with high sensitivity to any processes generating stress waves. The effect of different mix composition and amount of hemp fibers on the acoustic signal features such as the energy, counting and amplitude is including in this research. The obtained acoustic emission results together with mechanical fracture parameters can serve as input values of material models used for modelling of structure response.

University of Technology and University of Belgrade, are presented in this paper.

[PO-F2] Poster Session 2
Symposium F
Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-43] Design of spontaneous formation-based 3D plasmonic optical structure, using multyphysics modeling

○Jihwan Song[1], Inhee Choi[2], Yonghee Shin[3], SoonGweon Hong[5], Younggeun Park[5], Dongchoul Kim[4], Taewook Kang[3], Luke Lee[5]　(1.Dept. of Mechanical Engineering, Hanbat National University, Korea, 2.Dept. of Life Science, University of Seoul, Korea, 3.Dept. of Chemical and Biomolecular Engineering, Sogang University, Korea, 4.Dept. of Mechanical Engineering, Sogang University, Korea, 5.Dept. of Bioengineering and Berkeley Sensor and Actuator Center, University of California, Berkeley, United States of America)

[P2-44] Characterization of $K_xNa_{1-x}NbO_3$ powders and ceramics prepared by hydrothermal synthesis

○Jing Yang, Aifen Tian, Xuan Xi, Huiling Du　(Dept. of Materials Science and Engineering, Xi An Univ. of Science and Technology, China)

[P2-45] Numerical and experimental investigation of liquid metal dealloying of Cu-Ni alloy in liquid silver.

○Pierre-Antoine Geslin[1,2,3], Takumi Suga[2], Takeshi Wada[2], Hidemi Kato[2]　(1.INSA Lyon/CNRS, France, 2.Institute for Materials Research, Tohoku University, Japan, 3.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan)

[P2-46] Application of DLVO theory to predict dispersion stability of ZrO_2 submicron particles in electrolyte solutions

○Ming-Hong Chiueh, Tien-Jung Huang　(Industrial Technology Research Institute, Taiwan)

[P2-47] Multi-GPU large-scale phase-field lattice Boltzmann simulation of dendrite growth with thermal-solutal convection

○Shinji Sakane[1], Tomohiro Takaki[1], Munekazu Ohno[2], Yasushi Shibuta[3], Takayuki Aoki[4]　(1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.The University of Tokyo, Japan, 4.Tokyo Institute of Technology, Japan)

[P2-48] Stress analysis of 4H-SiC power devices via FEM and Raman spectroscopy

○Hiroki Sakakima[1], Asuka Hatano[1], Akihiro Goryu[2], Kenji Hirohata[2], Satoshi Izumi[1]　(1.The Univ. of Tokyo, Japan, 2.Toshiba, Japan)

[P2-49] A Functionally Graded Multi-Phase Micromechanical Model for Carbon Nanotube - Polymer Composites

○Vahidullah Tac[1,2], Ercan Gurses[1]　(1.Middle East Technical University, Turkey, 2.Turkish Aerospace Industries, Turkey)

[P2-50] Atomic surface treatment of copper nanowires by electron beam irradiation simulated by first principle calculation

○Shih Kuang Lee　(National Chiao Tung University, Taiwan)

[P2-51] Molecular-Dynamic Simulation of Rapid Solidification of Dipolar Molecular Crystal from Its Melt

○Xianqi Xu, Yang Yang　(East China Normal University, China)

[P2-52] Intrinsic Analysis of Structural Order Parameter at Equilibrium Crystal-Melt Interfaces

○Wenliang Lu, Hongtao Liang, Yang Yang （EAST CHINA NORMAL UNIVERSITY, China）

[P2-53] Multiscale Modelling of Indirect-to-Direct Band Gap Transition in Silicon Nanosheets

○Byung-Hyun Kim[1], Chan-Woo Lee[1], Mina Park[2], Gyubong Kim[2], Kersti Hermansson[3], Peter Broqvist[3], Heon-Jin Choi[4], Kwang-Ryeol Lee[2] （1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Computational Science Research Center, Korea Institute of Science and Technology, Korea, 3.Dept. of Chemistry-Ångström Laboratory, Uppsala University, Sweden, 4.Dept. of Materials Science and Engineering, Yonsei University, Korea）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-43] Design of spontaneous formation-based 3D plasmonic optical structure, using multyphysics modeling

○Jihwan Song[1], Inhee Choi[2], Yonghee Shin[3], SoonGweon Hong[5], Younggeun Park[5], Dongchoul Kim[4], Taewook Kang[3], Luke Lee[5]　(1.Dept. of Mechanical Engineering, Hanbat National University, Korea, 2.Dept. of Life Science, University of Seoul, Korea, 3.Dept. of Chemical and Biomolecular Engineering, Sogang University, Korea, 4.Dept. of Mechanical Engineering, Sogang University, Korea, 5.Dept. of Bioengineering and Berkeley Sensor and Actuator Center, University of California, Berkeley, United States of America)

Oil droplets in water or water droplets in oil have been generated fascinating science and utilized in enormous applications from medicine to energy harvesting. However, the creation of integrated three-dimensional architectures by liquid droplet and immiscible liquid interface is relatively less investigated. Here we report interfacial energy-driven and spontaneous formation of plasmonic cavity at room temperature without an external force. With the multiphysics approach considering the densities and interfacial energies of two different liquids, we simulated the spontaneous formation of cavity when a liquid water droplet meets immiscible liquid interface. At the interface, the metal ions in the liquid droplet are automatically reduced and they form the interfacial plasmonic layer onto the cavity surface. Due to the both optical cavity and integrated plasmonic structure, the significantly enhanced fluorescence is obtained by 1000 times. We believe our findings could offer a new avenue and advance in a variety of photonic and plasmonic materials and devices.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-44] Characterization of $K_xNa_{1-x}NbO_3$ powders and ceramics prepared by hydrothermal synthesis

○Jing Yang, Aifen Tian, Xuan Xi, Huiling Du　(Dept. of Materials Science and Engineering, Xi An Univ. of Science and Technology, China)

There is an increasing demand to replace $Pb(Zr,Ti)O_3$-based piezoelectric materials with lead-free alternatives, because of the toxicity of lead oxide which is largely used during the production process. $K_xNa_{1-x}NbO_3$ (KNN) is considered as one of the most promising candidates for lead free piezoelectric ceramics due to its high Curie temperature and good electrical properties.

$K_xNa_{1-x}NbO_3$ ceramics can be used for several applications such as high frequency transducers, ultra-sonic diagnostics and tunable micro-wave components. However, it is well known that dense and well-sintered $K_{0.5}Na_{0.5}NbO_3$ ceramics are very difficult to obtain by the ordinary sintering process owing to the high volatility of alkali elements at high temperatures. The major strategy to overcome this problem is simply to synthetized KNN powders at low temperature. One method of making dense $(K_xNa_{1-x})NbO_3$ ceramics is to use refined powder with improved sintering activity, prepared in the molten salt process, sol-gel routine or hydrothermal process. In this work, $(K_xNa_{1-x})NbO_3$ powders and ceramics were prepared by hydrothermal synthesis. X-ray diffraction and scanning electron microscope were performed to investigate the structure and surface morphology of the $(K_xNa_{1-x})NbO_3$ powders and ceramics. The results showed that all the KNN powders possessed the pervoskite structure and a handful of second phases. The $K_{0.7}Na_{0.3}NbO_3$ ceramic prepared by the powders exhibits relatively good properties (relative dielectric constant ε = 416 and piezoelectric coefficient d_{33}=40 pC/N).

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-45] Numerical and experimental investigation of liquid metal dealloying of Cu-Ni alloy in liquid silver.

○Pierre-Antoine Geslin[1,2,3], Takumi Suga[2], Takeshi Wada[2], Hidemi Kato[2] （1.INSA Lyon/CNRS, France, 2.Institute for Materials Research, Tohoku University, Japan, 3.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan）

Liquid metal dealloying has emerged as a promising technique to produce finely porous structures of various nature (non-noble metals, refractory metals or semi-conductors) presenting a high surface area, valuable in a numerous applications (catalysis, battery materials, sensors,...). This process consists in emerging a binary precursor alloy (i.e. Cu-Ni) in a liquid metal (Ag) chosen such that only one element of the precursor alloy (Cu) dissolves into the metallic melt while the other element (Ni) reorganizes into a porous structure. We investigated the formation of this microstructure based on the ternary phase diagram of the Ni-Cu-Ag system. First, we developed a quantitative phase-field model to investigate the initiation of this dealloying process. The phase-field method is particularly adapted to investigate this kind of free-boundary problem and the complex morphogenesis of the structures, but is enable to reach the experimental time and size-scales. In a multi-scale approach, we use phase-field results and experimental observations to develop a macroscopic diffusion model able to reproduce the kinetics and the composition profiles obtained experimentally. Also, based on this work on the Cu-Ni-Ag model system, we were able to generalize our findings to other systems and assess the potential of other systems to form finely porous microstructures upon dealloying.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-46] Application of DLVO theory to predict dispersion stability of ZrO_2 submicron particles in electrolyte solutions

○Ming-Hong Chiueh, Tien-Jung Huang   (Industrial Technology Research Institute, Taiwan）

In the manufacturing process of multi-layer ceramic capacitors (MLCC), electronic components often used in modern mobile phones, dispersion stability of ZrO_2 submicron particles can be improved by altering the pH of electrolyte solution. In this study we used the DLVO theory to predict the energy barriers of interaction forces between two ZrO_2 particles in various electrolyte solutions at different pH. The electrolyte solutions may be strong basic, weakly acidic, or strong acidic. The distance-dependent potentials of van der Walls force and electrical double layer force were calculated. The calculation results show that weakly acidic solution induces larger energy barrier between ZrO_2 particles, because of stronger electrical double layer force. This larger energy barrier can prevent aggregation of ZrO_2 particles and lead to dispersion stability.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-47] Multi-GPU large-scale phase-field lattice Boltzmann simulation of dendrite growth with thermal-solutal convection

○Shinji Sakane[1], Tomohiro Takaki[1], Munekazu Ohno[2], Yasushi Shibuta[3], Takayuki Aoki[4] （1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.The University of Tokyo, Japan, 4.Tokyo Institute of Technology, Japan）

Thermal-solutal convection, that inevitably occurs during terrestrial solidification of an alloy, drastically changes the dendrite morphology and microsegregation. Although phase-field method is the most powerful computational tool for predicting the dendrite morphology and microsegregation, we need many computational costs in the phase-field simulation taking the thermal-solutal convection into account. In this study, we enable a large-scale simulation for phase-field lattice Boltzmann model, which can express the dendrite growth with the transport of solute and heat and the fluid flow. Here, to reduce the computational cost, we employ a multi-level mesh and multi-level time step when solving phase-field equation, advection-diffusion equations for heat and solute, and lattice Boltzmann equation for computing the fluid flow. In addition, to accelerate the large-scale simulation, we implement the parallel computation using multiple graphics processing units (GPU). By employing the developed scheme, we perform the dendrite growth simulation during directional solidification of a binary alloy with thermal-solutal convection and investigate the effects of thermal-solutal convection on the dendrite morphology.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-48] Stress analysis of 4H-SiC power devices via FEM and Raman spectroscopy

○Hiroki Sakakima[1], Asuka Hatano[1], Akihiro Goryu[2], Kenji Hirohata[2], Satoshi Izumi[1] （1.The Univ. of Tokyo, Japan, 2.Toshiba, Japan）

We developed a scheme to analyze the stress distribution of 4H-SiC power devices by FEM and Raman spectroscopy. Raman spectroscopy is widely applied as a method for evaluating stress distribution of semiconductor devices. However, the relationship between phonon frequency, which is measured by Raman spectroscopy, and stress tensor is not clarified for 4H-SiC. In addition, it is impossible to evaluate the distribution of the stress tensor having six components only by Raman spectroscopy since the phonon frequency is a scalar quantity. To solve these problems, we detected phonon deformation potentials, which are the relationships between phonon frequency and stress tensor, and developed the analysis method combining FEM and Raman spectroscopy. Firstly, phonon deformation potentials were detected by first principle calculation. The phonon frequency of the strained crystal is calculated. All components of the phonon deformation potential constants were obtained from the relationship between the magnitude of stress and the phonon frequency shift. The calculated deformation potential constants were validated by previous experimental results. Secondly, multi-step thermal-stress FEM analysis which reproduces actual fabrication process was conducted for a pin diode. Young's modulus, linear expansion coefficient and intrinsic stress of thin films formed on SiC substrates were measured. The obtained stress distribution was converted into the distribution of the phonon frequency shift and validated through comparison with the result of the micro Raman spectroscopy. The obtained stress distribution and its origin will be presented. This work was supported by Council for Science, Technology and Innovation(CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), "Next-generation power electronics/Consistent R&D of next-generation SiC power electronics" (funding agency: NEDO)

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-49] A Functionally Graded Multi-Phase Micromechanical Model for Carbon Nanotube - Polymer Composites

○Vahidullah Tac[1,2], Ercan Gurses[1] (1.Middle East Technical University, Turkey, 2.Turkish Aerospace Industries, Turkey)

Carbon nanotubes (CNT) are widely known for their superior stiffness as well as strength since their discovery in 1991. While our current level of understanding of carbon nanotubes prevent us from using them in structural parts per se, embedding them in polymers for strengthening and stiffening purposes shows a great potential. However practical efforts towards designing, manufacturing and employing such nanocomposite materials have not yet fully culminated largely due to a lack of understanding of the bonding between the nanotube and the polymer.

Latest experimental and molecular mechanical observations of the region around a carbon nanotube embedded inside a polymer indicate the presence of at least four distinct "phases" in nanocomposites; the CNT, the thin interfacial gap between the CNT and the polymer, a large portion of polymer around the CNT with linearly varying properties, and the bulk polymer phase.

Hence, to accurately model nanocomposite material the varying nature of polymer in the proximity of the CNT has to be taken into account, among other things.

We adopt a multi-phase micromechanical model that allows gradual degradation/upgradation of the constituent phases to study the mechanical properties of CNT-Polymer composites. Using this model the mechanical properties of the polymer is gradually enhanced in the vicinity of the CNT. We also study the effect of the gap between the CNT and the polymer and the role it plays in such nanocomposites. The results of our analyses are then compared to experimental data and discussed in detail.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-50] Atomic surface treatment of copper nanowires by electron beam irradiation simulated by first principle calculation

○Shih Kuang Lee (National Chiao Tung University, Taiwan)

Atomic surface treatment of copper nanowires by electron beam irradiation simulated by first principle calculation

Alex Lee [a],Ting-Yi Lin [a], Yu-Chieh Lo [a], and Wen-Wei Wu [a]

[a] Department of Materials Science and Engineering, National Chiao Tung University 1001 University Road, Hsinchu 300, Taiwan 300

[*] Correspondence and requests for materials should be addressed to W.W.W (email:

WWWu@mail.nctu.edu.tw)

Recently, the techniques of atomic surface treatment by electron beam etching has developed vigorously. However, the improvement and more details should be understood specially in atomic scale. In the experiment when we applied the electron beam on copper nanowires with copper oxide (111) surface without heating, it was found the reduction reaction and the following Cu clusters slip on Cu (111) surface. For further complete the mechanism, we provide the Vienna ab initio simulation package (vasp) to perform the GGA calculation with PAW pseuodopotentials. For reduction reaction, we compare the energy between the theoretical structure of Cu with oxide surface and Cu (111) surface to predict the binding energy of oxygen. For the slip of Cu clusters, we calculate the energy mapping of slip path on Cu (111) surface to find the most probable routine of slip. The calculation data should help us control the intensity of electron beam radiation when we do the surface treatment of material and be the complement of slip observation.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-51] Molecular-Dynamic Simulation of Rapid Solidification of Dipolar Molecular Crystal from Its Melt

○Xianqi Xu, Yang Yang （East China Normal University, China）

We present results of molecular dynamics (MD) simulations of crystal growth from the melt. The work focuses on a face-centered-cubic molecular crystal consist with molecules modeled by an extended point dipole model. We will present results of non-equilibrium MD growth simulations as a function of temperature and molecular dipole moment. An analysis of the interfacial position as the function of simulation time was employed to extract the steady-state, and the data of the kinetic coefficients vs. molecular dipole moments and their anisotropies were calculated and will be presented. Values of the kinetic coefficient for the (100), (110) interfaces are compared quantitatively to the prediction of Mikheev-Chernov (MC) theory. Our study suggest that incorporating a second relaxation time due to the dipolar fluctuation beside the relaxation time of density waves, is necessary for extending MC theory to be applicable for molecular crystals.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-52] Intrinsic Analysis of Structural Order Parameter at Equilibrium Crystal-Melt Interfaces

○Wenliang Lu, Hongtao Liang, Yang Yang （EAST CHINA NORMAL UNIVERSITY, China）

We present atomistic simulations of precisely equilibrated crystal-melt interface under ambient pressure, for pure Ni and Fe. We demonstrate the capillary waves roughen the surface, but the intrinsic interfaces can be sharply defined. We use different types of local structural order-parameter together with a reference lattice to characterize the intrinsic interface. The statistical analysis on the structural order-parameters for the interfacial solid and interfacial liquid atoms represents universal scaling behavior, nearly independent of the order parameter type, crystal structure and interface orientations. We will discuss the potential application of such intrinsic analysis to the investigations of crystal nucleation and steady-state crystallization from melt.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-53] Multiscale Modelling of Indirect-to-Direct Band Gap Transition in Silicon Nanosheets

○Byung-Hyun Kim[1], Chan-Woo Lee[1], Mina Park[2], Gyubong Kim[2], Kersti Hermansson[3], Peter Broqvist[3], Heon-Jin Choi[4], Kwang-Ryeol Lee[2] (1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Computational Science Research Center, Korea Institute of Science and Technology, Korea, 3.Dept. of Chemistry-Ångström Laboratory, Uppsala University, Sweden, 4.Dept. of Materials Science and Engineering, Yonsei University, Korea)

Two-dimensional (2D) nanomaterials such as graphene, boron nitride (BN), and MoS_2 have attracted great attention owing to their exceptional and tuneable properties, which are distinguishable from those of their bulk phases. Recently, Si nanosheets (Si NSs) have been synthesized by various experimental techniques. Compared to other materials, Si-based nanostructures have great advantages when it comes to commercialization, as Si is compatible with the conventional device manufacturing processes in the microelectronics industry.

In experiments, (111) Si NSs showed thickness-dependent light emissions in the visible wavelength regime, originating from quantum confinement effects. This observation indicates that thin (111) Si NSs have a direct band gap, whereas bulk Si normally has an indirect band gap. However, the question of the physical origin behind this nano-effect of Si left unanswered.

The effect of biaxial strain on the band structure of 2D Si NSs with (111), (110), and (001) exposed surfaces was investigated by means of a multiscale modelling approach combining molecular dynamics simulations with a reactie force field and the density functional theory. For all the considered Si NSs, an indirect-to-direct band gap transition occurs as the lateral dimensions of Si NSs increase, i.e. increasing lateral biaxial strain from compressive to tensile always enhances the direct band gap characteristics. Further analysis revealed the mechanism of the transition which is caused by preferential shifts of the conduction band edge at a specific k-point due to their bond characteristics. Our results explain a photoluminescence result of the (111) Si NSs [U. Kim *et al.*, *ACS Nano* **2011**, *5*, 2176-2181] in terms of the plausible tensile strain imposed in the unoxidized inner layer by the surface oxidation.

[PO-G2] Poster Session 2

Symposium G
Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-54] Component-wise Effect of Incompatibility Tensor on Misorientation Development in Lath Block Structure Model based on FTMP

○Yuta Amano, Tadashi Hasebe, Yasutaka Matsubara （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P2-55] Construction of virtual ITZ specimens using extended stochastic optimization and evaluation of their permeability

○Se-Yun Kim, Tong-Seok Han （Dept. of Civil and Environmental Engineering, Yonsei Univ., Korea）

[P2-56] Estimation for probabilistic distribution of material response according to microstructural characteristics

○JI-SU KIM, Tong-Seok Han （Yonsei Univ., Korea）

[P2-57] Hypervelocity impact and shock behavior of pillared graphene foams

○Stefano Signetti, Seunghwa Ryu （Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-54] Component-wise Effect of Incompatibility Tensor on Misorientation Development in Lath Block Structure Model based on FTMP

○Yuta Amano, Tadashi Hasebe, Yasutaka Matsubara　(Dept. of Mechanical Engineering, Kobe Univ., Japan)

Modeling complex microstructures, e.g., those like lath martensite structures in high Cr ferritic heat resistant steels, are one of the critical issues in multiscale modeling of materials, although neither conventional schemes exist nor effective methodologies have been developed to date. In the present study, FTMP (Field Theory of Multiscale Plasticity)-based Di-CAP (Deformation-induced Context-dependent Autonomic Pluripotency) concept is applied to computationally fabricate complex microstructured samples to be further utilized in various deformation analyses based on, e.g., FEM. Here, we focus on the process of modeling single lath-block structures, which can be obtained in preliminary bi-axial compression analyses, provided the corresponding eigenstrain distributions based on the Bain lattice correspondence is initially introduced. One of the keys for the lath-block modeling is the development of misorientation across the lath boundaries, roughly satisfying K-S variant, together with the attendant internal stress fields. FTMP-based approach exhibits spontaneous evolution of such misorientation when substantial contribution of the incompatibility tensor is introduced in the hardening law. Here we decompose the incompatibility tensor into (a)pure deformation and pure rotation, (b)edge and screw, and (c)spherical (isotropic) and deviatoric components, respectively, to examine the mechanisms for the misorientation developments. Analyses are conducted using two basic models for a single lath block structure, i.e., vertical and horizontal models, where lath sub-blocks are aligned vertically and horizontally to the [111] axis, respectively. Demonstrated for (a) is that the pure deformation part shows relatively larger contributions to the misorientation developments, while, for (b), dominant contributions of the screw component are confirmed. For (c), on the other hand, the weighted spherical part is shown to have weak but basically the same contribution.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-55] Construction of virtual ITZ specimens using extended stochastic optimization and evaluation of their permeability

○Se-Yun Kim, Tong-Seok Han　(Dept. of Civil and Environmental Engineering, Yonsei Univ., Korea)

The external substance penetrates into an interfacial transition zone (ITZ) that is located between an aggregate and bulk cement paste and has a relatively high porosity than the bulk cement paste. However, it is difficult to confirm the 3-D microstructure of the ITZ with the functionally graded void distribution to evaluate its permeability. In this study, 3-D microstructures of bulk cement pastes with three kinds of porosities and the void gradient of the ITZ obtained from 2-D SEM image are used to construct the virtual 3-D microstructures of the ITZ. Based on the two information, the phase distribution characteristics of the ITZ are generated, and they are used for constructing the virtual ITZ specimen using a stochastic optimization. The stochastic optimization is an appropriate method to construct a random heterogeneous material [1], but the ITZ has the functionally graded void distribution, which depends on the distance from the aggregate. To construct the functionally graded microstructure, an extended stochastic optimization is proposed. In addition, an efficient iteration method for stochastic optimization is proposed and utilized for construction of the virtual ITZ specimens, which improved the computational cost. The permeability of the virtual ITZ

specimens are evaluated by a finite element method. The effect of the ITZ from the penetration of the external substances is confirmed by the permeability analysis using the virtual ITZ specimen. This study shows that the proposed extended stochastic optimization process is effective for constructing functionally graded phase distribution, while the real 3-D microstructure is difficult to obtain from experimental techniques. This study also confirms that the virtual experiment procedure can be synergistically used with the real experimental approaches.

[1] S. Torquato, Random Heterogeneous Materials: microstructure and macroscopic properties, vol. 16, Springer Science &Business Media, Berlin, 2013.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-56] Estimation for probabilistic distribution of material response according to microstructural characteristics

○JI-SU KIM, Tong-Seok Han （Yonsei Univ., Korea）

There is a strong correlation between the material microstructure and its response [1]. It is expected that the statistical distribution of material response has a relation with that of the microstructure characteristics, so that the effect of the microstructure to the response can be investigated. In this study, the sensitivity of the material responses due to microstructural characteristics is investigated using a first-order second moment (FOSM) method [2]. The FOSM method is a probabilistic method, which determines the mean and deviation of a function of responses with random input variables. For applying the FOSM method, specimens with certain microstructure characteristics might have to be reconstructed. For this reason, the reconstruction process [3] to generate the target specimens are needed. The area of lineal-path function and porosity of cement paste specimens are selected as random input variables, and the stiffness and strength evaluated by phase field fracture model are selected as output variables. The result of sensitivity analysis from the FOSM method is compared to the simulation results using whole specimens. From this result, the sensitivity of material response to microstructure is estimated using two reconstructed specimens, and the FOSM method is confirmed to reduce the time and cost for evaluating the probabilistic distribution of properties.

[1] Mindess, S., Young, J. F., and Darwin, D. Concrete. 2nd ed. Prentice Hall U.S.A. (2003) 57-80.

[2] Lee, T.-H. Probabilistic Seismic Evaluation of Reinforced Concrete Structural Components and Systems. University of California, Berkeley (2005).

[3] Chung, S.-Y., Han, T.-S., Kim, S.-Y., and Lee, T.-H. Investigation of the permeability of porous concrete reconstructed using probabilistic description methods. Construction and Building Materials (2014) 66:760-770.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-57] Hypervelocity impact and shock behavior of pillared graphene foams

○Stefano Signetti, Seunghwa Ryu （Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea）

The effectiveness of graphene as material for impact protection has been confirmed both by atomistic simulations [1] and microscale experiment [2] obtaining unprecedented impact toughness up to ˜50 MJ/kg at the nanoscale [1]. However, specific energy absorption could be, in principle, further increased by tailoring inter-layer interaction [3] via interface structuring or functionalization. In this study we present a modified graphene nanoarmor concept obtained by the introduction of pillar structures in the form of carbon nanotubes [4] of variable spatial density, aspect ratio, and size which allow the realization of stable graphene multilayers with variable spacing. Impact strength and shock behavior of such structures are investigated via molecular dynamics (MD) simulations and the effect of foam geometry on the specific energy absorption capability is evaluated across different size-scales.

References

[1] S. Signetti, S. Taioli, N.M. Pugno. 2D Materials Armors Showing Superior Impact Strength of Few Layers. *ACS Applied Materials &Interfaces* 8:40820-40830, 2017.

[2] J. Lee, P.E. Loya, J. Lou, E.L. Thomas. Dynamic mechanical behaviour of multilayer graphene via supersonic projectile penetration. *ACS Applied Materials &Interfaces* 346(632):1092-1096, 2014.

[3] S. Signetti, N.M. Pugno. Evidence of optimal interfaces in bio-inspired ceramic-composite panels for superior ballistic protection. *Journal of the European Ceramic Society* 34:2823-2831, 2014.

[4] S. Lee, D. Kang, I. Oh. Multilayered graphene-carbon nanotube-iron oxide three-dimensional heterostructure for flexible electromagnetic interference shielding film. *Carbon* 111:248-257, 2017.

[PO-H2] Poster Session 2

Symposium H
Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-58] Studying the kinetics of a self-propelled cruiser in 2D granular media under gravity
○Guo-jie Jason Gao （Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan）

[P2-59] A Discrete Tetris model showing two flow regimes for hard particles exiting a hopper with an adjustable obstacle
○Tomoya Yasuno[1,2], Guo-jie Jason Gao[1] （1.Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan, 2.Dept. of Complex Systems Science, Nagoya Univ., Japan）

[P2-60] Effect of water molecules on polymer chain motion in dense chain ensembles of nafion membrane
○Isamu Riku, Ryoma Oka, Koji Mimura （Osaka Prefecture Univ., Japan）

[P2-61] A Coarse-Grained Model for Competitive Adsorption on the Surface of Inorganic Nanomaterials
○Stefano Poggio[1], Hender Lopez[2], David Power[1], Vladimir Lobaskin[1] （1.School of Physics, University College Dublin, Ireland, 2.Institute Laue-Langevin, Grenoble, France）

[P2-62] Molecular Dynamics of Inorganic and Organic Interfaces with Force-Field Parameters Based on DFT Simulations
○Kosuke Ohata, Hiroya Nitta, Kenta Chaki, Taku Ozawa （JSOL Corporation, Japan）

[P2-63] **Molecular dynamics screening for developing compounds of electrolytes with high performance in lithium ion batteries**
○Yoshihiro Takai[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] （1.Graduate school of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan）

[P2-64] Molecular dynamics study on transmission mechanism of torsional deformation in cellulose nanofibers with hierarchical structure
○Kentaro Takada[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] （1.Graduate School of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan）

[P2-65] Bubble dynamics of foam flow around an obstacle
○Antti Puisto, Juha Koivisto, Leevi Viitanen, Mikko J Alava （Aalto University, Department of Applied Physics, Finland）

[P2-66] Shape Deformation and Mechanical Relationship of Ionic Droplet Under An Electric Field
Bo-Yu Shih[1], ○Wei-Chun Lin[1], Alice Hu[2], Hsuan-Teh Hu[1], Yu-Chieh Lo[3] （1.Department of Civil Engineering,National Cheng Kung University, Taiwan, 2.Department of Mechanical and Biomedical Engineering, City University of Hong Kong, Hong Kong, 3.Department of Materials Science and Engineering, National Chiao Tung University, Taiwan）

[P2-67] Multiscale modeling of surface functionalized graphene/polymer nanocomposites: insight into the effect of covalent grafting
○Jeong-ha Lee[1], Seunghwa Yang[2] （1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea）

[P2-68] Durability analysis on the environmental aging of epoxybased nanocomposite

○Sunyong Kwon[1], Man Young Lee[2], Seunghwa Yang[3] （1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Agency for Defense Development, Korea, 3.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-58] Studying the kinetics of a self-propelled cruiser in 2D granular media under gravity

○Guo-jie Jason Gao （Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan）

Experimentally and numerically, it has been shown that placing an obstacle near the orifice of a hopper can locally enhance the flow rate for hard discs leaving the hopper under gravity. Besides, the enhanced flow rate happens regardless the interparticle friction, the obstacle geometry, or particle dispersity. In this study, we propose a Tetris model to further clarify the physics behind this phenomenon. The model sequentially moves one particle at a time towards the hopper orifice, governed by Gaussian displacement functions. A particle can move as long as the movement creates no overlap between the particle and the others, the obstacle, or the boundaries of the hopper. Our model reduces the dynamics in the system to its minimal and allows no interparticle collaborative motion due to Newtonian dynamics. Using this model, we successfully reproduce the locally enhanced flow rate, which can be explained by a flow rate difference between its value near the obstacle and its maximal value without an obstacle. Our results show that the flow rate difference is the fundamental reason causing this phenomenon - universal with minimal dynamics involved.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-59] A Discrete Tetris model showing two flow regimes for hard particles exiting a hopper with an adjustable obstacle

○Tomoya Yasuno[1,2], Guo-jie Jason Gao[1]   (1.Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan, 2.Dept. of Complex Systems Science, Nagoya Univ., Japan）

Placing an obstacle near the orifice of a hopper has been shown experimentally and numerically to locally enhance the flow rate for hard particles leaving the hopper under gravity. A flow rate difference between its value near the obstacle and its maximal value without an obstacle can explain this phenomenon with minimal dynamics involved. When the obstacle sits close to the hopper orifice, the flow rate near the obstacle is smaller than the maximal value, which corresponds to a fluidized flow regime. On the other hand, when the obstacle is placed further from the orifice, the flow rate near the obstacle becomes larger than the maximal value and a clogging flow regime appears. In this study, we employ a Tetris model in 2D discretized space and successfully demonstrate the two flow regimes. Without creating overlap between any objects in the system, our model sequentially relocates one particle at a time into its von Neumann or Moore neighborhood closer to the hopper orifice. Our results show that in the fluidized regime, where flow rate is low, the Moore protocol, which allows higher freedom to move particles, gives higher flow rate than the von Neumann protocol. The trend reverses in the clogging regime, where higher freedom to move particles renders lower flow rate.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-60] Effect of water molecules on polymer chain motion in dense chain ensembles of nafion membrane

○Isamu Riku, Ryoma Oka, Koji Mimura （Osaka Prefecture Univ., Japan）

Because of the high power density, high efficiency, fast start-up, and zero emission at the point of use, proton exchange membrane fuel cells (PEMFCs) are the most promising candidates for replacing internal combustion engines in automobiles, and are also being developed for portable and distributed stationary power generation applications.

However, the life of PEMFCs is currently limited by the mechanical endurance of polymer electrolyte membranes (PEMs). The failure of PEM is believed to be the result of a combined chemical and mechanical effect acting together. Recently, it is found that cyclic hydration of the membrane during the operation cycles (start/shut down) of the fuel cell may cause mechanical degradation of the membrane.

Therefore, in this paper, to investigate such mechanical degradation of the membrane subjected to fuel cell cycles, we perform a series of molecular dynamic simulations for the membrane made from the sulfonated tetrafluoroethylene copolymer with the trade name Nafion. The effect of the water molecules on the polymer chain motion in dense chain ensembles of nafion membrane is to be clarified.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-61] A Coarse-Grained Model for Competitive Adsorption on the Surface of Inorganic Nanomaterials

○Stefano Poggio[1], Hender Lopez[2], David Power[1], Vladimir Lobaskin[1] （1.School of Physics, University College Dublin, Ireland, 2.Institute Laue-Langevin, Grenoble, France）

The increased use of nanoparticles (NP) and nanomaterials is pushing scientific research into trying to understand the mechanisms governing interactions between biomolecules and inorganic materials. It is known that, once a NP is in contact with a biological medium, a protein corona forms on its surface, and that the nature of the corona is what regulates the interaction between the NP and the other biomolecules.

In this work we propose a method to coarse grain the interactions of inorganic nanomaterials in contact with biological fluids of arbitrary composition. Biomolecules (lipids, proteins and carbohydrates) are coarse grained by mapping their main chemical fragments onto single beads, and their interaction with the NP surface is described a potential of mean force from atomistic simulations [2]. The NP is represented by a two-layer model where the surface interacts with the molecule beads by using the beads PMF with a slab of the material, corrected by a geometric factor, while the core interacts with via van der Waals forces calculated using Lifshitz theory. This model can describe the kinetics of competitive adsorption of biomolecules on the surface of a NP.

We have studied the kinetics of adsorption and the corona composition of Au NPs in a biological environment with the typical composition of lung lining fluid and blood plasma. This methodology can then be combined with adverse outcome pathway analysis to build mechanism-based predictive schemes for toxicity assessments.

[1] M. Rahman, S. Laurent, N. Tawil, L. Yahia, and M. Mahmoudi, Protein-Nanoparticle Interactions, volume 15 of Springer Series in Biophysics. Springer-Verlag, 2013
[2] E. Brandt and A. P. Lyubartsev. Molecular dynamics simulations of adsorption of amino acid side chain analogues and a titanium binding peptide on the TiO_2 (100) surface. J. Phys. Chem. C, 119:18126, 2015.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-62] Molecular Dynamics of Inorganic and Organic Interfaces with Force-Field Parameters Based on DFT Simulations

○Kosuke Ohata, Hiroya Nitta, Kenta Chaki, Taku Ozawa （JSOL Corporation, Japan）

Nanocomposites are important in the engineering field. However, the controlling of the properties of interfaces between inorganic solid fillers and organic molecules is one of the key issues. We have investigated the interaction between solids and polymers with a combination of Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations. DFT is a reliable method for calculating potential energy surface (PES). The force field parameters for MD simulations were determined by using our scheme for interfacial systems based on the DFT simulation. Then the scheme was applied to a solid-polymer interface. Utilizing the determined coarse-grained and full-atomistic force field parameters, the MD simulations were conducted. In this study, we utilized SIESTA for the QM simulation and J-OCTA for the system modeling and the MD simulation.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-63] Molecular dynamics screening for developing compounds of electrolytes with high performance in lithium ion batteries

○Yoshihiro Takai[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] （1.Graduate school of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan）

Recently, there is great interest in development of electric vehicles, so it demands improvement in performance of Lithium-ion Battery (LIB). For higher performance, it is important to develop new substances used for electrolyte or electrode. In particular, electrolyte is an important chemical factor for moving lithium ions between positive and negative electrodes in the battery. When the amount of ions moving is enhanced, the performance of the battery will be effectively improved. But there are hundreds of thousands of compounds as candidates for electrolytes, so we need to screen and choose ones from these many compounds. In this research, we perform atomistic evaluation about various characteristics of possible compounds of electrolyte (such as viscosity, ionic conductivity, degree of dissociation and diffusion coefficient) by mainly using molecular dynamics (MD) simulations. In evaluating at a molecular level, we can understand how the molecular level structure and properties affect the behavior of electrolyte. Molecule models we are using are ethylene carbonate (EC), fluoro ethylene carbonate (FEC), propylene carbonate (PC), butylene carbonate (BC), γ-butyrolactone (GBL), γ-valerolactone (GVL), dimethyl carbonate (DMC), ethyl-methyl carbonate (EMC), diethyl carbonate (DEC), and lithium hexafluorophosphate ($LiPF_6$). An electrolytes system in which 1 mol of $LiPF_6$ is mixed per 1 L of single solvent (solvent + 1M-$LiPF_6$) is simulated. The results suggest that we can determine a criterion for the screening of superior compounds based on information about molecular structures and properties of electrolyte. It is found that the smaller solvent molecules that easily diffuse contribute to the higher ionic conductivity of electrolytes. This is because diffusion coefficient of Li cation is greatly affected by that of solvent molecules. It is also found that solvation structure and size around Li cation take large effect on its diffusivity.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-64] Molecular dynamics study on transmission mechanism of torsional deformation in cellulose nanofibers with hierarchical structure

○Kentaro Takada[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] （1.Graduate School of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan）

Cellulose nanofiber (CNF) has high strength comparable to steel, and it shows low environmental load during a cycle of production and disposal. Beside it has many excellent properties and functions such as high rigidity, light-weight, flexibility and shape memory effect, so it is expected as a next-generation new material. CNF is a fibrous and nano-sized substance produced by decomposition of bulk-type cellulose which is a main component of plants. Usually it is constituted by many cellulose micro fibrils (CMFs) in which molecular chains of cellulose are aggregated in a crystal structure. It is also possible to make composite material of CNF together with other components, and then a new material with lightweight as well as high strength and high toughness will be realized. In such case, knowledge of mechanical properties for each CMF units is important. Since actual fibrils are complicatedly intertwined, it is also crucial to elucidate the transmission mechanism of force and deformation not only in one fibril but also in between fibrils. Indeed, how the dynamic and hierarchical structure composed of CMFs responds to bending or torsion, which includes gradient of stress and strain, is an interesting issue. However, little is known on torsional characteristics (shear modulus, torsional rigidity, etc.) concerning CMF. In general, in a wire-like structure, it is difficult to enhance torsional rigidity and strength, compared with tensile ones. Therefore, in this study, we try to build a hierarchical model of CNF by multiplying CMF fibers and to conduct molecular dynamics simulation for torsional deformation, by using a hybrid modeling between all-atoms and united-atoms models. First, shear modulus was estimated for one CMF fibril and it showed a value close to the experimental values. In addition, it is revealed that intermolecular hydrogen bonds (HBs) are dynamically changed and the HB mechanism is likely to work as strong resistance in torsional deformation.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-65] Bubble dynamics of foam flow around an obstacle

○Antti Puisto, Juha Koivisto, Leevi Viitanen, Mikko J Alava （Aalto University, Department of Applied Physics, Finland）

Foams are one of the rare examples of simple yield stress fluids. Formed of bubbles embedded in liquid they are often studied in the context of jamming [1]. Foam flow is interesting not only because the start-up requires a dynamical unjamming transition (yielding), but also due to novel technological applications related to forming technologies [2].

Here, we study a foam flow through a 2D Hele-Shaw shell with an obstacle, forming a constriction. For this purpose, we use bubble scale dynamics model (the Durian bubble model), which we extend with the appropriate descriptions for the boundary effects coming from the walls and the top and bottom plates. We

observe a negative wake behind the obstacle, analogous to the one observed in gas bubble motion in a viscoelastic medium. There, the medium is succesfully described by an Oldroyd-B model. This suggests that in the present conditions, the foam acts as a typical viscoelastic fluid, rather than the expected elastoviscoplasticity [3]. We compare the simulations data against experiments, foam intruder experiments, where we find a similar flow pattern. We find a reasonable agreement in the flow dynamics and the overshoots between the experimental data and the bubble model. Finally, we identify a viscoelastic timescale, which determines the magnitude of the velocity overshoot.

[1] G. Katgert, B. P. Tighe, M. van Hecke, Soft Matter 9, 9739 (2013).
[2] A. M. Al-Qararah, T. Hjelt, A. Koponen, A. Harlin, J. A. Ketoja, Colloids Surf. A 467, 97 (2015).
[3] S. Bénito, C. -H. Bruneau, T. Colin, C. Gay, F. Molino, Eur. Phys. J. E 25, 225 (2008)

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-66] Shape Deformation and Mechanical Relationship of Ionic Droplet Under An Electric Field

Bo-Yu Shih[1], ○Wei-Chun Lin[1], Alice Hu[2], Hsuan-Teh Hu[1], Yu-Chieh Lo[3] （1.Department of Civil Engineering,National Cheng Kung University, Taiwan, 2.Department of Mechanical and Biomedical Engineering, City University of Hong Kong, Hong Kong, 3.Department of Materials Science and Engineering, National Chiao Tung University, Taiwan）

Nano-sized symmetric double Taylor cone forms a capillary liquid bridge while electric field applied on Ionic liquids (2-dimethyl-3-propylimidazolium- bis(trifluoromethylsulphonyl)imide). This ionic liquid bridge size is around 20 nm. We attempt to understand the critical dimensions and stability criteria for nano-bridge forming mechanism. Therefore, we conduct molecular dynamics simulation under electric field to investigate ionic droplets electrohydrodynamic behavior with different structures and potential functions. Factors that affect liquid bridge size through extensive parameter are studied thoroughly in this work. We also investigate the influence of changing velocity field and shape deformation under different electric field conditions. The mechanical relationship between electric stress, Coulomb electrostatic force and the intermolecular interactions are analyzed. Through this complete studies, surface tension coefficient and ionic liquid viscosity are obtained. Results show that shape deformation and size of liquid bridge are mainly controlled by surface tension coefficient and viscosity.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-67] Multiscale modeling of surface functionalized graphene/polymer nanocomposites: insight into the effect of covalent grafting

○Jeong-ha Lee[1], Seunghwa Yang[2] （1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea）

Polymer nanocomposites is applied in various industries to improve their mechanical, electrical, thermal properties instead of using pure polymer. In view of improving mechanical properties of polymer nanocomposites, graphene nanosheets is typical reinforcement due to its excellent properties. However, agglomeration of graphene nanosheets in polymer reduces their mechanical and thermal properties. Besides,

weak cohesive energy between graphene and polymer by poor van der waals interaction causes slip condition in their interfacial region. To improve their intrinsic weak interfacial strength and dispersion properties between graphene and polymer nanocomposites, surface treatment of graphene such as covalent grafting or functionalization on graphene nanosheets have been generally used in graphene/polymer nanocomposites.

In this study, multiscale modeling approach for pristine and covalently functionalized graphene included polypropylene nanocomposites is implemented. Representative unit cell consists single-layered graphene and polypropylene matrix is modeled with three-dimensional periodic boundary conditions. Different number of covalent grafting on graphene is considered to investigate effect of grafting density. In molecular dynamics simulations, reactive forcefield for hydrocarbon structure is used to describe carbon-carbon bond breakage in graphene. Through statistical ensemble simulations, thermoelastic behavior of graphene/polypropylene nanocomposites are determined with grafting density differences at single-layered graphene interface. For equivalent continuum modeling to account for covalent grafting, the mean field micromechanics model is supplemented to characterize interfacial and interphase properties of nanocomposites in accordance with number of covalent grafting. In heat of vaporization perspective, correlation of covalent grafting and dispersion inside the polymer matrix is examined.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-68] Durability analysis on the environmental aging of epoxybased nanocomposite

○Sunyong Kwon[1], Man Young Lee[2], Seunghwa Yang[3]　(1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Agency for Defense Development, Korea, 3.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea)

Aging is a slow and steady process which occurs by various environmental factors including moisture, uv light, changes in temperature and pressure. Hygroscopic aging of polymer nanocomposite occurs by consistent exposure to moisture in service condition. As bounded water in the material causes microscopic changes in chemical and physical structure of the composite material, it eventually leads to swelling, plasticization, degradation of mechanical and interfacial properties. Thus, to properly examine the long-time process of aging, correlation between aging time-structure-corresponding properties should be developed. Therefore, in this study, multiscale bridging method incorporating atomistic approach of molecular dynamics (MD) simulation and continuum modeling is presented.

To define the relationship between aged structure and corresponding properties, MD simulation is firstly adopted. Different crosslinking ratio of 30% to 70% is established by crosslinking reaction between bisphenol F type epoxy (EPON862®) resin and triethylenetetramine (TETA) curing agent. A single layered defect-free graphene is added as fiber reinforcement in the nanocomposite structure. Also, to observe the hygroelastic behavior of nanocomposite, weight fraction of 0, 2, 4wt% water is included in the nanocomposite unit cell. After isobaric-isothermal (NPT) ensemble simulation, diffusion coefficient of water, coefficient of moisture expansion (CME), elastic modulus and cohesive zone law of epoxy/graphene nanocomposite models are predicted. Based on the results of MD simulation, equilibrium hygroelastic constitutive models incorporating interfacial properties between epoxy and graphene are used to accurately measure the nanoscale effect observed in MD simulations with moisture.

[PO-I2] Poster Session 2
Symposium I
Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-69] Topological evolution of the microstructures of thin films during grain growth

○Ahu Oencue[1], Thorsten Halle[2], Dana Zoellner[3] （1.Institute of Experimental Physics, Otto-von-Guericke University Magdeburg, Germany, 2.Institute of Materials and Joining Technology, Otto-von-Guericke University Magdeburg, Germany, 3.B CUBE Center for Molecular Bioengineering, TU Dresden, Germany）

[P2-70] Molecular dynamics simulations of phase transformations in nanocrystalline NiTi shape-memory alloys

○Won-Seok Ko （University of Ulsan, 93 Daehak-ro, Nam-gu, Ulsan, 44610, Korea）

[P2-71] An attempt to connect migration of grain boundaries to their atomic structures with help of Molecular Dynamics

Zakaria El Omari, ○Sylvain Queyreau, Charlie Kahloun, Brigitte Bacroix （Universite Paris XIII, Sorbonne Paris Cite, Laboratoire des Sciences des Procedes et des Materiaux, LSPM UPR 3407, France）

[P2-72] Disconnection interaction in Cu grain boundaries

○Christian Brandl （Karlsruhe Institute of Technology, Germany）

[P2-73] Phase-field Approach to Thermo-mechanical Behavior of Through-silicon Vias

Wooju Lee, ○jaekeun yoon, Dongchoul Kim （Sogang Univ., Korea）

[P2-74] Grain-Growth in Nanocrystalline Metals under Ion Irradiation: A Thermal Spike Model

○Djamel Kaoumi[1], Robert Birtcher[2], Arthur Motta[3] （1.North Carolina State University, United States of America, 2.Argonne National Laboratory, United States of America, 3.Penn State University, United States of America）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-69] Topological evolution of the microstructures of thin films during grain growth

○Ahu Oencue[1], Thorsten Halle[2], Dana Zoellner[3] (1.Institute of Experimental Physics, Otto-von-Guericke University Magdeburg, Germany, 2.Institute of Materials and Joining Technology, Otto-von-Guericke University Magdeburg, Germany, 3.B CUBE Center for Molecular Bioengineering, TU Dresden, Germany)

Historically, metallography has been the two-dimensional characterization of materials microstructures by optical microscopy. Consequential problems have long been known: A two-dimensional section through a three-dimensional object gives us only a very poor idea about size and form of the object. The same holds for the complex grain boundary networks of various kinds of polycrystalline materials. Therefore, many attempts have been made to gain three-dimensional information experimentally. Nevertheless, in simulations and analytical theories thin films are commonly still treated as two-dimensional objects making comparisons with three-dimensional experimental data rather hard.

In the present work, based on experimental measurements, grain growth in metallic thin films is investigated in detail by three-dimensional Monte Carlo Potts model simulations focusing particularly on the transition from bulk-like growth to columnar microstructures. Changes not only in average growth behaviour from a linear increase of the average grain area with annealing time to near-stagnation, but particularly temporal changes in local topology and individual growth kinetics, e.g., in terms of the Lewis-law as well as of the von Neumann-Mullins-law are discussed.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-70] Molecular dynamics simulations of phase transformations in nanocrystalline NiTi shape-memory alloys

○Won-Seok Ko (University of Ulsan, 93 Daehak-ro, Nam-gu, Ulsan, 44610, Korea)

Molecular dynamics simulations are performed to investigate temperature- and stress-induced phase transformations in nanocrystalline nickel-titanium shape-memory alloys. Our results provide detailed insights into the origins of the experimentally reported characteristics of phase transformations at the nanoscale, such as the decrease of the transformation temperature with grain size and the disappearance of the plateau in the stress-strain response. The relevant atomic scale processes, such as nucleation, growth, and twinning are analyzed and explained. We suggest that a single, unified mechanism--dominated by the contribution of a local transformation strain--explains the characteristics of both temperature- and stress-induced phase transformations in nanocrystalline nickel-titanium.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-71] An attempt to connect migration of grain boundaries to their atomic structures with help of Molecular Dynamics

Zakaria El Omari, ○Sylvain Queyreau, Charlie Kahloun, Brigitte Bacroix （Universite Paris XIII, Sorbonne Paris Cite, Laboratoire des Sciences des Procedes et des Materiaux, LSPM UPR 3407, France）

Grain Boundary (GB) migration is at the origin of microstructure evolutions in a large variety of crystalline materials. One of the many challenges to fully understand GB motion has to do with the GB vast panel of atomic configurations and existence of several motive forces or impacting parameters. In this context, atomistic simulations have proven to be particularly useful since GB migration can be investigated under well defined conditions, and large scale systematic investigations are now possible (i.g. [1]).

In this work we report a Molecular Dynamics investigation of the migration of a large panel of CSL GB in fcc Ni. In order to construct lesser known GB with mixed tilt+twist or asymmetric character, we orient and constrain the simulation domain to the CSL lattice defined by the two crystal orientations, in a fashion very similar to the approach proposed in [2]. GB motion may be initiated by a synthetic driving force as defined in [3]. As a result, very different temperature behaviour are observed ranging from athermal, to thermally activated and non monotonous thermal behaviour. Different behaviours are sometimes observed for very similar GBs, confirming the important of the GB atomic structure over the macroscopic geometrical parameters describing GB.

In an attempt to rationalise these results we developed an automated post-processing of the atomic configurations into a discrete modelling of GB in terms of intrinsic dislocations and disconnections when present. This analysing tool is applied to a dozen of simple GB and a correlation is made when possible between elementary migration mechanisms -atomic shuffling or disconnection motion- and discrete structure of GB.

[1] DL Olmsted, EA Holm, SM Foiles, Acta Mater. 57, 3704 (2009).
[2] AD Banadaki, S Patala. J. Appl. Cryst. 48, 585 (2015).
[3] K.G.F. Janssens, D. Olmsted, E.A. Holm, S.M. Foiles, S.J. Plimpton, P.M. Derlet, Nat. Mater. 5, 124 (2006).

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-72] Disconnection interaction in Cu grain boundaries

○Christian Brandl （Karlsruhe Institute of Technology, Germany）

Recent molecular dynamics (MD) simulations and transmission electron microscopy indicate that the grain boundary (GB) migration in asymmetric GB plane orientation is mediated by the nucleation and migration of disconnections in the GB plane. The collective motion and reaction of disconnections also initiates the formation of facets as the agglomeration of disconnections into a disconnection arrays.

In MD simulations we address the interaction of disconnection and disconnection dipoles at zero stress in S3 and S7 GBs. The diffusive rearrangement at finite temperate is analyzed in terms of one-dimensional random walks and the drift signatures are used to deduce the interaction strength and the disconnection core interaction. The implications of the disconnection-interaction on the collective migration of asymmetrical GBs is discussed in context of grain coarsening in fcc metals at elevated temperatures and the transition to stress-driven grain coarsening in nanocrystalline metals.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-73] Phase-field Approach to Thermo-mechanical Behavior of Through-silicon Vias

Wooju Lee, ○jaekeun yoon, Dongchoul Kim （Sogang Univ., Korea）

Three-dimensional stacking of silicon chips via *Through-silicon vias (TSVs)* is an innovative technique for electronic devices due to the drastically shortened electrical path which leads to the faster operation. When TSVs are exposed to high temperature, the higher coefficient of thermal expansion (CTE) of Cu generate the out-of-plane extrusion of Cu from TSV, so-called Cu pumping, which may damage the above lying silicon chip. Furthermore, the thermal expansion is irreversible because the Cu grains are coarsened during the annealing. The comprehensive understanding of Cu pumping mechanism according to the geometry of TSV and annealing conditions is indispensably required to ensure the reliability of electronic devices. A finite element analysis has been used to predict the Cu pumping. However, the finite element method does not incorporate the grain coarsening mechanisms that reduce the elastic energy generated by the thermal expansion. Here, we propose a phase field model that is modified to consider the thermal expansion of Cu polycrystalline during annealing process. The phase field model is the most suitable method to model the evolution of microstructures, since it has benefits for incorporating multiple mechanisms simultaneously. In this study, the significant mechanisms of Cu pumping, including grain boundary migration, thermal expansion, and interfacial characteristics, are considered into the free energy functional of the phase field model

---

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-74] Grain-Growth in Nanocrystalline Metals under Ion Irradiation: A Thermal Spike Model

○Djamel Kaoumi[1], Robert Birtcher[2], Arthur Motta[3] （1.North Carolina State University, United States of America, 2.Argonne National Laboratory, United States of America, 3.Penn State University, United States of America）

Grain growth was observed in nanocrystalline metallic foils in situ in a transmission electron microscope in a wide range of irradiation doses, temperature (from 20K to 773K) for four different pure metals (Zr, Pt, Cu and Au). The average grain size increased monotonically with ion fluence and similarly to thermal grain growth, the ion-irradiation induced grain growth curves could be best fitted with curves of the type:. With respect to temperature, the experimental results showed the existence of a low-temperature regime (below about 0.15-0.22Tm), where grain growth is independent of the irradiation temperature, and a thermally assisted regime where grain growth is enhanced with increasing irradiation temperature. A model is proposed to describe grain growth under irradiation in the temperature-independent regime, based on the direct impact of the thermal spikes on grain boundaries. In the model, grain-boundary migration occurs by atomic jumps, within the thermal spikes, biased by the local grain-boundary curvature driving. The experimental results will be presented as well as the model proposed to describe grain-growth kinetics in the low-temperature regime (cryogenic temperatures).

[PO-N2] Poster Session 2

Symposium N
Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-75] Why the structure-property relationship in metallic glasses should be established beyond short-range order: Insight from potential energy landscape

○Dan Wei[1,2], Yunjiang Wang[1,2], Lanhong Dai[1,2] （1.University of Chinese Academy of Sciences, China, 2.Institute of Mechanics, Chinese Academy of Sciences, China）

[P2-76] Vacancy segregation analysis near grain boundaries in metallic systems by long-time atomistic simulations

○Shotaro Hara （Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan）

[P2-77] EXPERIMENTAL AND DENSITY FUNCTIONAL THEORY STUDIES OF PRECIPITATE INTERFACES IN ALUMINIUM ALLOYS, WITH FOCUS ON β " & β

○Haris Rudianto, Deni Hariadi, Andriansyah Andriansyah （Gunadarma University, Indonesia）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-75] Why the structure-property relationship in metallic glasses should be established beyond short-range order: Insight from potential energy landscape

○Dan Wei[1,2], Yunjiang Wang[1,2], Lanhong Dai[1,2] （1.University of Chinese Academy of Sciences, China, 2.Institute of Mechanics, Chinese Academy of Sciences, China）

For crystals, structures provide all information needed for predicting material properties. However, what determines non-crystalline solids properties remains elusive for many years. Extensive work has been performed to identify structures playing an important role in glass, but a key question arises that what is the hidden rule of structural feature that can predict properties. Here we calculate an atom's activation energy (the system's long-time property) for thermally activated relaxation with the Activation-Relaxation Technique (ART) and correlate the searched local potential energy landscape with several of the successful structural predictors. We find a common nature in the successful structural predictors that spatial correlation of structural information matters a lot once they tend to determine an atom's properties. There exists a critical correlation length of about sub-nanometer which is corresponding to the second shell of the pair correlation function of glassy structures. We further demonstrate this concept by manipulating the cutoff distance of local structural entropy - one of the successful structural feature - that only if this local structure is defined beyond the short-range order it can predict activation of local atom rearrangement in the model metallic glass. In this way, we question the prevailing approach of materials science aimed at identifying simple structural motifs responsible for metallic glass properties.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-76] Vacancy segregation analysis near grain boundaries in metallic systems by long-time atomistic simulations

○Shotaro Hara （Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan）

Long-term degradation phenomena in metallic systems under a high temperature, such as creep voiding, are governed by the vacancy diffusion, accumulation and growth processes at an atomistic scale around the material heterogeneities like grain boundaries. However, the basic properties such as the equilibrium vacancy concentrations and the kinetics near grain boundaries are not still understood because a molecular dynamics simulation often suffers from tracking thermally-activated processes due to its limited time scale. In this study, the vacancy segregation behavior at grain boundary has been analyzed using diffusive molecular dynamics simulations, which is a novel approach for exploring the atomic level mass action along the chemical potential gradient at diffusive time scale. The equilibrium vacancy concentrations and the chemical potential distributions at grain boundaries are computed for the different grain boundary character. The correlation between the grain boundary energies and their concentrations have also been considered. Furthermore, the kinetic nature of grain boundary sliding was investigated using this new scheme and the effect of stress on the sliding was discussed.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-77] EXPERIMENTAL AND DENSITY FUNCTIONAL THEORY STUDIES OF PRECIPITATE INTERFACES IN ALUMINIUM ALLOYS, WITH FOCUS ON $\beta"$ & β

○Haris Rudianto, Deni Hariadi, Andriansyah Andriansyah （Gunadarma University, Indonesia）

Aluminium is the third most abundant element in the Earth's crust, after oxygen and silicon. Before the start of the last century, aluminium started to come into wide use as a structural material. Since then, it has reached the position of being the second most used metal in the world, with only steel beating it to the throne. One important structural limitation of aluminium is their fatigue strength. Precipitation hardening is utilized to strengthen a wide variety of alloy systems especially for Aluminum Alloys. An example is the class of commercially important Al-Mg-Si based alloys which are strengthened by a number of metastable precipitate phases, where the needle-shaped β''-Mg5Si6 precipitates are often the main contributor to hardening. Beginning with the supersaturated solid solution (SSS), the generic precipitation sequence in Al-Mg-Si alloys is generally believed to be :

SSS -> Mg/Si clusters -> Guinier-Preston zones -> β'' -> β' -> β

In practice, the sequence can be even more complex and a number of other metastable phases, depending on alloy composition and the heat treatment time and temperature. In this research, interface energy was calculated by Quantum Espresso with super cells designed on VESTA. For comparison, in this research, experimental was also carried out to determine effects of strengthening precipitates on mechanical properties. T6 heat treatment was done starting from solid solution treatment, quenching and finished my artificial aging. Hardness was done to determine mechanical properties and SEM-EDS and XRD were done to characterize the materials.

Keywords; Aluminum Alloys, DFT, Strengthening Precipitates, Heat Treatment

Poster Session | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[PO-O2] Poster Session 2
Symposium O
Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-78] Adsorption of Volatile Organic Compounds (VOCs) on Silicene by Density Functional Theory Calculations

○Thi Viet Bac Phung[1], Trong Lam Pham[1], Van An Dinh[1,2] （1.Nanotechnology Program, Vietnam Japan University - Vietnam National University, Viet Nam, 2.Center for Atomic and Molecular Technologies, Graduate School of Engineering, Osaka University, Japan）

[P2-79] Atomistic insights into defect formation mechanism in single crystal SiC based on molecular dynamics simulation

○Kenji Nishimura[1], Koji Miyake[1], Ken-ichi Saitoh[2] （1.AIST, Japan, 2.Kansai Univ., Japan）

[P2-80] Potential cathode material Na_xVOPO_4 for rechargeable Sodium - ion batteries: DFT investigation

○Duc Huu Luong[1], An Van Dinh[1,2], Yoshitada Morikawa[3], Yoji Shibutani[2,1] （1.Nano Technology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan, 3.Department of Precision Science and Technology, Graduate School of Engineering, Osaka University, Japan）

[P2-81] Two-dimensional Na_xSiS as a promising anode material for rechargeable Sodium-based batteries: Ab initio material design.

Thi Dung Pham[1], ○Van An Dinh[1,2], Kazunori Sato[3], Yoji Shibutani[1,2] （1.Nanotechnology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan, 3.Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, Japan）

[P2-82] Modelling and analysis of SiO2 interfaces of non-firing solids

○Tomohiro Sato[1], Ken-ichi Saitoh[1], Masayoshi Fuji[2], Chika Yamashita Takai[2], Hadi Razavi[2], Masanori Takuma[1], Yoshimasa Takahashi[1] （1.Dept. of Mechanical Engineering, Kansai Univ., Japan, 2.Advanced Ceramics Reserch Center, Nagoya Institute of Technology, Japan）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-78] Adsorption of Volatile Organic Compounds (VOCs) on Silicene by Density Functional Theory Calculations

○Thi Viet Bac Phung[1], Trong Lam Pham[1], Van An Dinh[1,2] （1.Nanotechnology Program, Vietnam Japan University - Vietnam National University, Viet Nam, 2.Center for Atomic and Molecular Technologies, Graduate School of Engineering, Osaka University, Japan）

Cancer can be regarded as a rising threat towards modern societies. Detecting cancer at an early stage significantly improves the curability of the disease [1]; unfortunately, currently available methods for early diagnosis of cancer are scarce and inefficient. In fact, the concentration of VOCs in cancer patients in the breath is different from that in normal people [2]. Therefore, development of new sensors that can detect VOCs at low concentrations, corresponding to the early stage of cancer, is desirable. 2D materials are expected as attractive materials for these sensors due to their large surface area to volume ratio. In this work, we investigated the adsorption mechanism of some small-to-medium VOCs on the surface of silicene by the quantum simulation method. The images of the potential energy surfaces for different positions of the adsorbate on the silicene surface were explored by *Computational DFT-based Nanoscope* [3] for determination of the most stable configurations and diffusion possibilities. The adsorption energy profiles were calculated by three approximations of van der Waals interation: revPBE-vdW, optPBE-vdW, and DFT-D2. It is found that the adsorption energies of the VOCs in question vary in the range of 0.6-1.0 eV, which indicates that silicene is considerably sensitive with these VOCs. The charge transfer between the substrate and VOCs and the effect of an electric field on the adsorption configurations, energies, and band structures were also addressed.

References

[1] M. Hakim, Y. Y. Broza, O. Barash, N. Peled, M. Phillips, A. Amann, H. Haick Chem. Rev. 2012, 112, 11, 5949-5966.

[2] E. M. Gaspar, A. F. Lucena, J. D. da Costa, and H. C. das Neves. Journal of Chromatography A 2009, 1216, 14, 2749-2756.

[3] Developed by V. A. Dinh, Vietnam Japan University.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-79] Atomistic insights into defect formation mechanism in single crystal SiC based on molecular dynamics simulation

○Kenji Nishimura[1], Koji Miyake[1], Ken-ichi Saitoh[2] （1.AIST, Japan, 2.Kansai Univ., Japan）

Silicon carbide (SiC) is a promising next-generation semiconductor for high-power, high-temperature, and high-voltage devices because of its wide bandgap, high breakdown field, and high thermal conductivity. However, the efficient and smooth machining of SiC is technically difficult due to its intrinsic nature of high hardness and brittleness as well as strong anisotropy. It is still a great challenge to understand machining

processes in which damage layers caused by stress-induced phenomena such as plastic deformation and fracture are introduced beneath grinding surface. In this study, we perform one million-atom molecular dynamics simulations of nanoindentation tests on cubic SiC single crystal using a nano-sized spherical indenter to clarify the plastic deformation mechanism and defect formation criteria in SiC. An analytical bond-order Tersoff-type interatomic potential for SiC developed by Erhart *et al.*, which reproduces the elastic, defect, and thermal properties, is adopted. The load-displacement curves of the nanoindentation tests obtained by our simulations demonstrate transition from elastic deformation to plastic deformation so-called "pop-in" event. Our results also predict the decrease of the CRSS (critical resolved shear stress) of single crystal SiC with increasing temperature from 300 K to 2000 K for both (001) and (111) indent, which means less energy is required to activate slip systems at higher temperature. These results are similar to the feature of ductile materials such as metals, although SiC is known as brittle materials. In addition, we identify crystalline slips and defects generated beneath the indenter after the pop-in event by means of a novel type of structural analysis method using sub-lattice of Si or C which is based on common neighbor analysis. The structural analysis we propose reveals that dislocation loops in {111} planes which correspond to the slip plane of SiC are developed with increasing indenter depth. Furthermore, we find that for lower temperature perfect dislocations are dominantly formed, while for higher temperature partial dislocations together with stacking faults are superior to the perfect dislocations, resulting in the dramatic increase of the partial dislocations.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-80] Potential cathode material Na_xVOPO_4 for rechargeable Sodium - ion batteries: DFT investigation

○Duc Huu Luong[1], An Van Dinh[1,2], Yoshitada Morikawa[3], Yoji Shibutani[2,1] （1.Nano Technology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan, 3.Department of Precision Science and Technology, Graduate School of Engineering, Osaka University, Japan）

Using the density functional calculations, we investigated the crystal and electronic structures, electrochemical properties and ion diffusion mechanism of Sodium - polaron complex in Sodium Vanadyl phosphate $NaVPO_5$. A calculated voltage of 3.77 V (GGA+U) and 3.58 V (HSE06) corresponding to a redox reaction of potential couple V^{4+}/V^{5+} were in good agreement with experimental result [1]. The diffusion mechanism of charge carriers was explored using GGA+U. In the charge process, a Sodium ion is removed from the crystal structure so that the Sodium vacancy appears and a positive small polaron forms at one the two first nearest VO_6 octahedron. The diffusion of Na+ ion which is accompanied by a positive small polaron is described by three elementary diffusion processes, including single, crossing and parallel diffusions [2]. With the smallest activation energy of 395 meV, the pathway of Sodium diffusion along the [010] direction is the most favorable diffusion pathway and it is significantly higher than previous calculation which did not mention the small polaron formation. In the discharge process, Sodium ion is intercalated to structure of β - $VOPO_4$, then the negative small polaron forms at one of the nearest neighbour VO_6 octahedron. In addition, the elementary diffusion process of sodium ion is more favorable in the [010] direction. However, because of about 10% smaller volume, the diffusion activation energy (627 meV) is significantly higher than those required in the charge process. Compared with the other materials, it is obviously that this material would perform as well as some common materials for cathode such as Olivine.

[1] G. He, A. Huq, W. H. Kan, and A. Manthiramm, Chem. Mater. 2016, **28**, 1503−1512
[2] V. A. Dinh *et al.* App. Phys. Express, 2012, **5**, 045801

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-81] Two-dimensional Na$_x$SiS as a promising anode material for rechargeable Sodium-based batteries: Ab initio material design.

Thi Dung Pham[1], ◯Van An Dinh[1,2], Kazunori Sato[3], Yoji Shibutani[1,2] (1.Nanotechnology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan, 3.Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, Japan）

The rapidly rising demand of energy storage system for electronic devices presents an imperative need to develop sodium-ion batteries with high energy density, high conductivity, and low barrier energy. In this work, we present the density functional study on properties of the two-dimensional (2D) Na$_x$SiS as a promising anode material for rechargeable sodium ion batteries (SIBs). Energetically stable structures of Na-adsorbed *Silicene sulfide* Na$_x$SiS were explored. It is found that *silicene sulfide* has an adsorption energy to sodium atom about of -0.4 eV, which is large enough to ensure a good stability for sodium inserting into SiS during sodiate process. The electronic structure and capacity of Na$_x$SiS were calculated. The electronic structure of pristine SiS monolayer and Na adsorbed layer shows the distinction of a semiconductor material. The fully sodiated phase of SiS is Na$_{0.5}$SiS corresponding to a highest theoretical capacity of 187.2 mAh/g per one side layer. The diffusion mechanism of Na ions was also investigated by using NEB method. Two possible elementary processes are explored: one is along *a*-and the other is along *b*-direction. Most importantly, *Silicene sulfide* shows a good sodium mobility with an energy barrier along two dimension is only 183 meV, which is much smaller than that in Li$_x$SiS (430meV), 2D TiS$_2$ (220meV), and 2D MoS$_2$ (280-680 meV). Our investigations also reveal that SiS exhibits the better electrochemical performance as an anode in the SIBs than in the LIBs. All these characteristics suggest that 2D SiS can expected to be a promising anode material for sodium batteries.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-82] Modelling and analysis of SiO2 interfaces of non-firing solids

◯Tomohiro Sato[1], Ken-ichi Saitoh[1], Masayoshi Fuji[2], Chika Yamashita Takai[2], Hadi Razavi[2], Masanori Takuma[1], Yoshimasa Takahashi[1] (1.Dept. of Mechanical Engineering, Kansai Univ., Japan, 2.Advanced Ceramics Reserch Center, Nagoya Institute of Technology, Japan）

Generally, ceramics are manufactured by using sintering process. However, this process needs high temperature and loss a lot of fuels. CO2 emission in the process is also need to improve. So, non-fire process is focused to make ceramics products.

For non-fire process, surfaces of SiO2 particles are polished and put hydrogen on the activate surfaces. These SiO2 particles are compressed and put into water that is non-fire process of ceramics. In this study, SiO2 interface models were constructed for molecular dynamics simulation. Interactions between SiO2 and H2O were presented by using ReaxFF potential. At first, SiO2 interfaces model without OH as end groups were conducted. By put water molecules between SiO2 interfaces, some atoms were changed their combinations. Some of them achieved lower potential energy through the simulation. It is seemed that a part

of non-fire process was reproduced. For example, hydrogen atom connected the oxygen atom of SiO2. However, connection of SiO2 did not observed over SiO2 interfaces.

Then, SiO2 interfaces model with OH as end groups were conducted. At relaxation of the models, SiOH exists in the model. After relaxation, water molecules were put into the surfaces. However, changes of connection between SiO2 and H2O or SiO2 interfaces did not observed. Energetic or structural stability of SiOH surfaces were seemed to effect the result.

Distance of interfaces, conducting compressed SiO2 including OH as end groups models might be key to improve the ability of reaction between atoms.

Plenary Talk | Plenary Talk

[PL5] Plenary Talk 5

Property optimisation of titanium alloys based on phase stability evaluation and microstructure design
Chair: Dongsheng Xu(IMR-CAS, China)
Thu. Nov 1, 2018 8:30 AM - 9:20 AM Room1
Rui Yang

[PL5] Plenary Talk 5

○Rui Yang （Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China）

(Thu. Nov 1, 2018 8:30 AM - 9:20 AM Room1)

[PL5] Plenary Talk 5

Property optimisation of titanium alloys based on phase stability evaluation and microstructure design

○Rui Yang　(Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China)

Titanium alloys are extensively used in aircraft engines and have emerged as ideal materials for a wide range of biomedical implants. Applications of titanium alloys in such reliability sensitive components/devices require a thorough understanding and precise control of properties which are determined by the rich variety of phase transformations and multi scale microstructures. In many cases experimental investigations have already pointed to one or several key processes or parameters that dominate the properties and service performance of the alloys. Under such circumstances the computational and modelling tasks are relatively well defined and the results can be critical in clarifying and solving the problems. This talk will review work conducted in the past few years using such an experiment plus computation approach, taking examples from near-alpha titanium alloys and titanium aluminides for aero engine applications and from beta-type titanium alloys for biomedical use. The topics to be covered include alloying effects on the alpha phase and their relations to creep resistance and cold dwell fatigue propensity, alloying effects, phase stability and deformation mechanisms of high strength titanium aluminides, and metastable phases and stress induced transformations in beta-type titanium alloys.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C9] Symposium C-9

Chair: Vasily Bulatov(Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, United States of America)

Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room1

[SY-C9] Interstitial Shuffling Mechanism for Solute-Induced Embrittlement of Titanium

○Daryl C. Chrzan （Department of Materials Science and Engineering, University of California, Berkeley, United States of America）

[SY-C9] Screw dislocation mediated solution strengthening of substitutional α-Ti alloys - First principles investigation

○Piotr Kwasniak （Warsaw University of Technology, Poland）

[SY-C9] Microstructural effects on strain rate sensitivity in dual-phase titanium alloys

○Sana Waheed[1], Zebang Zheng[2], Daniel S. Balint[1], Fionn P. E. Dunne[2] （1.Dept. of Mechanical Engineering, Imperial College London , UK, 2.Dept. of Materials, Imperial College London , UK）

[SY-C9] **Understanding thermal alleviation in cold dwell fatigue in titanium alloys using crystal plasticity model**

○Zebang Zheng[1], Adam Stapleton[2], Kate Fox[2], Fionn P.E. Dunne[1] （1.Dept. of Materials, Imperial College London, UK, 2.Rolls-Royce plc, UK）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room1)

[SY-C9] Interstitial Shuffling Mechanism for Solute-Induced Embrittlement of Titanium

Invited

○Daryl C. Chrzan （Department of Materials Science and Engineering, University of California, Berkeley, United States of America）

The exceptional sensitivity of the strength of Ti alloys to low concentrations of interstitial O arises from a mechanism akin to steric hindrance [1]. The equilibrium interstitial sites of the O atoms are highly distorted and compressed during the passage of a dislocation. The presence of an O atom at this site resists this distortion and compression inhibiting the passage of the dislocation and strengthening the metal. However, this strength increase is also correlated with embrittlement of the metal. We identify a dislocation-induced interstitial shuffling mechanism that can explain the observed O-induced embrittlement of Ti [2]. Molecular dynamics simulations show that the passage of a dislocation can move a fraction of the O interstitials from their equilibrium octahedral sites into adjacent hexahedral sites. The excess number of O interstitials in hexahedral sites is metastable and will eventually return to equilibrium. However, simulations of the dislocation/O interstitial interaction predict that an O atom in the hexahedral site presents a weaker obstacle to dislocation slip than an O atom in the octahedral site. Under typical strain rates, the time between dislocation passage on the slip plane is less than the estimated typical residence time for an O atom in the hexahedral site. The implication is that the passage of the first dislocation on the slip plane leads to softening for the subsequent dislocations. Subsequent dislocations may the further soften the slip plane through the same mechanism. This slip plane softening is expected to lead to planar slip, and the stress concentrations associated with planar slip then lead to the embrittlement of the metal. This work is supported by the U. S. Office of Naval Research under grant N00014-16-1-2304 and employed computational resources of the National Science Foundation under grant ACI-1053575.

[1] Q. Yu *et al.*, Science 347, 635-639 (2015).

[2] M. Poschmann *et al.*, to be published.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room1)

[SY-C9] Screw dislocation mediated solution strengthening of substitutional α-Ti alloys - First principles investigation

○Piotr Kwasniak （Warsaw University of Technology, Poland）

The mechanical properties of hexagonal Ti alloys depend substantially on the glide of <*a*> type screw dislocations. The configurations and stabilities of these line defects are, however, known only in pure Ti and Ti + O solutions, where the locking-unlocking mechanism and a strong pinning effect control their activity. In this study, we investigated the unclear, screw dislocation mediated solution strengthening of substitutional α-Ti alloys. To this end, a first principle computational scheme was used to determine the structures and energies of the considered line defects during planar and cross-slip processes in the vicinity of the solute element. Two phenomena were determined that are crucial in terms of plastic deformation: (i) enhanced

polymorphism of the dislocation cores leading to multiple new core configurations, and (ii) relatively large positive and negative interaction energies between the solutes and the line defects. Both these effects are strongly affected by the valence configuration of the alloying elements. Due to their pronounced structure and energy variations, dislocation planar and cross slip processes can occur under different scenarios, through diverse non-planar core geometries. The calculations performed also indicate In as a potential alloy element for improving both the strength and ductility of Ti by stabilizing a special, compact core geometry able to spread on an arbitrary glide plane with a low energy barrier. All of the above effects are discussed in terms of the physical factors (solute size misfit, stacking fault energy and electronic structure) that affect the energy and geometry of dislocation cores.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room1)

[SY-C9] Microstructural effects on strain rate sensitivity in dual-phase titanium alloys

○Sana Waheed[1], Zebang Zheng[2], Daniel S. Balint[1], Fionn P. E. Dunne[2] (1.Dept. of Mechanical Engineering, Imperial College London , UK, 2.Dept. of Materials, Imperial College London , UK)

Cold dwell fatigue failure in titanium alloys is a major concern in aero-engine applications and is inherently linked to the strain rate sensitivity (SRS) of the material. Recent crystal plasticity finite element (CPFE) work has shown the material SRS to be influenced by a number of microstructural factors [1]. However, these higher-level modelling studies do not include discrete aspects of slip and considerably overestimate the material rate sensitivity as compared to experimental studies. Thus, the significance and mechanism of microstructural effects on experimentally observed strain rate sensitivity in titanium alloys remain unclear.

In this study, a planar discrete dislocation plasticity (DDP) model is set up explicitly incorporating dislocation penetration across phase boundaries and material heterogeneity arising from alpha and beta titanium phases to simulate realistic microstructures. Stress relaxation tests are performed to investigate microstructural effects, such as the presence of colony or basketweave microstructures, textured or non-textured crystallography and grain size effects, on the material strain rate sensitivity. The SRS coefficients obtained from the simulations match closely with experimental values. It is found that changing the microstructure from pure alpha, colony to basketweave, and reducing alpha grain sizes leads to a significant reduction in material rate sensitivity, whereas dislocation penetration is found to not be as significant as previously considered for small hold strains. The mechanistic basis for these effects is argued to be changes in dislocation mean free-path and the total amount of plasticity in the specimen. Finally, DDP results are compared with corresponding CPFE simulations, to show that discrete aspects of slip and hardening mechanisms have to be accounted for to capture experimentally observed rate sensitivity. These results provide increased understanding of the mechanism of cold dwell fatigue failure in titanium alloys and are relevant for the design of dwell-insensitive microstructures.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room1)

[SY-C9] Understanding thermal alleviation in cold dwell fatigue in titanium alloys using crystal plasticity model

$^{\bigcirc}$Zebang Zheng[1], Adam Stapleton[2], Kate Fox[2], Fionn P.E. Dunne[1]　(1.Dept. of Materials, Imperial College London, UK, 2.Rolls-Royce plc, UK)

Dwell fatigue facet nucleation has been investigated in isothermal rig disc spin tests and under anisothermal in-service engine conditions in titanium alloy IMI834 using α-HCP homogenised and faithful α-β lamellar microstructure crystal plasticity representations. The empirically observed facet nucleation and disc failure at low stress in the isothermal spin tests has been explained and originates from the material rate sensitivity giving rise to soft grain creep accumulation and hard grain basal stresses which increase with fatigue cycling until facet nucleation. The α-HCP homogenised model is not able to capture this observed behaviour at sensible applied stresses. In contrast to the isothermal spin tests, anisothermal in-service disc loading conditions generate soft grain slip accumulation predominantly in the first loading cycle after which no further load shedding nor soft grain creep accumulation is observed, such that the behaviour is stable, with no further increase in hard grain basal stress so that facet nucleation does not occur, as observed empirically. The *thermal alleviation*, which derives from in-service loading conditions and gives the insensitivity to dwell fatigue dependent on the temperature excursions, has been explained. A stress-temperature map for IMI834 alloy has been established to demarcate the ranges for which the propensity for dwell fatigue facet nucleation is high, threatening or low.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C10] Symposium C-10

Chair: Tomohito Tsuru(Japan Atomic Energy Agency, Japan)
Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room1

[SY-C10] First Principles Calculations of Dislocations in Model Engineering Alloys (Ni, Ni3Al, hcp-Ti, and a Refractory Metal BCC-HEA)
○Christopher Woodward （Air Force Research Laboratory, United States of America）

[SY-C10] **Hybrid QM/MM study of dislocation glide in tungsten in the presence of plasma components**
○Petr Grigorev[1], Tom Swinburne[2], James Kermode[1] （1.Warwick Centre for Predictive Modelling, UK, 2.Los Alamos National Laboratory, United States of America）

[SY-C10] First-principles Calculations of Deformation Twins in Hexagonal Titanium Alloys
○Daisuke Matsunaka, Ryosuke Amano （Dept. of Mechanical Engineering, Shinshu Univ., Japan）

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room1)

[SY-C10] First Principles Calculations of Dislocations in Model Engineering Alloys (Ni, Ni3Al, hcp-Ti, and a Refractory Metal BCC-HEA)

Invited

○Christopher Woodward （Air Force Research Laboratory, United States of America）

In order to understand the "chemistry of deformation" an adequate description of the strain field near the center (core) of dislocations is required. While continuum elasticity methods have been very successful in describing long-range stress fields of dislocations these methods diverge in the core region. Atomistic methods have shown that the forces produced at the dislocation core and their coupling to the applied stress can have a dramatic effect on plasticity. However, atomistic methods are limited by the fidelity of the assumed interaction model and for this reason are at best semi-empirical. Here the Lattice Greens Function is used with Density Functional Theory to calculate the equilibrium core structure of isolated screw dislocation in four model-engineering alloys. These include Ni, $L1_2$ Ni_3Al, and a c+a pyramidal dislocation in hcp Ti. Pipe diffusion along the dissociated partial dislocations in Ni has been evaluated for self-diffusion and Co solutes. Recent progress extending a 3-d lattice Greens function to model screw dislocations in a refractory bcc high entropy (high concentration solid solutions) will be reviewed.

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room1)

[SY-C10] Hybrid QM/MM study of dislocation glide in tungsten in the presence of plasma components

○Petr Grigorev[1], Tom Swinburne[2], James Kermode[1] （1.Warwick Centre for Predictive Modelling, UK, 2.Los Alamos National Laboratory, United States of America）

Tungsten has been chosen as the diverter armour material in ITER and is the main candidate material for plasma-facing components for future fusion reactors.Interaction of plasma components with the material is unavoidable and will lead to degradation of the performance and the lifetime of the in-vessel components.From this point of view it is important to gain an understanding of dislocation mobility as well as the influence of fusion plasma components (H and He) on the mechanism.

Dislocation glide is governed by the localised rearrangement of atoms inside the dislocation core but is tightly coupled to the stress and strain fields on larger length scale.Thus, a correct description of the process requires chemically accurate treatment of the dislocation core atoms together with the use of the systems large enough to accommodate the corresponding stress fields.On the one hand, Density Functional Theory (DFT) provides an accurate description of the interatomic bonding, however the computational cost of the method does not allow one to study large enough systems and requires usage of periodic cells (i. e. with dislocation dipoles and quadrupoles with complex symmetry). On the other hand, classical interatomic potentials are much more computationally affordable allowing to study systems of required size, but the accuracy and transferability of the description of dislocation core is poor, especially for multi-element systems.

In this study we use a hybrid multiscale approach, namely quantum mechanics/molecular mechanics

(QM/MM) combining an accurate local QM description of the dislocation core atoms with a classical model for the rest of the system. We apply a recently developed QM/MM implementation of the virtual work principle to compute energy barriers. The effect of H and He atoms in the material on the dislocation core structure together with the energetics of dislocations and impurities are investigated. The obtained results are analysed by comparison with pure DFT studies from literature together with machine learning based Gaussian Approximation Potential (GAP) model.

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room1)

[SY-C10] First-principles Calculations of Deformation Twins in Hexagonal Titanium Alloys

○Daisuke Matsunaka, Ryosuke Amano （Dept. of Mechanical Engineering, Shinshu Univ., Japan）

Because of the excellent strength-to-density ratio and the high corrosion resistance, titanium (Ti) and Ti alloys have attracted much attention as aerospace and biomedical materials. One of the methods to improve mechanical properties of Ti is addition of solid solution atoms. For example, the tensile and fatigue strengths of Ti increase with oxygen content, although compromising ductility and toughness. For further development of titanium alloys, detailed understanding of effects of alloying elements on individual deformation modes, various slip and deformation twinning, in hexagonal alpha-titanium alloys is important.

In this study, we investigate twin boundaries and interaction of solute atoms such as Al in alpha-titanium alloys by first-principles calculations. For {11-22} twin, the mirror glide structure is stable, compared with the mirror reflection one and the {10-12} twin boundary. While the {10-12} twin boundary can migrate easily, the energy barrier for migration of the {11-22} twin boundary is relatively high. The interaction of solute atoms with the {10-12} twin boundary depends on the distance and the corresponding boundary sites, i.e., expansion and compression sites. On the other hand, the interaction of solute atoms with the {11-22} twin boundary is complex due to the mirror glide boundary structure.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C11] Symposium C-11

Chair: Nikhil Chandra Admal(University of California Los Angeles, United States of America)
Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room1

[SY-C11] A Multi-Scale Dislocation Language - Data Mining, Statistical Analysis, and Steps Towards a Community-Driven Data Base

○Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

[SY-C11] **The effect of dislocation character on dislocation line tension in bcc tungsten and its impact on kink-pair enthalpy**

○David Cereceda[1], Vasily Bulatov[3], Jaime Marian[2] （1.Dept. of Mechanical Engineering, Villanova University, United States of America, 2.Department of Materials Science and Engineering, University of California Los Angeles, United States of America, 3.Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, United States of America）

[SY-C11] Atomistic modeling of thermally activated plasticity in UO_2

Aurélien Soulié[1], ○Jean-Paul Crocombette[1], Antoine Kraych[1], Frédérico Garrido[2], Gaël Sattonnay[2], Emmanuel Clouet[1] （1.CEA Saclay, SRMP, France, 2.CSNSM, CNRS-IN2P3-Université Paris-Sud, France）

[SY-C11] **FTMP-based Simulations and Evaluation of Geometrically-Necessary Boundaries (GNBs) of Dislocation**

○Shiro Ihara, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[SY-C11] Improved phase field model of dislocation intersections

○Songlin Zheng[1], Yong Ni[2] （1.China Academy of Engineering Physics, China, 2.University of Science and Technology of China, China）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room1)

[SY-C11] A Multi-Scale Dislocation Language - Data Mining, Statistical Analysis, and Steps Towards a Community-Driven Data Base

Invited

○Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

Dislocations are simplistic objects: they are one-dimensional, their motion is constrained by the crystallography and they are surrounded by a stress field that decays with $1/r$. However, once dislocations start to interact with themselves or with other microstructures, their collective behavior becomes extremely complex. This - despite the apparent simplicity of the individual object - is still far from completely being understood.

Simulation methods, such as the Molecular Dynamics (MD) or the Discrete Dislocation Dynamics (DDD) have been very successfull in predicting the evolution of dislocation microstructures along with the resulting structure-property relations. However, up to now, there is no common "language" that allows to directly compare different dislocation structures - not even if they are obtained from the same simulation method. This makes statistical analysis and data mining on the level of the dislocations difficult.

An overview over state of the art methods for analyzing systems of dislocations will be given. Subsequently, the "Multi-scale Dislocation Language" (MuDiLingo) will be introduced, which allows to extract important geometrical properties of dislocations along with the corresponding energies. Based on examples from MD and DDD it will be shown (i) how this approach can be used to quantitatively compare dislocation microstructures, (ii) how valuable input for simulation methods on higher length scales can be provided by data-mining, and (iii) how MuDiLingo will enable us to create a data base of dislocation data, which might be of great benefit to the community.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room1)

[SY-C11] The effect of dislocation character on dislocation line tension in bcc tungsten and its impact on kink-pair enthalpy

○David Cereceda[1], Vasily Bulatov[3], Jaime Marian[2] （1.Dept. of Mechanical Engineering, Villanova University, United States of America, 2.Department of Materials Science and Engineering, University of California Los Angeles, United States of America, 3.Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, United States of America）

In addition to the well-characterized elastic contribution, the energy of a dislocation contains an inelastic, or 'core', term that reflects the loss of validity of elasticity theory at dislocation segments. While the elastic part is known to be symmetric about its maximum value for the edge orientation (minimum for screw), in bcc metals, the core energy displays an asymmetry that can be characterized using atomistic calculations. In kink-pair configurations on screw dislocations, this asymmetry leads to a difference in energy between 'right' and 'left' kinks that is not captured in elastic models. In this work, we calculate dislocation segment self-energies as a function of dislocation character in bcc tungsten and kink-pair enthalpies as a function of stress. To avoid finite-size artifacts in atomistic simulations, we develop continuum models of kink-pair configurations based on full elasticity and line tension approaches, parameterized with a substrate Peierls potential and dislocation self-energies obtained from atomistic calculations.

The elastic and line tension models represent specific situations of the environment of these kink-pair configurations, and we discuss our results in terms of the range of validity of each as well as the effect of self-energy asymmetry on kink-pair enthalpy. To match the continuum results to direct atomistic simulations, we vary the core radius of elasticity theory and discuss the implications of the values obtained.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room1)

[SY-C11] Atomistic modeling of thermally activated plasticity in UO$_2$

Aurélien Soulié[1], ○Jean-Paul Crocombette[1], Antoine Kraych[1], Frédérico Garrido[2], Gaël Sattonnay[2], Emmanuel Clouet[1]   (1.CEA Saclay, SRMP, France, 2.CSNSM, CNRS-IN2P3-Université Paris-Sud, France)

We investigate the thermally activated glide mobility of dislocations in uranium dioxide (UO$_2$) from an atomistic point of view using a variable charge many-body empirical potential, the Second Moment Tight-Binding potential with charge equilibration (SMTB-Q). In order to determine the main glide system, we model the dislocation core structures for edge and screw orientations lying in different glide planes. Uncommon core structures with a double periodicity and a charge alternation are obtained. Straight dislocations motion is first considered to obtain the Peierls stress of each dislocation. We then address the thermally activated motion of the dislocations by the nucleation of kink pairs. Atomistic simulations give us the structure as well as the formation and migration energies of kink pairs. This information is finally combined with an elastic interaction model for kink pairs to obtain the dislocation velocities and the evolution of the critical resolved shear stress as a function of temperature. These quantities are compared to experimental critical resolved shear stress and dislocation velocity measured on urania single crystals.

Reference : Acta Materialia 150, 248-261 (2018)

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room1)

[SY-C11] FTMP-based Simulations and Evaluation of Geometrically-Necessary Boundaries (GNBs) of Dislocation

○Shiro Ihara, Tadashi Hasebe   (Dept. of Mechanical Engineering, Kobe Univ., Japan)

Rational as well as practically-feasible treatments of spatio-temporally distributed discrete dislocation ensembles have been a long-standing issue and still a challenging problem inevitable in completion of multiscale modeling of metallic materials. Unlike 2D cases, which cannot be simply reduced down to continuously-distributed density function-like pictures, 3D counterparts need to deal, more or less, with its configurational complexities explicitly. We have recently been tackling these based on FTMP (Field Theory of Multiscale Plasticity), focusing on continuum descriptions of dislocation aggregates. Among others, quantitative stability/instability assessments of wall structures are critically important, in the sense that they substantially dominates both the micro/macro mechanical properties of the material systems concerned. The present study targets GNBs (Geometrically Necessary Boundaries) in terms of their stability/instability criteria and some dynamic interactions with in-coming dislocations, whose details about the consisting dislocations recently have been experimentally identified and theoretically evaluated by Hong, Winther, et al. Dislocation dynamics simulations on five typical GNBs, i.e., GNBs 2, 3, 4, 7 and 8, are conducted by utilizing Zbib code

and ParaDis code, and FTMP-based evaluations are performed against them. Duality diagram representations revealed a possible overall picture that governs the GNBs, i.e., all the GNBs exhibit a common tendency to converge ultimately to a single point, i.e., the ideal value for a hexagonal network-based GNB that yields the lowest energy as well as the smallest incompatibility, located in the most lower-left on the diagram.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room1)

[SY-C11] Improved phase field model of dislocation intersections

○Songlin Zheng[1], Yong Ni[2] （1.China Academy of Engineering Physics, China, 2.University of Science and Technology of China, China）

Revealing the long-range elastic interaction and short-range core reaction between intersecting dislocations is crucial for understanding dislocation-based strain hardening mechanisms in crystalline solids. Phase field model (PFM) has shown great potential in modeling dislocation dynamics with employing the continuum microelasticity theory to describe the elastic interactions and incorporating the -surface into the crystalline energy to enable the core reactions. Since the crystalline energy is approximately formulated by linear superposition of interplanar potential of each slip plane in the previous PFM, it does not fully account for the reactions between dislocations gliding in intersecting slip planes. In this study, an improved PFM of dislocation intersections is proposed through updating the crystalline energy by coupling the potential of two intersecting planes, and then applied to study the collinear interaction compared with the previous PFM model. Collinear annihilation captured only in the improved PFM is found to strongly affect the junction formation and plastic flow in multislip systems. The results indicate that the improvement is essential for PFM of dislocation intersections.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C12] Symposium C-12

Chair: Irene Beyerlein(University of California at Santa Barbara, United States of America)
Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room1

[SY-C12] Modeling the interaction between martensitic phase transformations and dislocation dynamics

○Rachel Derby, Michael Budnitzki, Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

[SY-C12] The effect of microscopic slip deformation on the yield stress in dispersion hardened alloys analyzed by using crystal plasticity FEM

○Yelm Okuyama[1], Masaki Tanaka[1], Tatsuya Morikawa[1], Tetsuya Ohashi[2] （1.Dept. of Materials Science and Engineering, Kyushu University, Japan, 2.Dept. of Engineering, Kitami Institute of Technology, Japan）

[SY-C12] Deformation Behaviour for Two-Phase Composites under Large Deformations using Micromechanical Analysis

○Srihari Dodla （Madanapalle Institute of Technology (MITS) Madanapalle, India）

[SY-C12] Dislocation dynamics simulation of FCC single crystals in high strain rate deformation

○Ronan MADEC （CEA, DAM, DIF, France）

[SY-C12] Comparison of two methods to cross-slip modeling by means of mathematical theory of moving curves

○Miroslav Kolar, Jan Kratochvíl, Petr Pauš, Michal Beneš （Czech Technical University in Prague, Czech Republic）

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room1)

[SY-C12] Modeling the interaction between martensitic phase transformations and dislocation dynamics

○Rachel Derby, Michael Budnitzki, Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

Two of the most important deformation mechanisms in TRIP-Steel are the martensitic phase transformations (MT) and elastic/plastic deformation due to the motion of dislocations. Martensitic phase transformations are desirable because they enhance the strength of TRIP-steels, however, dislocations can lower the strength of the material. These two phenomena are strongly coupled due to their contributions of strain to the system, resulting in an effect on the final macroscopic properties of the material. Thus, both dislocations and phase transformations must be considered simultaneously when modeling TRIP-Steels.

While MD simulations are inherently able to treat both dislocations and MT, such simulations suffer from a high computational cost and, hence, are not able to reach relevant time scales. Phenomenological continuum models for plasticity can be coupled with phase field approaches for the MT and can reach larger time scales; they do not capture the dynamics of the dislocations.

In our model, the dynamics of dislocations is described by a continuum dislocation dynamics (CDD) model, where instead of individual dislocations, a dislocation density is considered. This approach reduces the computational cost and enables the modeling of larger length scales. We use a coupled CDD/phase field approach to study the interaction of dislocation plasticity and the martensitic phase transformations. Our main focus is on the influence of different initial values and on the history dependence of the material. This will allow us to discuss, among others, what happens to dislocations in regions that undergo a MT - an information of big importance for continuum models operating on larger length scales.

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room1)

[SY-C12] The effect of microscopic slip deformation on the yield stress in dispersion hardened alloys analyzed by using crystal plasticity FEM

○Yelm Okuyama[1], Masaki Tanaka[1], Tatsuya Morikawa[1], Tetsuya Ohashi[2] （1.Dept. of Materials Science and Engineering, Kyushu University, Japan, 2.Dept. of Engineering, Kitami Institute of Technology, Japan）

The relationship between yield stress and the distribution of microscopic plastic deformation was investigated in dispersion hardened alloys using crystal plasticity FEM. Dispersed particles were randomly distributed in a 3D box in the calculation model. A plate region was extracted from the 3D box, and was used as a finite element model. The length factor in the Orowan equation was determined form the particle distribution in the 3D box. The critical resolved shear stress in local was set to a function of the length factor in the model. The length factor was defined as the average spacing of the particles, which surround the element, on the slip plane. The crystal plasticity analysis elucidates that the initiation and propagation of local slip deformation depends on the length factor. In this study, the relationship between the length factor and macroscopic mechanical response, *i.e.* yield stress and work hardening rate, is discussed.

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room1)

[SY-C12] Deformation Behaviour for Two-Phase Composites under Large Deformations using Micromechanical Analysis

○Srihari Dodla （Madanapalle Institute of Technology (MITS) Madanapalle, India）

This study presents a micromechanics approach for the elasto-viscoplastic behaviour of eutectic materials and structures. In this approach, the high-fidelity generalised method of cells (HFGMC) is applied for the prediction of the effective behaviour of two cold-drawn Cu-Ag composites with different drawing strains and to obtain the field (deformation gradient and stress) distributions in the composite. Both phases (Cu or Ag) are rate-dependent crystal plasticity material constituents. HFGMC is applied for analysing the deformation behaviour of two-phase Cu-Ag composites under uniaxial compression. The micromechanical analysis has been verified by comparison with experimental and finite element simulation results. Results in terms of deformation behaviour and field distributions are given for two different cold-drawn composites.

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room1)

[SY-C12] Dislocation dynamics simulation of FCC single crystals in high strain rate deformation

○Ronan MADEC （CEA, DAM, DIF, France）

In the range of high strain rate deformations from 10^4 to 10^6 s^{-1} or more, the mobile dislocation density significantly increases and some dislocations may reach a large fraction of sound velocity. The extent of this mobile dislocation multiplication stage depends upon material, experimental or simulation conditions. It also strongly depends on the initial dislocation density. When the total dislocation density reaches a certain value, it may saturate [1].

Molecular dynamics simulations are well suited for very high strain rates (10^7 s^{-1} or more). Hoverver, owing to the extremely small volumes and simulation times, it cannot deal with smaller strain rates. As a consequence, another type of simulation is needed for strain rates below 10^6 s^{-1} and dislocation dynamics simulations appears to be the most suitable method for this purpose.

The first dislocation dynamics studies at high strain rates were performed in small volumes (2-5 microns) of copper single crystals [2-5]. The dislocation fluxes and artefacts such as self annihilations were not carefully handled [6]. In addition, plastic strains were quite small (less than 0.2%) for such volume sizes and the saturation of the mobile dislocation density was difficult to reach even for the lowest strain rate. Nevertheless, the effect of inertia above 10^3 s^{-1} [2] and, above all, the importance of cross-slip [3-5] were established.

With growing computing power, larger volumes and deformations can be reached and the end of the multiplication stage of high strain rate deformation can be reached. So this topic deserves being revisited. Results about dislocation velocities, mobile and total dislocation densities, as well as the anisotropic response of copper single crystal as a function of stain rate and the effect of cross-slip will be discussed.

[1] L. Zepeda-Ruiz, A. Stukowski, T. Oppelsturp, V.V. Bulatov, Nature 550, 492-495 (2017)
[2] Z.Q. Wang, I.J. Beyerlein, R. Lesar, Phil. Mag. 87, 2263-2279 (2007)

[3] Z.Q. Wang, I.J. Beyerlein, R. Lesar, Model. Simul. Mater. Sci. Eng. 15, 675-690 (2007)

[4] Z.Q. Wang, I.J. Beyerlein, R. Lesar, Phil. Mag. 88, 1321-1343 (2008)

[5] Z.Q. Wang, I.J. Beyerlein, R. Lesar, Int. J. Plast. 25 26-48 (2009)

[6] R. Madec, B. Devincre, L. Kubin, Solid mechanics and its applications 115, 35-44 (2004)

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room1)

[SY-C12] Comparison of two methods to cross-slip modeling by means of mathematical theory of moving curves

○Miroslav Kolar, Jan Kratochvíl, Petr Pauš, Michal Beneš （Czech Technical University in Prague, Czech Republic）

The contribution focuses on the comparison of two different methods of dislocation cross-slip modeling, both based on the theory of evolving curves. The cross-slip is understood as deterministic, stress-driven dislocation process. In certain geometrical configuration, the criterion based on evaluation of driving stresses in the primary plane and in the cross-slip plane is employed. As an illustrative example, we consider a scenario where the cross-slip is forced by the repulsive stress exerted by a spherical obstacle with realistic repulsive stress. The result of this scenario is the double cross-slip.

The employed model for the dislocation motion can be schematically written as the curvature driven flow in the form

normal velocity = curvature + force.

In the first method, the dislocation motion law is based on the isometric projection. The cross-slip plane is tilted to the primary plane so that dislocation motion remains planar. When the dislocation enters the cross-slip plane, the appropriate physical quantities are recalculated accordingly.

The second method is based on the exploitation of the model of curves evolving on smooth surfaces and driven by the geodesic curvature. The smoothness of the the glide surface is ensured by regularizing the sharp interfaces between the primary plane and the cross-slip plane.

For both methods, the dislocations are described as parametrized curves. In numerical simulations, the flowing finite volume method is used. The results of the numerical simulations for both methods are compared to demonstrate their agreement.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E9] Symposium E-9

Chairs: Andrej Ostapovec(Institute of Physics of Materials ASCR, Czech Republic), Yujie Wei(Chinese Academy of Sciences, China)
Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room2

[SY-E9] The motion of a single dislocation from molecular dynamics simulations and its physical interpretation

○Yujie Wei[1,2], Shenyou Peng[1,2]　(1.Chinese Academy of Sciences, China, 2.School of Engineering Sciences, University of Chinese Academy of Sciences, China)

[SY-E9] Atomistic study on the super-elasticity of single crystal bulk NiTi shape memory alloy under adiabatic condition

○Bing Wang[1], Guozheng Kang[1], Qianhua Kan[1], Wenping Wu[2], Kun Zhou[3], Chao Yu[1]　(1.School of Mechanics and Engineering, Southwest Jiaotong University, China, 2.School of Civil Engineering, Wuhan University, China, 3.School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapore)

[SY-E9] Atomistic Modelling of Fracture with Non-Linear Elastic Boundary Conditions

○Punit Patel, James Kermode　(University of Warwick, UK)

[SY-E9] Atomistic simulation of the deformation and crack nucleation mechanisms in titanium alloys

○Dongsheng Xu　(Institute of Metal Research, Chinese Academy of Sciences, China)

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room2)

[SY-E9] The motion of a single dislocation from molecular dynamics simulations and its physical interpretation

Invited

○Yujie Wei[1,2], Shenyou Peng[1,2]　(1.Chinese Academy of Sciences, China, 2.School of Engineering Sciences, University of Chinese Academy of Sciences, China）

The dependence of dislocation mobility on stress is the fundamental ingredient for the deformation in crystalline materials. Strength and ductility, the two most important properties characterizing mechanical behavior of crystalline metals, are in general governed by dislocation motion. Experimentally, recording the position of a moving dislocation in a short time window is still challenging, and direct observation to deduce the speed-stress relationship of dislocations is still missing. Here we report the motion of an obstacle-free twinning partial dislocation in face centred cubic crystals with spatial resolution at the angstrom scale and temporal picosecond temporal information. The dislocation exhibits two limiting speeds: The first is subsonic and occurs when the resolved shear stress is on the order of hundreds of megapascal. While the stress is raised to gigapascal level, an abrupt jump of dislocation velocity occurs, from subsonic to supersonic regime. The two speed limits are governed respectively by the local transverse and longitudinal phonons associated with the stressed dislocation, as the two types of phonons influence dislocation gliding at different stress levels. In contrast, the kinetics of a screw dislocation is distinct from that of edges. We demonstrate that a screw dislocation can move steadily at the speed of shear wave velocity, or even move supersonically.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room2)

[SY-E9] Atomistic study on the super-elasticity of single crystal bulk NiTi shape memory alloy under adiabatic condition

○Bing Wang[1], Guozheng Kang[1], Qianhua Kan[1], Wenping Wu[2], Kun Zhou[3], Chao Yu[1]　(1.School of Mechanics and Engineering, Southwest Jiaotong University, China, 2.School of Civil Engineering, Wuhan University, China, 3.School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapore）

The temperature-induced phase transition and the super-elasticity (from the stress-induced phase transition) of equiatomic single crystal bulk NiTi shape memory alloys are investigated by the molecular dynamics method. By the simulation to the thermo-mechanical response of the single crystal NiTi alloy along the $<001>_{B2}$ under the compression/unloading and an adiabatic condition, the temperature change and the nucleation and growth of martensite transformation during the compression/unloading are discussed. The simulated results of molecular dynamics show that the single crystal bulk NiTi shape memory alloy exhibits a significant temperature change during the martensite transformation and its reverse under an adiabatic condition; moreover, a localized instability occurs apparently in the process of martensite transformation, which is closely related to the nucleation and growth rates of martensite phase; finally the effect of model size and strain rate on the thermo-mechanical response of the single crystal bulk NiTi alloy is also discussed, and no instability is observed in the simulated stress-strain curves if the model size is relatively larger, e.g., $8V_0$ and $13.824V_0$.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room2)

[SY-E9] Atomistic Modelling of Fracture with Non-Linear Elastic Boundary Conditions

○Punit Patel, James Kermode （University of Warwick, UK）

Atomistic simulations of crack propagation are key to understanding the fracture behaviour of materials. Cracks involve strong coupling across the scales, with bond breaking on the quantum scale driven by long range stress fields. Current QM methods are limited to simulation sizes too small to accurately describe fracture dynamics and improved QM/MM methods are able to adequately capture elastic effects [1]. However these methods are still heavily limited temporally and to coarse grain into the continuum scale while maintaining the overall fracture dynamics an expanded multiscale approach is required.

Applications in covalently bonded single crystals to complex alloys are underway. Screened classical potentials [2] predict a brittle response in both silicon carbide (SiC) and diamond, giving confidence in their applicability. DFT SiC surface energy calculations produced predictions in good agreement with experiment [3]. Extension of a multiscale approach for fracture includes a novel approach in correcting for finite domain boundary conditions, in which a non-linear continuum boundary correction is applied to help reduce the required system size, in order to compute energy barriers for crack extension bridging DFT and long time scale MD [4].

[1] N. Bernstein *et al.*, Rep. Prog. Phys. 72, 026501 (2009).
[2] L. Pastewka *et al.*, Phys. Rev. B. 87, 205410 (2013).
[3] G. Sernicola *et al.*, Nat. Commun. 8, 108 (2017)
[4] P. Patel, L. Pastewka, C. Ortner and J. R. Kermode, In Prep, (2018)

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room2)

[SY-E9] Atomistic simulation of the deformation and crack nucleation mechanisms in titanium alloys

○Dongsheng Xu （Institute of Metal Research, Chinese Academy of Sciences, China）

Titanium alloys are widely used in aero-space and chemical industries, but due to the complicated hierarchical microstructure formed in these systems, the deformation and fatigue life control is not easy. Multi-scale simulations were carried out on the deformation and microstructure evolution of titanium alloys in order to understand deformation and fatigue behavior under different conditions. The dislocation nucleation, interaction, debris accumulation and their effects on the deformation and fatigue crack nucleation were investigated. It was shown that, upon cyclic deformation, point defects and small dislocation loops can be formed in slip band by dipolar reaction. This will consume mobile dislocations, and make the operating slip system hardened; at the same time, they can provide deformation mechanism upon further increase of the stress. Comparing with perfect lattice, the lattice with point defects under tension perpendicular to the slip plane can be weakened by these point defects, therefore they may serve as fatigue crack nucleation sites and propagating paths. These understanding gained by simulations may provide important clue to the fatigue resistance design for titanium alloys.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E10] Symposium E-10

Chairs: Irene Beyerlein(University of California at Santa Barbara, USA), Dongsheng Xu(Institute of Metal Research, CAS, China)
Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room2

[SY-E10] **Study of atomic trajectories during twinning transformation in magnesium**
○Andrej Ostapovec[1], Tomáš Káňa[1], Václav Paidar[2] （1.Institute of Physics of Materials ASCR, Czech Republic, 2.Institute of Physics ASCR, Czech Republic）

[SY-E10] **Understanding nanocontact plasticity through massive MD simulations**
○Jorge Alcala[1], Javier Varillas[2,1], Jordi Torner[2], Jan Očenášek[1] （1.Universidad Politecnica de Catalunya, Spain, 2.New Technologies Research Centre, Czech Republic）

[SY-E10] **Atomistically informed mesoscale modeling of fracture**
○Hamad ul Hassan[1], Johannes Möller[2,3], Erik Bitzek[2], Alexander Hartmaier1[1], Rebecca Janisch[1] （1.ICAMS, Ruhr-Universität Bochum, Germany, 2.Friedrich-Alexander Universität Erlangen-Nürnberg , Germany, 3.Fraunhofer Institut für Werkstoffmechanik, Freiburg, Germany）

[SY-E10] **Lattice Distortion Effect on Cross-Slip in High Entropy Alloys and Lennard-Jones Systems for Face-Centered Cubic**
○Chao-Chun Yen[1], Junping Du[2,3], Jia-An Lin[4], Yu-Chieh Lo[4] （1.National Tsing Hua University, Taiwan, 2.Kyoto University, Japan, 3.Osaka University, Japan, 4.National Chiao Tung University, Taiwan）

[SY-E10] **Atomic structure of gamma/alpha2 interface and its influence on plastic deformation of lamellar TiAl alloys**
○Hao Wang[1], Aidong Tu[1], Yanxia Liu[2], Dongsheng Xu[1], Rui Yang[1] （1.Institute of Metal Research, CAS, China, 2.Dept. of Physics, Liaoning University, China）

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room2)

[SY-E10] Study of atomic trajectories during twinning transformation in magnesium

○Andrej Ostapovec[1], Tomáš Káňa[1], Václav Paidar[2]   (1.Institute of Physics of Materials ASCR, Czech Republic, 2.Institute of Physics ASCR, Czech Republic)

Deformation twinning is important mode of plastic deformation in magnesium and its alloys. Study of twinning mechanisms has long tradition. However, there is still opened questions in this field. There is some speculations in the literature, which connects possibility of non-Schmid behavior of mechanical twinning to type of atomic trajectories during twinning transformation. However, such theoretical considerations often use simplified descriptions of atomic motions. For instance, some authors made conclusions about macroscopic behaviour of twinning on the basis of linear or circular atomic trajectories. In a broader picture, real atomic paths should be quite complicated. They are consequence of disconnection glide along twin boundary. In this study we would like to discuss atomic trajectories obtained from modeling using EAM potentials as well as from ab-initio calculations.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room2)

[SY-E10] Understanding nanocontact plasticity through massive MD simulations

○Jorge Alcala[1], Javier Varillas[2,1], Jordi Torner[2], Jan Očenášek[1]   (1.Universidad Politecnica de Catalunya, Spain, 2.New Technologies Research Centre, Czech Republic)

This presentation concerns comprehensive molecular dynamics (MD) simulations of nanocontact plasticity in body-centered cubic (BCC) and face-centered cubic (FCC) crystals. The main focus is on the understanding of the evolution of the nanoscale material hardness with increasing tip penetration through detailed analyses of the distinct defect nucleation processes which result in the formation of a permanent imprint. It is shown that the gradual development of an entangled defect structure essentially governs the evolution of material pileup at the contact boundary, a feature that explains the different FCC and BCC imprint morphologies and topographies that develop depending on loading orientation. The present analyses provide a fundamental background to understand why BCC surfaces are harder than FCC surfaces at the nanoscale, including the role of the elastic response of the indented crystals. Novel MD simulations for crystals containing a preexisting (dense) dislocation network further confirm the pivotal role of the incepted defects upon indenter tip penetration. Our analyses contribute to the understanding of indentation size effects in submicrometer-sized material volumes, where a physical rationale to the validity of strain gradient plasticity and geometrically necessary dislocations is essentially lacking. Finally, our investigation leads to the finding of a general correlation between the nanohardness and the yield strength measured at the nanoscale under uniaxial loading conditions.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room2)

[SY-E10] Atomistically informed mesoscale modeling of fracture

○Hamad ul Hassan[1], Johannes Möller[2,3], Erik Bitzek[2], Alexander Hartmaier1[1], Rebecca Janisch[1]　(1.ICAMS, Ruhr-Universität Bochum, Germany, 2.Friedrich-Alexander Universität Erlangen-Nürnberg , Germany, 3.Fraunhofer Institut für Werkstoffmechanik, Freiburg, Germany）

At the engineering scale, continuum mechanics provides an efficient way to model fracture based on stresses, stress intensity factors, and energy release rates. At the atomic scale, in contrast, the breaking of atomic bonds is caused by critical forces acting on individual atoms. Therefore, a scaling methodology is required to apply information from atomistic scale to the continuum level problems, which are governed by engineering length and time scales.

Fracture at the continuum level can be described using state of the art methods such as cohesive zone-based modeling, which requires a material-specific traction-separation law (T-S law). Here, we present a mesh independent approach for atomistic-to-continuum level scaling of the stress and displacement measures, which are used in the T-S law. Our approach is based on a detailed analysis of the forces acting between the atoms in front of a crack tip, as well as between two semi-infinite half-crystals. Such a constellation is used to calculate the properties of cohesive zones based on atomistic simulations. The analysis shows, that the interatomic forces at a crack tip can be directly related to the restoring tractions between the two planar surfaces. This allows for an unambiguous scaling of the critical stresses and displacements, from GPa / Åon the atomic level, to the order of hundreds of MPa and nm on the mesoscale. A series of finite element simulations are performed for K_I loading based on the scaled input data for the T-S law and the critical stress intensity factors are calculated and compared with results from the atomistic simulations. We demonstrate and examine the ability of the atomistically informed finite element simulation to directly reproduce results from atomistic simulations.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room2)

[SY-E10] Lattice Distortion Effect on Cross-Slip in High Entropy Alloys and Lennard-Jones Systems for Face-Centered Cubic

○Chao-Chun Yen[1], Junping Du[2,3], Jia-An Lin[4], Yu-Chieh Lo[4]　(1.National Tsing Hua University, Taiwan, 2.Kyoto University, Japan, 3.Osaka University, Japan, 4.National Chiao Tung University, Taiwan）

The superior mechanical properties of high-entropy alloys (HEAs) make an outstanding success in material science and engineering. In recent years, more efforts have been devoted to the effect of severe lattice distortion, which is one of the core effects of HEAs. Previous studies have shown the impacts of severe lattice distortion on plastic deformation, including the influences on nucleation and propagation of dislocation. One of the most common mechanism is cross-slip in metals, which is a fundamental process of screw dislocation motion and plays an important role in dislocation annihilation and work hardening. However, there is no sufficient reference so far that can provide a clear correlation between the cross-slip and lattice distortion in HEAs. This may result from the difficulties of finding the cause of local lattice strain through experimental approach. Nevertheless, atomistic simulations can overcome the dilemma. Here, we create a binary system containing two different sizes of atoms. In order to focus on the lattice distortion caused only by size difference, a large-scale molecular dynamics simulation is performed using Lennard-Jones potentials to provide a size-controllable system where different sizes of atoms are assumed to be the same chemical potential. Therefore, we can systematically discuss the influence of the lattice distortion on cross-slip of HEAs. Furthermore, we apply nudged elastic band method on modified embedded-atom method potentials of CoCrFeMnNi and Lennard-Jones potentials to calculate the activation energy of cross slip for screw

dislocation respectively, and compare both results for further investigation.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room2)

[SY-E10] Atomic structure of gamma/alpha2 interface and its influence on plastic deformation of lamellar TiAl alloys

○Hao Wang[1], Aidong Tu[1], Yanxia Liu[2], Dongsheng Xu[1], Rui Yang[1]　(1.Institute of Metal Research, CAS, China, 2.Dept. of Physics, Liaoning University, China)

TiAl alloys with the γ-TiAl/α_2-Ti$_3$Al lamellar structure exhibit excellent high temperature performance. However, the strong anisotropy of the lamellae leads to the strong dependence of mechanical properties, in particular the fatigue behavior, on lamella orientation, thickness, volume fraction, etc. In the present work, molecular dynamics with the embedded-atom potential is employed to investigate the energy of both the coherent and incoherent γ/α_2 interfaces. The interface coherency is found to depend on the volume ratio of the γ lamellae over the α_2 lamellae, resulting in a critical volume ratio, below/above which the interface is coherent/incoherent. Loading perpendicular and parallel to the lamella interface indicates that the yield strength of coherent interface is higher than that of the incoherent interface. Plastic deformation mostly occurs first in the γ region and transmits to the α_2 region via dislocations or twinning across the γ/α_2 interface. Subsequent fracture behavior also depends on the γ/α_2 volume ratio. With the coherency and incoherency interfaces, crack nucleates within the γ region and at the γ/α_2 interface, respectively. The present result thus contribute to the evaluation of the structural stability and the improvement of mechanical performance of TiAl alloys.

[SY-E11] Symposium E-11

Chairs: Xiaoyu Yang(Computer network information center, CAS, China), Denise Reimann(ICAMS, Ruhr-Universität Bochum, Germany)
Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room2

[SY-E11] Thermodynamically consistent directional distortional hardening of wrought Mg alloys: experimental investigation and constitutive modeling

○Baodong Shi[1], Yan Peng[1], Chong Yang[1], Jianliang Sun[1], Fusheng Pan[2] （1.NECSR, School of Mechanical Engineering, Yanshan Univ., China, 2.NERC-MA, Chongqing Univ., China）

[SY-E11] **A computational infrastructure for multiscale materials simulation**

○Xiaoyu Yang （Computer network information center of the Chinese Academy of Sciences, China）

[SY-E11] Using machine learning methods to homogenize damage from micro- to macroscale

Denise Reimann[1], Hamad ul Hassan[1], Tobias Glasmachers[2], ○Alexander Hartmaier[1] （1.ICAMS, Ruhr-Universität Bochum, Germany, 2.Institut für Neuroinformatik, Ruhr-Universität Bochum, Germany）

[SY-E11] Graph theory analysis of rich fiber-scale data yields very fast simulations of damage evolution in composites

jerry quek[2], ○brian n cox[1] （1.arachne consulting, United States of America, 2.IHPC, Singapore）

[SY-E11] A deep learning-based constitutive model for finite element analysis

Fariborz Ghavamian[1], ○Angelo Simone[2,1] （1.Delft University of Technology, Netherlands, 2.University of Padova, Italy）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room2)

[SY-E11] Thermodynamically consistent directional distortional hardening of wrought Mg alloys: experimental investigation and constitutive modeling

Invited

○Baodong Shi[1], Yan Peng[1], Chong Yang[1], Jianliang Sun[1], Fusheng Pan[2] （1.NECSR, School of Mechanical Engineering, Yanshan Univ., China, 2.NERC-MA, Chongqing Univ., China）

As a lightweight structural material, magnesium alloy exhibits strong anisotropy due to texture, which limits its use in energy-saving lightweight structures. This pronounced anisotropy cannot be captured by only classical isotropic or kinematic hardening due to the constant shape evolution of yield surfaces during plastic deformation. Therefore, the shape evolution of yield surface, named as distortional hardening is the main approach to capture the anisotropic behavior of Mg alloy. Moreover, stress state is changing during forming process such as deep drawing, i.e., the loading history effect during plastic deformation cannot be ignored. Thus, focusing on loading path dependent distortional hardening of AZ31 Mg alloy, experimental investigation on the evolution of anisotropy is performed, moreover, a constitutive model with distortional evolution of yield surfaces is developed based on elasto-plasticity theory at finite strain. Thermodynamical consistency is proved. The anisotropic mechanical behavior of AZ31 Mg alloy is demonstrated after model parameters calibrated with experiments.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room2)

[SY-E11] A computational infrastructure for multiscale materials simulation

○Xiaoyu Yang （Computer network information center of the Chinese Academy of Sciences, China）

Bridging materials models and passing materials-related data and information across length scales is critical for the quantitative and predictive modelling of materials development. However, lacking of acceptable linkage software and tools is an obstacle. It is recommended in the report by the Minerals, Metals &Materials Society that "establishing an infrastructure for multiscale materials data is the first programmatic recommendations". Currently we are developing such an infrastructure to address this need based on a high-throughput computational infrastructure MatCloud[1]. The core of this multiscale simulation infrastructure is a linking software tool and technologies that contains a workflow designer and a workflow engine. The workflow designer aims to support the design of simulations involving running quantum mechanics scale ABINIT simulation and molecular scale LAMMPS simulation by drag &drop approach. The workflow engine is responsible for parsing and processing the workflow of multiscale materials simulation created by the workflow designer. As a test case, the multiscale materials simulation linking tool will be used to develop a particular interatomic potential through data-driven approach. In this talk, we will report our progress and challenges encountered.

Reference:

[1]. Yang X. et al , MatCloud: A High-throughput Computational Infrastructure for Integrated Management of Materials Simulation, Data and Resources, Computational Materials Science, Volume 146, 15 April 2018,

---

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room2)

[SY-E11] Using machine learning methods to homogenize damage from micro- to macroscale

Denise Reimann[1], Hamad ul Hassan[1], Tobias Glasmachers[2], ○Alexander Hartmaier[1]   （1.ICAMS, Ruhr-Universität Bochum, Germany, 2.Institut für Neuroinformatik, Ruhr-Universität Bochum, Germany）

Micromechanical models are in general able to describe microstructural influences, such as texture and grain size distribution, on damage evolution. A homogenization from the micro to the macro scale is, however, conceptually demanding. Hence, a new approach involving machine learning algorithms is suggested. In this work, numerical data based on micromechanical simulations is used to train the machine learning algorithm, which in turn describes macroscopic damage evolution as function of loading conditions and microstructure. The micromechanical simulations are based on representative volume elements (RVE) of realistic microstructure models, using crystal plasticity and damage mechanics to describe plastic deformation and damage evolution on the grain level.
Local quantities from these RVE simulations, such as stress, strain and damage, are homogenized into global averages. The trained machine learning algorithm is then able to predict global damage evolution as a function of the macroscopic loading state (e.g. equivalent strains, equivalent and hydrostatic stresses), elastic-plastic material properties and microstructure information (e.g. grains size distribution, crystallographic texture, etc.). The results are compared with well-accepted closed-form damage models such as Chaboche or Lemaître for validation. Furthermore, different machine learning algorithms such as artificial neural networks, support vector machines and random forest are used and their results are compared with each other as well.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room2)

[SY-E11] Graph theory analysis of rich fiber-scale data yields very fast simulations of damage evolution in composites

jerry quek[2], ○brian n cox[1]   （1.arachne consulting, United States of America, 2.IHPC, Singapore）

Simple mechanistic arguments suggest that the loci of cracks that initiate and propagate among fine-scale, stochastic, heterogeneous material domains might be predictable by fast graph theoretic methods, without executing explicit fracture mechanics simulations. Here we explore the usefulness of graph theoretic methods for analyzing the microcracking that develops in continuous fiber composites loaded transversely to the fiber direction. We use graph theoretic methods to analyze rich data published elsewhere for two types of fiber composite. The data describe the irregularity of the spatial distribution of the fiber population, and meandering of fibers within the population, which is seen when the fibers are tracked along the nominal fiber direction. Graph analysis yields very fast predictions of the likely sites of crack initiation in the fiber composite, as well as plausible indications of the likely direction in which an initiated crack will grow, the developing shape of the crack, and the frequency of instances of fibers that will bridge the crack obliquely, thereby raising the composite fracture resistance. From the results of the graph analysis, we infer a stochastic population of effective defects in the composite, whose location and effective strength are related to the

Euclidean and topological characteristics of the fiber population in the vicinity of the defect. We propose that, if the predicted distribution of defects is entered as an initial material condition in an homogenized finite element simulation of the composite, then the important effects of the stochastic fiber distribution, in regard to crack initiation, preferred directions of growth, and toughening due to fiber-bridging, can be captured in a simulation of tractable size. This strategy carries the pertinent spatial information content of any measured random distribution of fibers into a simulation in which the fibers are not represented explicitly.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room2)

[SY-E11] A deep learning-based constitutive model for finite element analysis

Fariborz Ghavamian[1], ○Angelo Simone[2,1]   (1.Delft University of Technology, Netherlands, 2.University of Padova, Italy)

A deep learning model is simply a function that maps a given input to a desired output. In spite of the simple nature of a deep learning model, over the past decade it has revolutionized natural language processing (NLP) and image understanding (IU). One can name three fundamental reasons to explain this astonishing accomplishment: 1) availability of large amount of data for NLP and IU over the past decade; 2) the fact that the performance of a deep learning model keeps increasing by increasing the training data (unlike other machine learning models); and 3) the recently available hardware and software infrastructures which are tailored for deep learning.

In this contribution we leverage the power of deep learning to construct a deep learning-based constitutive model. More specifically, we develop a novel neural network architecture which is tailored for simulations of history-dependent material behavior, and we discuss its implementation in a finite element model.

A possible application of this deep learning-based constitutive model is to serve as an efficient surrogate to a representative volume element (RVE) in a multi-scale finite element analysis. In this application large amount of training data can readily be generated from the RVE. As a proof of concept, we train our deep learning model on a set of data collected from a viscoplastic constitutive model and employ it a finite element model. Through numerical experiments we show that the structural level response of the finite element model is adequately approximated when using the deep learning-based constitutive model in place of the viscoplastic one.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E12] Symposium E-12

Chairs: Baodong Shi(NECSR, School of Mechanical Engineering, Yanshan Univ., China), Ligang Zhang(Central South University, China)
Thu. Nov 1, 2018 4:00 PM - 5:00 PM Room2

[SY-E12] **Diffusivities and atomic mobilities in bcc Ti-Mo-Nb-Ta-Zr alloys**

○Weimin Bai[1], Guanglong Xu[2], Libin Liu[1], Ligang Zhang[1] （1.School of Materials Science and Engineering, Central South Univ., China, 2.Tech Inst. for Advanced Materials &School of Materials Science and Engineering, Nanjing Tech Univ., China）

[SY-E12] Design of Ti-alloy by Integrating High Throughput Experiments and Calculations

○Ligang Zhang, Libin Liu, Di Wu　（Central South University, China）

[SY-E12] Simulation of Plasticity in Amorphous Solids

○Shingo Urata[1], Takahiro Murashima[2], Shaofan Li[3]　（1.Innovative Technology Research Center, Asahi Glass Co., Ltd (AGC)., Japan, 2.Dept. of Physics, Tohoku University, Japan, 3.Dept. of Civil and Environmetal Engineering, Univ. of California Berkeley, United States of America）

[SY-E12] Computational generation of the yield surfaces using stress based loading

○mayank chouksey, Sumit Basu　（Indian Institute of Technology, Kanpur, India）

(Thu. Nov 1, 2018 4:00 PM - 5:00 PM Room2)

[SY-E12] Diffusivities and atomic mobilities in bcc Ti-Mo-Nb-Ta-Zr alloys

○Weimin Bai[1], Guanglong Xu[2], Libin Liu[1], Ligang Zhang[1] （1.School of Materials Science and Engineering, Central South Univ., China, 2.Tech Inst. for Advanced Materials &School of Materials Science and Engineering, Nanjing Tech Univ., China）

Titanium and its alloys are widely used in biomedical field due to the low elastic modulus comparable to bone as well as high specific strength and high corrosion resistance. β-type (with bcc structure) and near β titanium alloys comprising non-toxic and non-allergic elements have been extensively investigated in the past decades to achieve low Young's modulus and good mechanical properties. Researchers suggested that Zr, Nb, Ta and Mo are the most desirable alloying elements in β-type bio-Ti alloys which have ability to effectively increase strength and reduce elastic modulus according to electronic structural calculations. Recently, a number of low-modulus biomedical β-titanium alloys have been developed, for example, Ti-29Nb-13Ta-4.6Zr (TNTZ), Ti-24Nb-4Zr-7.9Sn and Ti-8Mo-4Nb-2Zr.

Diffusivities play important roles when we manipulate above phase transformations and control microstructure development. The diffusion paths and phase fractions during homogenization and precipitation are precisely predicted with the help of thermodynamic and kinetic data by means of the Thermo-Calc and DICTRA software [2,3]. The microstructure evolution during heat treatment can be not only statistically explained via the classical nucleation and growth model equipped with accurate diffusivities, but also represented by the phase field modeling allying with diffusion kinetic database of multi- component and multi-phase systems.

In this work, the diffusivities of sub-ternary systems in Ti-Mo-Nb-Ta-Zr were extracted from composition profiles of diffusion couples using Whittle-Green [4] and Hall [5] methods. Based on the experimental results and thermodynamic descriptions, a self-consistent atomic mobility database of bcc Ti-Mo-Nb-Ta-Zr alloys were assessed using DICTRA software. All the kinetic descriptions were further verified by comprehensive comparisons between various model-predicted diffusion properties and the experimental data. The general agreement validates the potential application of the present atomic mobility database to simulate the diffusion in higher orders.

[1] J.-O. Andersson and J. Ågren, J. Appl. Phys. 72 (1992) 1350-1355.

[2] J.-O. Andersson et al., Calphad. 26 (2002) 273-312.

[3] D.P. Whittle and A. Green, Scr. Metall. 8 (1974) 883-884

[4] L.D. Hall, J. Chem. Phys. 21 (1953) 87-89.

(Thu. Nov 1, 2018 4:00 PM - 5:00 PM Room2)

[SY-E12] Design of Ti-alloy by Integrating High Throughput Experiments and Calculations

○Ligang Zhang, Libin Liu, Di Wu （Central South University, China）

The Speed for development of next materials is too slow and it has been emerging as the bottleneck for the innovation of the manufacturing technology. However, application of the computer and information technology to the materials science and engineering has made it possible for us to estimate the properties for single phases, model the microstructure evolutions, and predict the material properties. On the other hand, in order to verify the calculation results, we should develop and use the high throughput methods. In this talk, we introduce some new progress in materials calculation and high throughput experiments, especially the high throughput determination of the phase diagram, diffusion coefficients, and thermal-physical properties, and the high throughput verification of the response of the materials microstructure and properties to the compositions and heat treatment temperatures. Some preliminary results on the attempt of development of high strength and high toughness Ti alloys has been introduced.

(Thu. Nov 1, 2018 4:00 PM - 5:00 PM Room2)

[SY-E12] Simulation of Plasticity in Amorphous Solids

○Shingo Urata[1], Takahiro Murashima[2], Shaofan Li[3] （1.Innovative Technology Research Center, Asahi Glass Co., Ltd (AGC)., Japan, 2.Dept. of Physics, Tohoku University, Japan, 3.Dept. of Civil and Environmetal Engineering, Univ. of California Berkeley, United States of America）

A Multiscale model to simulate mechanical response of amorphous solids has been developed by coupling molecular mechanics and finite element method. In this method, an atomistic-based representative sampling cell (RS-cell) is embedded into each element to represent inelastic deformations in amorphous materials. Because the method employs a Parrinello-Rahman molecular dynamics based Cauchy-Born rule to construct an atomistically-informed constitutive model at continuum level, it is possible to quantitatively measure amorphous plastic deformations. In other words, the method intrinsically embeds a potential shear-transformation-zone (STZ), and thus the evolution of RS-cells can naturally allow molecular clusters having irreversible microstructure rearrangements at microscale in response to applied loads without using any phenomenological modeling. By using the proposed method, we obtained inelastic hysteresis loops for the amorphous materials under cyclic loading and also shear band formation at macroscale by using the Lennard-Jones binary glass (LJBG) model. In addition, we extended the method to apply to silicate glasses by considering electrostatic interaction. We would also demonstrate fracture simulation of the oxide glasses by coupling the method with Multiscale Cohesive Zone Model.

(Thu. Nov 1, 2018 4:00 PM - 5:00 PM Room2)

[SY-E12] Computational generation of the yield surfaces using stress based loading

○mayank chouksey, Sumit Basu （Indian Institute of Technology, Kanpur, India）

Ductile fracture in metals proceeds through nucleation, growth and coalescence of microvoids. Determination of the yield surface of a ductile porous material is necessary to simulate onset and evolution of ductile damage in a metal. Since the early work by Gurson where yield function for concentric spherical void inside a spherical RVE was considered, several extensions have emerged. It has been shown that the void

shape and anisotropy of the bulk matrix modify the yield function significantly. All these predictions of yield rely on limit analysis of the RVE based on the upper bound theorem and Hill-Mandal homogenization. These models have not accounted for onset of yield through localization of plastic strain.

Recently the competition between localization and uniform yield via the Gurson model has been compared. We have extended this work by performing stress controlled computational homogenization over sub-spaces of the principal stress space, to probe the yield surface of perfectly plastic materials with different void shapes. A special four-noded user element is developed in ABAQUS, that, is tied to a RVE with periodic boundary condition, restrained rigid body rotation and subjected to either macroscopic deformation gradient or Cauchy stress. The macroscopic plastic dissipation rate is monitored to detect yield. As a result, yield due to both uniform plastic deformation and localization are captured. We have compared the results of our computationally determined yield surfaces with the theoretical upper bound estimates. We show that over a significant section of the principal stress sub-space, localization modifies the yield surface. For prolate voids, localization hastens yield while for oblate it is delayed over estimates provided by models based on the upper bound theorem. The comparison gives us a rich insight into the competition between macroscopic yield through uniform proliferation of plasticity and localization.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F9] Symposium F-9

Chair: Ernst Kozeschnik(Institute of Materials Science and Technology, TU Wien, Austria)
Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room3

[SY-F9] Programmable Materials - tuning effective materials response

○Peter Gumbsch[1,2], Chris Eberl[1,3], Claudio Findeisen[1,2], Alexander Butz[1], Jan Pagenkopf[1,2]
（1.Fraunhofer IWM, Germany, 2.Karlsruhe Institute of Technology (KIT), Germany, 3.Albert-Ludwigs-Universität Freiburg, Germany）

[SY-F9] Equilibrium crystal shape of GaAs by ab-initio thermodynamics

In Won Yeu[1,2], Gyuseung Han[1,2], Cheol Seong Hwang[2], ○Jung-hae Choi[1]　（1.Center for Electronic Materials, Korea Institute of Science and Technology, Korea, 2.Department of Materials Science and Engineering, and Inter-university Semiconductor Research Center, Seoul National University, Korea）

[SY-F9] Elastic field of lattice defects in low-dimensional nano-carbon materials

○Xiao-Wen LEI[1], Akihiro NAKATANI[2], Tomoya TANIGUCHI[1]　（1.Dept. of Mechanical Engineering, Univ. of Fukui, Japan, 2.Dept. of Adaptive Machine Systems, Osaka Univ. , Japan）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room3)

[SY-F9] Programmable Materials - tuning effective materials response

Invited

○Peter Gumbsch[1,2], Chris Eberl[1,3], Claudio Findeisen[1,2], Alexander Butz[1], Jan Pagenkopf[1,2] （1.Fraunhofer IWM, Germany, 2.Karlsruhe Institute of Technology (KIT), Germany, 3.Albert-Ludwigs-Universität Freiburg, Germany）

The design of materials and materials microstructures to specific materials properties requires mechanistic materials modelling over multiple length scales to avoid tedious trial-and-error procedures and excessive experimentation. The feasibility of such multiscale modelling has now been demonstrated in several cases including the explicit modelling of the microstructural evolution during processing. As an example, I will explain the manufacturing process of a steel component, for which the local microstructure and the resulting material properties after deep drawing can be predicted.

On the component level, locally different processing conditions result in locally different materials properties which are often dealt with as a nuisance. I would like to take this further and ask whether we are able to design materials such that their locally varying properties are used for component functionality. Conceptually this can be regarded as locally *programming a material* to achieve component functionality. It will require large-scale structural optimization, predictive materials models for materials with significantly varying properties. I will give examples how this can be achieved. The approach can most easily be demonstrated using additively built metamaterials. With such metamaterials one can even go further and design them such that their effective materials properties can still be changed after manufacturing to achieve intrinsically *programmable materials*.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room3)

[SY-F9] Equilibrium crystal shape of GaAs by ab-initio thermodynamics

In Won Yeu[1,2], Gyuseung Han[1,2], Cheol Seong Hwang[2], ○Jung-hae Choi[1] （1.Center for Electronic Materials, Korea Institute of Science and Technology, Korea, 2.Department of Materials Science and Engineering, and Inter-university Semiconductor Research Center, Seoul National University, Korea）

The growth of the III-V compound semiconductors on Si is crucial to adapt their superior electronic properties to the silicon-based CMOS technology. In order to achieve the high-quality hetero-epitaxy preventing defects such as dislocation, crack, and anti-phase boundary, the selective area growth (SAG) method has been developed. To optimize this process, the atomic scale understanding is essential in terms of both the thermodynamics and kinetics. In this study, we establish a thorough methodology to calculate the surface energy as a function of temperature (T) and pressure (P) for the III-V compound materials in the combined framework of density functional theory (DFT) calculations and thermodynamics [1], which is competitive compared the previous DFT studies providing the surface energy as a function of chemical potential. Then, we construct the equilibrium crystal shape of GaAs as a function of T and P, including the effects of surface vibration. The calculated equilibrium shapes in various T and P conditions are compared with the experimentally grown shapes and explained in the viewpoint of the surface vibration, twin formation and kinetic factors.

[1] In Won Yeu *et al.,* Sci. Rep. 7, 10691 (2017).

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room3)

[SY-F9] Elastic field of lattice defects in low-dimensional nano-carbon materials

○Xiao-Wen LEI[1], Akihiro NAKATANI[2], Tomoya TANIGUCHI[1] （1.Dept. of Mechanical Engineering, Univ. of Fukui, Japan, 2.Dept. of Adaptive Machine Systems, Osaka Univ. , Japan）

Carbon atoms build themselves into different materials such as fullerenes, diamond nano-thread, carbon nanotube (CNT), and graphene sheet (GS) in nanometer-scale. The materials are formally classified into point, line, and surface materials, which correspond to zero-, one- and two-dimensional materials, respectively. Many literatures report that the lattice defects affected mechanical properties and electronic properties. Lattice defects in such low-dimensional nano-carbon are limited into special atomic structures rather than bulk (three-dimensional) materials, but the properties of these low-dimensional materials depend on the lattice defects as well as bulk materials. Continuum theory, such as dislocation theory, has been developed sophisticatedly for very long years. In low-dimensional materials, however, theoretical approaches for lattice defects are just developing. In this study we discuss the elastic field of lattice defects in low-dimensional nano-carbon, e.g. Stone-Wales (SW) defects on single-walled carbon nanotubes (SWCNTs) and GS. The various equilibrium configurations of atomistic models with defects are obtained using LAMMPS. The site potential energy and stress distribution of each atom are evaluated in the vicinity of defects. We also measure a curvature and bond length to identify the out-of-plane deformation and in-plane deformation. We also study the dependence of elastic field on the chirality of CNT and the interaction of two SW defects in details. Formation energy significantly depends on chirality, i.e. diameter, of nanotube as well as the orientation and position of SW defect in SWCNT and GS. The results obtained for atomistic models are compared with an classical analytical solutions of plane stress which is established ideally with assumption of only in-of-plane deformation, and the effect of out-of-plane deformation of low-dimensional nano-carbon is discussed.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F10] Symposium F-10

Chair: Ricardo Lebensohn(Los Alamos National Laboratory, United States of America)
Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room3

[SY-F10] **Data Analytics for Mining Process-Structure-Property Linkages for Hierarchical Materials**

○Surya Raju Kalidindi （Georgia Tech, United States of America）

[SY-F10] Maximization of strengthening effect of microscopic morphology in duplex elastoplastic solids

○Ikumu Watanabe[1], Gaku Nakamura[2], Kohei Yuge[2] （1.National Institute for Materials Science, Japan, 2.Seikei University, Japan）

[SY-F10] Assessment of formability limit diagram prediction by crystal plasticity finite element method

○Duancheng Ma （Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria）

[SY-F10] Analysis of gradient microstructures using crystal plasticity

○Balaji Selvarajou, Jerry Quek Siu Sin （IHPC, Singapore, Singapore）

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room3)

[SY-F10] Data Analytics for Mining Process-Structure-Property Linkages for Hierarchical Materials

Invited

○Surya Raju Kalidindi （Georgia Tech, United States of America）

A majority of the materials employed in advanced technologies exhibit hierarchical internal structures with rich details at multiple length and/or structure scales (spanning from atomic to macroscale). Collectively, these features of the material internal structure are here referred to as the material structure, and constitute the central consideration in the development of new/improved hierarchical materials. Although the core connections between the material's structure, its evolution through various manufacturing processes, and its macroscale properties (or performance characteristics) in service are widely acknowledged to exist, establishing this fundamental knowledge base has proven effort-intensive, slow, and very expensive for most material systems being explored for advanced technology applications. The main impediment arises from lack of a broadly accepted framework for a rigorous quantification of the material's structure, and objective (automated) identification of the salient features that control the properties of interest. This presentation focuses on the development of data science algorithms and computationally efficient protocols capable of mining the essential linkages from large ensembles of materials datasets (both experimental and modeling), and building robust knowledge systems that can be readily accessed, searched, and shared by the broader community. The methods employed in this novel framework are based on digital representation of material's hierarchical internal structure, rigorous quantification of the material structure using n-point spatial correlations, objective (data-driven) dimensionality reduction of the material structure representation using data science approaches (e.g., principal component analyses), and formulation of reliable and robust process-structure-property linkages using various regression techniques. This new framework is illustrated through a number of case studies.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room3)

[SY-F10] Maximization of strengthening effect of microscopic morphology in duplex elastoplastic solids

○Ikumu Watanabe[1], Gaku Nakamura[2], Kohei Yuge[2] （1.National Institute for Materials Science, Japan, 2.Seikei University, Japan）

An inverse analysis method based on nonlinear finite element analysis is developed to find an optimized morphology of periodic microstructure for improving the macroscopic mechanical properties in duplex elastoplastic solids. Here a gradient-based computational optimization method and two types of homogenization methods are employed. In this study, the optimization problem is defined as the maximization of the sum of macroscopic external works for several macroscopic deformation modes, enabling us to obtain a high strength material. The morphologic strengthening effect is discussed through a comparison with experiments and classical theories.

In a homogenization method based on finite element analysis, a representative volume element of an objective microstructure is modeled with finite elements and the deformation analysis is conducted under periodic boundary condition in control of macroscopic stress or strain. As the numerical results, the deformation state of microstructure is obtained along with the corresponding macroscopic material response. By coupling with this computational homogenization method and a mathematical optimization

method, the microstructure corresponding to a required performance can be found efficiently.

In this study, a computational optimization method for microstructure is applied to maximize the strength of a dual-component elastoplastic solid. A standard metal plasticity is employed to describe the material responses of each components and the material constants are determined from the macroscopic experiments of the corresponding single-component materials. For optimization calculations, the distributions of two densities are considered with node-based discretization under a constraint condition to finally segregate two components. And here simple strain-constant analytical homogenization method, so-called mixture rule, is applied to handle the mixture state during the optimization process.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room3)

[SY-F10] Assessment of formability limit diagram prediction by crystal plasticity finite element method

○Duancheng Ma （Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria）

This study is inspired by the recent development of "virtual material testing laboratory" in which the main equipment are full field crystal plasticity models. Ample examples have demonstrated its applications to sheet forming operations. In those applications, the mechanical anisotropy originated from the crystallographic texture can be adequately described, such as r-values and earing. Formability is also another very important property in sheet metal forming, which yet have not been equipped in these virtual laboratories. Though theoretical models for formability can be dated back to 1800s, all popular models at the moment suffer respective limitations. In this study, we make an attempt to the prediction of formability limit diagram by crystal plasticity finite element method, with the objective of overcoming the limitations posed by the current theoretical models. The focus is placed on the texture dependence of the formability limit diagram

---

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room3)

[SY-F10] Analysis of gradient microstructures using crystal plasticity

○Balaji Selvarajou, Jerry Quek Siu Sin （IHPC, Singapore, Singapore）

Gradients in microstructural features such as grain size, initial dislocation density and crystallographic texture occur in many engineering applications such as shot peened regions and heat affected zone of welds. While such microstructures may be desirable to improve mechanical properties, modelling of such microstructures require integration of appropriate length scales into the constitutive model. Crystal plasticity finite element method (CPFEM) offers an appropriate route to integrate the crystallographic and grain shape/size effects into the same descriptor for deformation; thus it allows for the probing of the deformation behaviour of complex gradient microstructures. In this work, we implement a CPFEM model that accounts for the effect of the grain boundaries and thus bringing in a length scale effect. The model is used to perform mesoscale simulations of realistic microstructures. Emphasis is on the role of the distribution of grain size, shape and crystallographic texture on the deformation behaviour. Corroboration with the fracture behaviour of such microstructures are also made.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F11] Symposium F-11

Chair: Peter Gumbsch(Fraunhofer IWM, Germany)
Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room3

[SY-F11] Mesoscale plasticity models of polycrystalline materials for efficient computation of microstructure/property relationships

○Ricardo Lebensohn （Los Alamos National Laboratory, United States of America）

[SY-F11] Development of a new consistent discrete Green operator for FFT-based methods to solve heterogeneous problems with eigenstrains

○Komlavi Senyo ELOH[1,2,3], Alain JACQUES[2,1], Stéphane BERBENNI[1,3] （1.University of Lorraine, France, 2.Institut Jean Lamour, France, 3.Laboratoire d'etudes de microstructures et de mé canique des matériaux, France）

[SY-F11] Efficient FFT-based Homogenisation without Linear Reference Medium

○Till Junge （EPFL, Mech. Engineering, Multiscale Mechanics Modeling, Switzerland）

[SY-F11] Multiscale modelling of the effective viscoplastic behavior of constituents of the mantle transition zone (Mg_2SiO_4 wadsleyite and ringwoodite): bridging atomic and polycrystal scales

Olivier Castelnau[1], Katell Derrien[1], Sebastian Ritterbex[2], Philippe Carrez[2], ○Patrick Cordier[2] （1.Process and Engineering in Mechanics and Materials, CNRS/ENSAM/CNAM, Paris, France, 2.Unité Matériaux et Transformations, CNRS / Univ. Lille, Lille, France）

[SY-F11] Scalable and Directionally-Sensitive Three-Dimensional Quantifying of Orientation and Dislocation Density Gradients in Crystal Plasticity Computer Simulations

○Markus Kuehbach, Franz Roters （Max-Planck-Institut fur Eisenforschung GmbH, Germany）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room3)

[SY-F11] Mesoscale plasticity models of polycrystalline materials for efficient computation of microstructure/property relationships

Invited

○Ricardo Lebensohn （Los Alamos National Laboratory, United States of America）

Models based on crystal plasticity are increasingly used in engineering applications to obtain microstructure-sensitive mechanical response of polycrystalline materials. Three key elements of these models are: a proper consideration of the single crystal plastic deformation mechanisms, a representative description of the microstructure, and an appropriate scheme to connect the microstates with the macroscopic response. The latter can be based on homogenization (e.g. self-consistent methods [1]), which relies on a statistical description of the microstructure, or be full-field solutions, which requires a spatial description of the microstructure (e.g. spectral methods [2]). Full-field models are numerically intensive, making their direct embedding in multiscale calculations computationally demanding. On the other hand, they can be used to generate reference solutions for assessment of homogenization-based approaches. In this talk we will review our recent efforts to develop material models based on polycrystal plasticity to capture anisotropic strength, along with their integration with emerging characterization methods in Experimental Mechanics (e.g. [3]), and their embedding in Finite Elements formulations (e.g. [4]) to solve problems involving complex geometries and boundary conditions with microstructure-sensitive material response.

[1] R.A. Lebensohn, C.N. Tomé and P. Ponte Castañeda: "Self-consistent modeling of the mechanical behavior of viscoplastic polycrystals incorporating intragranular field fluctuations". *Phil. Mag.* 87, 4287-4322 (2007).
[2] R.A. Lebensohn, A.K. Kanjarla and P. Eisenlohr: "An elasto-viscoplastic formulation based on fast Fourier transforms for the prediction of micromechanical fields in polycrystalline materials". *Int. J. Plast.* 32-33, 59-69 (2012).
[3] R. Pokharel, J. Lind, A.K Kanjarla, R.A. Lebensohn, S.F. Li, P. Kenesei, R.M. Suter and A.D. Rollett: "Polycrystal plasticity: comparison between grain scale observations of deformation and simulations". *Ann. Rev. Cond. Matter Phys.* 5, pp. 317-346 (2014).
[4] J. Segurado, R.A. Lebensohn, J. Llorca and C.N. Tomé: "Multiscale modeling of plasticity based on embedding the viscoplastic self-consistent formulation in implicit finite elements". *Int. J. Plast.* 28, 124-140 (2012).

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room3)

[SY-F11] Development of a new consistent discrete Green operator for FFT-based methods to solve heterogeneous problems with eigenstrains

○Komlavi Senyo ELOH[1,2,3], Alain JACQUES[2,1], Stéphane BERBENNI[1,3] （1.University of Lorraine, France, 2.Institut Jean Lamour, France, 3.Laboratoire d'etudes de microstructures et de mécanique des matériaux, France）

A new expression of the periodized discrete Green operator using the Discrete Fourier Transform method and consistent with the Fourier grid is derived from the classic "Continuous Green Operator" in order to

avoid the problem refered to as "aliasing" inherent to Discrete Fourier Transform methods. It is shown that the easy use of the conventional continous Fourier transform of the modified Green operator for heterogeneous materials with eigenstrains leads to spurious oscillations when computing the local responses of composite materials close to materials discontinuities like interfaces, dislocations, edges...We also focus on the calculation of the displacement field and its associated discrete Green operator which may be useful for materials characterisation methods like diffraction techniques.

The development of these new consistent discrete Green operators in the Fourier space allows to eliminate oscillations while retaining similar convergence capability. For illustration, the new discrete Green operators are implemented in a fixed-point algorithm for heterogeneous periodic composites knows as the Moulinec and Suquet (1994,1998) "basic scheme" that we extended to consider eigenstrain fields, as in Anglin, Lebensohn and Rollett(2014). Numerical examples are reported, such as the computation of the local stresses and displacement of composite materials with homogeneous or heterogeneous elasticiy combined with dilatational eigenstrain or representing prismatic dislocation loops. The mechanical fields obtained for cubic-shaped inclusion, spherical Eshelby and inhomogeneity, are compared with analytical solutions and the discretization method using the classic Green operator.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room3)

[SY-F11] Efficient FFT-based Homogenisation without Linear Reference Medium

○Till Junge （EPFL, Mech. Engineering, Multiscale Mechanics Modeling, Switzerland）

In the field of computational homogenisation of periodic representative volume elements (RVE), over the last two decades, fast Fourier transform (FFT)-based spectral solvers have emerged as a promising alternative to the finite element method (FE).

Most spectral methods are based on work of Moulinec and Suquet [1] and split an RVE's response into that of a linear reference medium and a periodic fluctuation due to heterogeneities. The main advantage of this formulation over FE is that it can be both significantly faster and memory-saving. The two main problems are 1) the choice of the reference medium, which is typically based on heuristics, non-trivial and has a strong impact on the method's convergence (A bad choice can render the method non-convergent), and 2) convergence is not uniform. Numerous studies have suggested mitigations to both of these problems (e.g. [2]), but they have remained substantial disadvantages compared to the more expensive, but also more robust FE.

Recent work by Zeman et al. [3] proposes a new formulation for spectral solvers which dispenses with the linear reference problem and converges unconditionally. We present Spectre, an open implementation of this novel method and use it to show that the new approach is more computationally efficient than its linear reference medium-based predecessors, converges in the presence of arbitrary phase contrast - including porosity - and eliminates or drastically reduces Gibbs ringing.

[1] H. Moulinec and P. Suquet. A numerical method for computing the overall response of nonlinear composites with complex microstructure. Computer Methods in Applied Mechanics and Engineering, 157(1):69-94, 1998
[2] M. Kabel, et al. Efficient fixed point and Newton-Krylov solvers for FFT-based homogenization of elasticity at large deformations. Computational Mechanics, 54:1497-1514, 2014
[3] J. Zeman, et al. A finite element perspective on non-linear FFT-based micromechanical simulations. Int. J. Num. Meth. Eng., 2016

[SY-F11] Multiscale modelling of the effective viscoplastic behavior of constituents of the mantle transition zone (Mg_2SiO_4 wadsleyite and ringwoodite): bridging atomic and polycrystal scales

Olivier Castelnau[1], Katell Derrien[1], Sebastian Ritterbex[2], Philippe Carrez[2], ○Patrick Cordier[2] （1.Process and Engineering in Mechanics and Materials, CNRS/ENSAM/CNAM, Paris, France, 2.Unité Matériaux et Transformations, CNRS / Univ. Lille, Lille, France）

The Earth mantle transition zone (an envelope of the Earth's interior between 410 and 660 km depth) is constituted by more than half from wadsleyite and ringwoodite. Waldseyite is present up to 525km depth, whereas ringwoodite appears below. In the transition zone, pressure ranges from 14 GPa to 24GPa, and temperature lies between 1880˚ K and 1900˚ K. Estimation of the viscoplastic behavior of these constituents, and the link with their microstructure (crystallographic texture), is crucial to better understand the structure of large scale convection cells in the mantle responsible for plate tectonic.

In this work, the viscoplastic behavior of wadsleyite and ringwoodite polycrystalline aggregates (cm scale) is obtained by bridging several scale transition models, starting from very fine scale (nm) of the dislocation core structure. This presentation will emphasize the grain-polycrystal scale transition.

Deformation resulting from thermally activated dislocation glide has been modeled in wadsleyite and ringwoodite at high pressures, for a wide range of temperatures, and under laboratory and *in situ* (*i.e.* mantle) strain-rates conditions. The model relies on the structure and kink pairs nucleation enthalpies of the rate controlling screw dislocations which have been modeled using the Peierls-Nabarro-Galerkin method and an elastic interaction model. Corresponding single slip critical resolved shear stresses (CRSS), and associated constitutive equations have been deduced from Orowan's equation in order to describe the average viscoplastic behavior at the grain scale, for all available slip systems.

These data are then implemented in two grain-polycrystal scale transition models, a statistical one (Second-Order Viscoplatic Self-Consistent scheme) allowing rapid evaluation of the effective viscosity of the polycrystalline aggregates, and a full-field method (FFT based method) allowing investigating many inter- and intra-granular features such as stress and strain localization in a typical microstructure, heterogeneous activation of slip systems, etc. Calculations have been performed for pressure, temperature, and strain-rates conditions corresponding to laboratory and *in situ* conditions. The obtained effective behavior is in very good match with available experimental data.

[SY-F11] Scalable and Directionally-Sensitive Three-Dimensional Quantifying of Orientation and Dislocation Density Gradients in Crystal Plasticity Computer Simulations

○Markus Kuehbach, Franz Roters （Max-Planck-Institut fur Eisenforschung GmbH, Germany）

In-grain orientation and dislocation density gradients, especially those building up at grain and phase boundaries, tune to significant extent a variety of microstructure evolution mechanisms: the nucleation and incipient stage of discontinuous dynamic recrystallization, deformation texture evolution, or phase transformations to name but a few. Despite being additionally also of relevance for stress and strain partitioning, their comprehensive quantification in three dimensions, though, has received little attention so far and remains elusive.

In this work we report on higher-order neighbor- and signed-distance-based techniques for quantifying such gradients; resulting in a tool applicable to point-cloud-based data. These are tracked for instance via integration point cloud sets in finite-strain-formalism full-field crystal plasticity computer simulations. Exemplarily, as such an evaluation of dislocation gradients resulting from Crystal Plasticity deformation simulations using the DAMASK spectral solver [1, 2] will be presented and their relevance for discontinuous dynamic recrystallization discussed.

[1] P. Eisenlohr, M. Diehl, R.A. Lebensohn, F. Roters: A spectral method solution to crystal elasto-viscoplasticity at finite strains, International Journal of Plasticity 46 (2013), 37 - 53

[2] P. Shanthraj, P. Eisenlohr, M. Diehl, F. Roters: Numerically robust spectral methods for crystal plasticity simulations of heterogeneous materials, International Journal of Plasticity 66 (2015) 31 - 45

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F12] Symposium F-12

Chair: Yasushi Shibuta(The University of Tokyo, Japan)
Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room3

[SY-F12] Microstructure formation in large-scale molecular dynamics simulation

○Yasushi Shibuta[1], Shin Okita[1], Eisuke Miyoshi[2], Shinji Sakane[2], Tomohiro Takaki[2], Munekazu Ohno[3] (1.The University of Tokyo, Japan, 2.Kyoto Institute of Technology, Japan, 3.Hokkaido University, Japan)

[SY-F12] Directed assembly of structured nanoparticles through rapid micromixing

○Arash Nikoubashman[1], Nannan Li[2], Athanassios Z. Panagiotopoulos[2] (1.Johannes Gutenberg University of Mainz, Germany, 2.Princeton University, United States of America)

[SY-F12] Various interfaces related to twinning in hexagonal metals

○Vaclav Paidar[1], Andriy Ostapovets[2] (1.Institute of Physics AS CR Prague, Czech Republic, 2.Institute of Physics of Materials AS CR Brno, Czech Republic)

[SY-F12] Multiscale mean-field modelling of mechanochemical processes in heterogeneous materials for energy storage

○Mikhail Poluektov[1], Łukasz Figiel[1,2] (1.International Institute for Nanocomposites Manufacturing, WMG, University of Warwick, UK, 2.Warwick Centre for Predictive Modelling, University of Warwick, UK)

[SY-F12] Impact of local symmetry breaking on the physical properties of tetrahedral liquids

○Rui Shi, Hajime Tanaka (University of Tokyo, Japan)

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room3)

[SY-F12] Microstructure formation in large-scale molecular dynamics simulation

Invited

○Yasushi Shibuta[1], Shin Okita[1], Eisuke Miyoshi[2], Shinji Sakane[2], Tomohiro Takaki[2], Munekazu Ohno[3]　(1.The University of Tokyo, Japan, 2.Kyoto Institute of Technology, Japan, 3.Hokkaido University, Japan)

Microstructure formation is discussed on the basis of large-scale molecular dynamics (MD) simulations of nucleation, solidification and subsequent grain grow for pure iron [1-3]. After the nucleation and solidification, the time change of volume of grains is directly estimated for 2D and 3D grain growths [1]. For the 2D grain growth, grains with seven and more neighboring grains generally grow larger, whereas those with five and less neighboring grains shrink and disappear [2], which basically agrees with von Neumann-Mullins law. For the 3D grain growth, threshold number of neighboring grains is estimated to be approximately 14 [2]. Moreover, the physical origin of the deviation from the ideal grain growth is investigated by the direct estimation of the reduced mobility (i.e., the product of the intrinsic grain boundary mobility and the grain boundary energy) and the geometric factor [3]. The new insights based on large-scale MD simulations up to billion atoms are achieved for the first time owing to a multi-graphics processing unit (GPU) parallel computation on the GPU-rich supercomputer.

[1] Y. Shibuta, et al., Nature Comm. 8 (2017) 10. [2] S. Okita, Y. Shibuta, ISIJ Int. 56 (2016) 2199. [3] S. Okita et al., submitted.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room3)

[SY-F12] Directed assembly of structured nanoparticles through rapid micromixing

○Arash Nikoubashman[1], Nannan Li[2], Athanassios Z. Panagiotopoulos[2]　(1.Johannes Gutenberg University of Mainz, Germany, 2.Princeton University, United States of America)

Tailored nanoparticles are increasingly sought after for many scientific and technological applications, such as optoelectronic devices and highly selective catalysts. However, both research and commercialization of these materials has been impeded by the lack of suitable fabrication techniques. One promising approach for overcoming this hurdle is flash nanoprecipitation, where (soft) nanoparticles are assembled through rapid micromixing of polymers in solution with a miscible poor solvent. This continuous process allows for high yields as well as precise control over particle size and morphology. We employed multiscale computer simulations of this process to understand its underlying mechanisms and to efficiently explore parameter space. We first performed explicit solvent molecular dynamics (MD) simulations of a bead-spring polymer model to study the microscopic properties of the fabrication process. Then, we fed the MD data into a kinetic Monte Carlo algorithm to reach macroscopic length- and timescales. We discovered that the nanoparticle size can be reliably tuned through the initial polymer concentration and the mixing rate. Further, we were able to fabricate a wide variety of structured colloids, such as Janus and core-shell particles, when polymer blends were used in the feed stream.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room3)

[SY-F12] Various interfaces related to twinning in hexagonal metals

○Vaclav Paidar[1], Andriy Ostapovets[2]　(1.Institute of Physics AS CR Prague, Czech Republic, 2.Institute of Physics of Materials AS CR Brno, Czech Republic)

The {10-12} twin mode is the one most commonly activated in hexagonal metals. A primary part of the lattice transition from the matrix to the twin orientation is shear deformation that converts the [0001] direction of the hexagonal axis in the matrix to a direction almost parallel to the [10-10] direction perpendicular to the <a> axis in the basal plane in the twin. In addition to primary mechanical twinning also several types of double-twins were observed as, for example, {10-11}-{10-12} or {10-12}-{10-12}. Surprisingly, the last one can occur in magnesium with the c/a ratio smaller than $\sqrt{3}$ but also in zinc with the c/a ratio larger than $\sqrt{3}$. Various types of symmetrical and asymmetrical interfaces including also basal/basal or prismatic/prismatic boundaries will be discussed and their impact on materials properties will be envisaged.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room3)

[SY-F12] Multiscale mean-field modelling of mechanochemical processes in heterogeneous materials for energy storage

○Mikhail Poluektov[1], Łukasz Figiel[1,2]　(1.International Institute for Nanocomposites Manufacturing, WMG, University of Warwick, UK, 2.Warwick Centre for Predictive Modelling, University of Warwick, UK)

Performance enhancement of energy storage devices, e.g. batteries, requires careful selection of materials. The microstructure of such materials can undergo a complex electro-chemo-mechanical cycling during battery exploitation, which involves extreme volumetric expansion of the active material during the chemical reaction. The expansion is causing mechanical stress, which, in turn, influences the kinetics of chemical reactions even up to their arrest [3]. Thus, to predict the mechanochemical behaviour of a multi-material battery electrode, both the multi-physics phenomena and microstructure must be taken into account.

Up to now, the major focus has been on development of coupling models between mechanics, diffusion and chemical reactions, e.g. [4], particularly, chemical reactions, such as lithiation and oxidation, that take place at a surface, e.g. [1-2]. When localised reactions are modelled, the thermodynamic consistency has to be maintained and the velocity of the chemical reaction front should not violate the entropy production inequality and the balance laws. One such model is based on the chemical affinity tensor [2]. This model was used to predict the kinetics and the arrest of the reaction front in free-standing Si particles of a battery anode [5].

The model presented in this talk builds on [5] and accounts for the lithiation kinetics of a collection of particles inside an effective matrix material. The battery microstructure is modelled using the multiscale mean-field framework based on the incremental Mori-Tanaka method. This is the first application of a multiscale mean-field technique to modelling lithiation reaction front kinetics in a complex anode microstructure within the finite-strain framework, and to linking the intraparticle kinetics with the macroscopic response of the battery.

References

[1] ZW Cui, F Gao, JM Qu (2013) J Mech Phys Solids 61:293-310

[2] AB Freidin, EN Vilchevskaya, IK Korolev (2014) Int J Eng Sci 83:57-75

[3] K van Havenbergh, S Turner, N Marx, G van Tendeloo (2016) Energy Technol 4:1005-1012

[4] VI Levitas, H Attariani (2014) J Mech Phys Solids 69:84-111

[5] M Poluektov, AB Freidin, L Figiel (2018) Int J Eng Sci accepted

---

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room3)

[SY-F12] Impact of local symmetry breaking on the physical properties of tetrahedral liquids

○Rui Shi, Hajime Tanaka （University of Tokyo, Japan）

Water and silica are the most important materials with local tetrahedral symmetry. They have similar crystalline polymorphs and exhibit anomalous density maximum in the liquid state. However, water and silica also show very different characteristics. For instance, the density of water varies much more sharply than that of liquid silica near the maximum as temperature changes. More notably, silica is a very good glass-former, but water is an extremely poor one. The physical origins of these similarities and differences still remain elusive, due to the lack of a microscopic understanding of the structural ordering in these two important liquids. Here, by accessing microscopic structural information by computer simulations, we reveal that local translational symmetry breaking is responsible for the density anomalies. On the other hand, the difference in the degree of local orientational symmetry breaking between water and silica, which originates from the difference in their bonding nature, causes not only the difference in the sharpness of density anomalies, but also their distinct glass-forming abilities. Our work not only shows the crucial roles of local translational and orientational symmetry breaking in the physical properties of the two extremely important materials, water and silica, but also provides a unified scenario applicable for other tetrahedral liquids such as Si, Ge, C, BeF_2, and GeO_2.

Symposium | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[SY-G5] Symposium G-5

Chairs: Keonwook Kang(Yonsei University, Korea), Akiyuki Takahashi(Tokyo University of Science, Japan)
Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room4

[SY-G5] Metallic materials under extreme pressure: Interplay of plasticity and phase transitions

○Nina Gunkelmann[1], Hoang-Thien Luu[1], Diego R. Tramontina[3], Carlos J. Ruestes[3], Yudi Rosandi[4], Herbert M. Urbassek[2] (1.Clausthal University of Technology, Germany, 2.University of Kaiserslautern, Germany, 3.National University of Cuyo, Argentine, 4.University of Padjadjaran, Indonesia)

[SY-G5] Dislocation dynamics modeling of fracture behavior with considering dislocation shielding effect

○Akiyuki Takahashi, Hayato Sugasawa, Masanori Nagura (Tokyo University of Science, Japan)

[SY-G5] Dynamic behaviors of dislocations and grain boundaries induced by phonon scattering in nanoscale

○Soon Kim, Sung Youb Kim (Dept. of Mechanical Engineering, UNIST, Korea)

[SY-G5] Investigation on 1/2<11-1>{112} and 1/2<11-1>{123} mixed dislocations in BCC iron by classical molecular dynamics

○Tomohisa Kumagai[1], Akiyoshi Nomoto[1], Akiyuki Takahashi[2] (1.Central Research Institute of Electric Power Industry, Japan, 2.Tokyo University of Science, Japan)

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room4)

[SY-G5] Metallic materials under extreme pressure: Interplay of plasticity and phase transitions

Invited

○Nina Gunkelmann[1], Hoang-Thien Luu[1], Diego R. Tramontina[3], Carlos J. Ruestes[3], Yudi Rosandi[4], Herbert M. Urbassek[2]　(1.Clausthal University of Technology, Germany, 2.University of Kaiserslautern, Germany, 3.National University of Cuyo, Argentine, 4.University of Padjadjaran, Indonesia)

Shock waves are ubiquitous in various fields of activity including space science and engineering. They are of key interest for materials engineering, where shock-induced phase transitions may be used to produce new materials with increased strength which might be stable at ambient conditions.

As prototypical materials, we consider iron and iron-carbon alloys showing a pressure induced phase transformation from the bcc to the hexagonal close-packed phase at around 13 GPa depending on the carbon content. We study waves in polycrystalline Fe using an interatomic potential that faithfully incorporates this phase transition at the desired equilibrium pressure.

Our simulations show that the phase transformation is preceded by plastic activity, leading to the so-called 3-wave structure: An elastic compression wave is followed by a plastic wave which then leads to a phase-transformation front. We show that the phase transformation from bcc to hcp and vice-versa helps to drive twinning and decreases the probability of multiple spallation and crack formation. In agreement with experiments, the fracture surface is influenced by the phase transition showing smooth spall surfaces.

Despite large differences in material properties, shock waves in aluminium nanofoams exhibit, similar to polycrystalline iron, a 3-wave structure indicating three wave regimes: an elastic precursor is pursued by plastic activity in the filaments before eventually the foam structure is crushed and a compact material results. The collapse of the foam is well described by an analytical compaction model.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room4)

[SY-G5] Dislocation dynamics modeling of fracture behavior with considering dislocation shielding effect

○Akiyuki Takahashi, Hayato Sugasawa, Masanori Nagura　(Tokyo University of Science, Japan)

Ductile-brittle transition (DBT) in ferric steels is a critical issue to ensure the structural integrity of nuclear power plants. The DBT is believed to be caused by the shielding effect of dislocations at the crack tip. Therefore, in order to make a deep understanding of the fracture behavior and the DBT mechanisms, it is necessary to develop a computational method that can take into account the dislocation nucleation, the dislocation behavior and the stress of dislocation around the crack tip, and can derive the fracture toughness as a result of dislocation-crack interactions. This paper presents a dislocation dynamics (DD) simulation technique for the fracture toughness calculation with the consideration of dislocation shielding effect. In this study, the crack is represented with discrete dislocations, and the crack problem is solved using the DD method. The dislocation nucleation from the crack tip is simply modeled with a critical shear stress in the immediate vicinity of the crack tip. The nucleated dislocations move in the material, and produce the stress at the crack tip. The complex system of crack-dislocation interactions can be solved only with the DD

method. In the DD method, the stress intensity factor at the crack tip can be easily computed by calculating the Peach-Koehler force, which is normally calculated in the DD simulations, acting at the crack tip dislocation. When the stress intensity factor reaches a critical value, the fracture toughness is determined by the applied stress. To demonstrate the potential of the developed DD method, we performed a simulation of dislocation shielding with various dislocation mobility, which imitates the temperature dependence of dislocation behavior and fracture toughness. The numerical result clearly shows that the higher dislocation mobility gives higher fracture toughness, which is qualitatively in agreement with experimental results.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room4)

[SY-G5] Dynamic behaviors of dislocations and grain boundaries induced by phonon scattering in nanoscale

○Soon Kim, Sung Youb Kim （Dept. of Mechanical Engineering, UNIST, Korea）

Conventional dislocation dynamics based on continuum theory is limited in its ability to describe motion of dislocations in nanoscale. This is because discrete characteristics are no longer ignored in nanoscale unlike in micro- or macroscales. Especially, the discreteness becomes a significant factor to describe core region of dislocation so that it contributes to nonlinear properties of the core. In a sense that the core determines mobility of dislocations and concerns interactions among them, the discrete approach must be carefully considered in nanoscale dislocation dynamics. To reflect the discrete characteristics in nanoscale, computer simulations and discrete lattice dynamics approach have been used to quantify properties of the dislocation core.

In our work, we carried out molecular dynamics simulation to study motion of the dislocation in nanoscale and found surprising behavior that internal stress of system where dislocation is inserted is dropped when the dislocation is in motion by externally applied stress. By using discrete lattice dynamics, we proved that this behavior occurs due to scattering of the wave emitted from breaking of atomic bond in the core [1].

Furthermore, we extended our approach to grain boundary since it can be assumed as a collection of dislocations if its misorientation angle is small enough. We simulated the grain boundaries for various misorentation angles under external stress. As a result, dropping of internal stress is also observed as in dislocation case. Not only the stress-drop, but the grain boundaries were curved during their motion and magnitude of the curvature and speed were inversely proportional to the misorientation angle. We analyzed these behaviors by using the discrete lattice dynamics and concluded that these are able to be appeared only in nanoscale materials.

References

[1] S. Kim, D. T. Ho, K. Kang, and S. Y. Kim, *Acta. Mater*, **115** (2016), p143-154.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room4)

[SY-G5] Investigation on 1/2<11-1>{112} and 1/2<11-1>{123} mixed dislocations in BCC iron by classical molecular dynamics

○Tomohisa Kumagai[1], Akiyoshi Nomoto[1], Akiyuki Takahashi[2]　(1.Central Research Institute of Electric Power Industory, Japan, 2.Tokyo University of Science, Japan）

Mixed dislocation motion of 1/2<11-1>{112} and 1/2<11-1>{123} slip systems in pure BCC iron was observed by using classical molecular dynamics (MD). Angles between Burgers vector and dislocation line, which is referred as mixed dislocation angle, were between 0 degree and 180 degree (i.e., 0 degree and 180 degree correspond to screw dislocation and 90 degree corresponds to edge dislocation). As an initial configuration, one mixed dislocation was introduced in the MD box. Then, shear strain parallel to the slip plane with constant strain rate was applied to glide the dislocation to calculate Peierls stress, or shear stress was applied to calculate mobility and friction stress.The directions of dislocation motion were both twinning and anti-twinning directions. Dislocation mobility and friction stress at 100K and 300K were evaluated as well as Peierls stress. High Peierls stress was observed on a mixed dislocation whose core structure was straight (i.e., it does not contain kinks) since all of the dislocation had to jump to the next position at the same time. On the other hand, low Peierls stress was observed on a mixed dislocation whose core structure contains kinks since it could gradually move through kink movement along with the dislocation line. There seemed that the friction stress and the mobility of the mixed dislocations were affected by the dislocation core structure at 100K; the friction stress was high and the mobility was low at the mixed dislocation angles where Peierls stress was high. On the other hand, there seemed to be less effect of the core structure on the friction stress nor the mobility at 300K. It is found that directions of dislocation motion have almost no effects on the Peierls stress, mobility and friction stress as a whole.

Symposium | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[SY-G6] Symposium G-6

Chairs: Akiyuki Takahashi(Tokyo University of Science, Japan), Keonwook Kang(Yonsei University, Korea)
Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room4

[SY-G6] Repulsive Correction in Tersoff Potential for Irradiated Si

○Youhwan Jo, Taeyeon Kim, Byeongchan Lee （Kyung Hee University, Korea）

[SY-G6] Phase-field modeling of microstructural evolution of Fe-Cr-Al system

○Kunok Chang （Kyung Hee Univ., Korea）

[SY-G6] Dissolution kinetics of ejecta in hydrogen at megabar pressure

○Arslan B. Mazitov[1,2], Artem R. Oganov[3,1,4], Alexey V. Yanilkin[1,2] （1.Dukhov Research Institute of Automatics (VNIIA), Moscow, Russian Federation, Russia, 2.Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation, Russia, 3.Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russian Federation, Russia, 4.International Center for Materials Discovery, Northwestern Polytechnical University, Xi'an, China）

[SY-G6] MD simulation study of displacement damage in bulk wurtzite GaN by proton irradiation

○SangHyuk Yoo, Yongwoo Kim, Keonwook Kang （Dept. of Mechanical Engineering, Yonsei Univ., Korea）

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room4)

[SY-G6] Repulsive Correction in Tersoff Potential for Irradiated Si

○Youhwan Jo, Taeyeon Kim, Byeongchan Lee （Kyung Hee University, Korea）

Engineering applications for nuclear fussion/fission facilities usually require a material with exceptional properties. Silicon carbide (SiC) and its composites are prospective materials for such usage due to low degradation of mechanical properties at high temperature as well as high resistance to irradiation. There are ongoing attempts to employ SiC/SiC composites like flow channel inserts (FCI) in dual coolant lead lithium (DCLL) blankets and fuel claddings for the Generation IV nuclear reactors. SiC/SiC composites are yet to be examined further before confirmed to be the best option. As an example, irradiation damages in SiC/SiC composites may cause a serious problem by interacting with various elements in nuclear operations.

Understanding the microstructural evolution under irradiation is critical to validate SiC/SiC composites and the resulting safety under irradiation, and Molecular dynamics (MD) is a viable option for that purpose. Nevertheless the reliability of MD simulations heavily depends on the accuracy of an interatomic potential. The Tersoff potential is a good candidate, but not particularly optimized for high-energy environment, resulting in a few pathological behaviors.

In this talk we propose a correction function that minimizes the problems of the Tersoff potential developed for bulk equilibrium. In particular, the correction function replaces the repulsive part of Tersoff within a threshold interatomic spacing. The function behaves monotonically and is continuous with the original repulsive part up to the third derivative at the threshold, and moreover, complexity does not increase significantly because the correction function introduces only two additional free parameters. By primary knock-on atom (PKA) simulations, the effect of the correction is examined. We evaluate a maximum penetration length and the number of Frenkel pairs and discuss a benefit from the correction.

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room4)

[SY-G6] Phase-field modeling of microstructural evolution of Fe-Cr-Al system

○Kunok Chang （Kyung Hee Univ., Korea）

After Fukushima nuclear power plant accident, the Accident Tolerant Fuel Cladding (ATFC) has attracted a great deal of attention. The Fe-Cr-Al system has been studied for a long time as a potential candidate for ATFC due to its excellent high-temperature oxidation resistance. To optimize the microstructure has been performed for a long period of time in order to enhance the mechanical stability of the Fe-Cr-Al alloy in the neutron irradiation environment. The spinodal decomposition generally takes place at nuclear power plants operation temperature, 290 Celsius degree and it is generally have negative effect on their performace. Therefore, we performed the phase-field modeling to predict the phase separation behavior in Fe-Cr-Al system to investigate a role of Cr and Al compositions on decomposition behavior. To obtain large-scale 3D microstructure, we applied CUDA parallelizing computing technique. I will also present comparative analysis

results with the microstructure obtained experimentally.

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room4)

[SY-G6] Dissolution kinetics of ejecta in hydrogen at megabar pressure

○Arslan B. Mazitov[1,2], Artem R. Oganov[3,1,4], Alexey V. Yanilkin[1,2] （1.Dukhov Research Institute of Automatics (VNIIA), Moscow, Russian Federation, Russia, 2.Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation, Russia, 3.Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russian Federation, Russia, 4.International Center for Materials Discovery, Northwestern Polytechnical University, Xi'an, China）

A process of metal particles, *ejecta*, transport in gases is the subject of recent researches in the field of nuclear energetics. Practical necessity of the study arises from the processes of inertial thermonuclear fusion, which are often accompanied by separation of ejecta particles from the interior surface of the fuel container. At the pressure of approximately 1 megabar, saturation of the ejecta with hydrogen adversely affect a fraction of pure fuel in the system. In this work, we studied a solution process of titanium ejecta in warm dense hydrogen at megabar pressure. Thermodynamic and kinetic properties of the process were investigated using classical and quantum molecular dynamics. We estimated such features as a solution time of ejecta, a degree of saturation of titanium atoms with hydrogen as well as a heat effect of the solution. It was found that particles with a radius of 1-10 mkm dissolve in hydrogen within a time of 10^{-1}-10^{-2} mks, while a mixing process can be described by diffusion law at discussed the conditions. Presented approach demonstrates the final state of the titanium-hydrogen system as a homogenized fluid with completely dissolved titanium particles. This result can be generalized to all external conditions under which titanium and hydrogen are an atomic fluids.

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room4)

[SY-G6] MD simulation study of displacement damage in bulk wurtzite GaN by proton irradiation

○SangHyuk Yoo, Yongwoo Kim, Keonwook Kang （Dept. of Mechanical Engineering, Yonsei Univ., Korea）

Gallium nitride (GaN) based optoelectronic devices including LED and HEMT (High Electron Mobility Transistor) are widely used in aerospace industry because of large, direct band gap, high breakdown voltage and high electron mobility. Those applications loaded in satellites will be damaged during operating on the low earth orbit by radiation, which is mostly consisted of protons. Previous experimental research showed the decrements of the electron mobility and LED light intensity according to the proton fluence [1, 2]. However, it is difficult to show which kind of point defects are created and affected to the device. In this study, authors conduct Primary Knock-on Atom simulations in order to predict displacement damage on bulk wurtzite GaN by proton irradiation. PKA energy used in the MD simulation are obtained from GEANT4 simulation and experimental results. And author will show favorable type of point defects induced by displacement damage.

Reference
1. Xinwen, H., et al., *Proton-irradiation effects on AlGaN/AlN/GaN high electron mobility transistors.* IEEE Transactions on Nuclear Science, 2003. **50**(6): p. 1791-1796.

2. Khanna, S.M., et al., *Proton energy dependence of the light output in gallium nitride light-emitting diodes.* IEEE Transactions on Nuclear Science, 2004. **51**(5): p. 2729-2735.

[SY-N5] Symposium N-5

Chair: Jutta Rogal(ICAMS Ruhr University Bochum, Germany)
Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room4

[SY-N5] Understanding the impact of extended defects on the behaviour of C atoms: a multi technique approach
○Christophe Domain[1], charlotte S becquart[2] （1.EDF, France, 2. Univ.Lille, CNRS, INRA, ENSCL, UMR 8207, UMET, Unité Matériaux et Transformations, France）

[SY-N5] Localised on-the-fly Kinetic Monte Carlo
○Johannes Bulin （Fraunhofer-Institut SCAI, Germany）

[SY-N5] A Preconditioning scheme for Minimum Energy Path finding methods
○Stela Makri, James Kermode, Christoph Ortner （University of Warwick, UK）

[SY-N5] Temperature Programmed Molecular Dynamics - Accessing rare events using a combination of finite time sampling and bias potentials
○Abhijit Chatterjee （Dept. of Chemical Engineering, Indian Institute of Technology Bombay, India）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room4)

[SY-N5] Understanding the impact of extended defects on the behaviour of C atoms: a multi technique approach

Invited

○Christophe Domain[1], charlotte S becquart[2] （1.EDF, France, 2. Univ.Lille, CNRS, INRA, ENSCL, UMR 8207, UMET, Unité Matériaux et Transformations, France）

The interaction at the atomistic scale of interstitial solutes such as carbon or nitrogen with extended point defects has consequences at the macroscopic level. Typical examples are the yield peak and Lü ders plateau, related to static strain aging or the Portevin-Le Chatelier effect (the presence of serrations on the plastic part of the stress-strain curve during tensile test) due to dynamic strain aging. In ferritic steels, these atypical behaviors are due to the interaction between dislocations and solute atoms (mainly C). Depending on aging time and temperature, solute atoms diffuse towards dislocations, forming Cottrell atmospheres, and reduce their mobility. Because of the time scale of C diffusion and the stresses created near the extended defects, typical atomistic approaches such as molecular dynamics (MD) or on-lattice atomistic kinetic Monte Carlo (on-lattice AKMC) approaches are not appropriate to investigate, at the atomistic level, these phenomena. In this talk, we will thus present the approach we have pursued to investigate the behavior of C atoms in the vicinity of extended defects (dislocations, dislocation loops ⋯) in Fe. We have applied different complementary techniques. Calculations based on the density functional theory (DFT) as well as with an empirical FeC atomistic potential have been used extensively to determine the strength of the interaction between carbon atoms and the various defects in stable or metastable configurations. On-lattice static Monte Carlo as well as off-lattice kinetic Monte Carlo approaches have been applied to build Cottrell atmospheres and study dynamically the behavior of C atoms in the vicinity of extended defects (dislocations, ⋯). Finally molecular dynamics (MD) simulations have been deployed to estimate the stress necessary to release the dislocations from the C atmospheres.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room4)

[SY-N5] Localised on-the-fly Kinetic Monte Carlo

○Johannes Bulin （Fraunhofer-Institut SCAI, Germany）

Various on-the-fly Kinetic Monte Carlo algorithms have been used to simulate the long-term evolution of atomistic systems. Unlike classical Kinetic Monte Carlo methods, these algorithms search for possible transitions/reactions only when necessary (hence on-the-fly), rather than relying on a previously-known set of transitions. Unfortunately, their performance deteriorates when large systems or systems with many similar transition mechanisms are investigated.

We will present a localised on-the-fly Kinetic Monte Carlo variant that is based on the k-ART algorithm by El-Mellouhi, Lewis, and Mousseau. This algorithm is capable of localising transition searches, enabling the simulation of significantly larger systems, and can also recycle known transition mechanisms. Unlike k-ART, which uses a graph-based technique to identify similar local environments, we use an RMSD (root mean square deviation) measure that is invariant under index permutations and rotations of local environments. This allows our algorithm to deal not only with highly-structured materials like crystals, but also with amorphous materials, which are difficult to classify with graphs.

We will conclude by demonstrating computational results of our algorithm, and discuss potential areas of application.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room4)

[SY-N5] A Preconditioning scheme for Minimum Energy Path finding methods

○Stela Makri, James Kermode, Christoph Ortner （University of Warwick, UK）

In transition state theory, the study of thermally activated transitions between energy minima is achieved by finding transition paths connecting the minima. These paths provide information on the energy barrier and reaction rates of the system without going through long and expensive simulations. To find them, current techniques use steepest descent-like minimisation to relax a discretised initial guess. However, steepest descent typically gives slow convergence rates in the presence of ill-conditioned potentials. In this talk I will be discussing how to reduce the condition number of the potential of an arbitrary system and improve the convergence speed and robustness of transition path finding methods, using a preconditioning scheme. Our key assumption is that the cost of constructing a preconditioner is much smaller than the cost of computing the potential; for density functional theory the cost of single point evaluations is much more expensive than the computation of a preconditioner and thus the proposed approach improves computing times significantly. We have developed a preconditioning scheme, where the preconditioner acts as a coordinate transformation of the discrete images along the path to aid the ill-conditioning in the transverse direction and a preconditioning scheme that considers the interactions between the images is currently in development. Finally, we are working towards a preconditioning scheme for finding energy barriers in hybrid quantum mechanical - molecular mechanical models.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room4)

[SY-N5] Temperature Programmed Molecular Dynamics - Accessing rare events using a combination of finite time sampling and bias potentials

Invited

○Abhijit Chatterjee （Dept. of Chemical Engineering, Indian Institute of Technology Bombay, India）

Rates of physical and chemical processes often obey Arrhenius law. Recently, we developed the temperature-programmed molecular dynamics (TPMD) method[1,2,3] that provides a convenient way of estimating the Arrhenius parameters of kinetic pathways even in situations where the underlying landscape is rugged. The TPMD method employs a temperature program with finite temperature MD in order to accelerate thermally activated events from a particular state of the system. Kinetic pathways are sought from a collection of states without any prior knowledge of these pathways. Since kinetic pathways are selected with a probability that is proportional to their rate constants, we find that slow pathways with small pre-exponential factors and large activation barriers are rarely sampled with TPMD. We introduce a procedure to overcome this limitation by bias potentials. This additional feature in the TPMD method dramatically improves its ability to estimate Arrhenius parameters. Examples of the variation of the TPMD method are provided for metal surface diffusion

in presence of solvent.

1. V Imandi, A Chatterjee, Estimating Arrhenius parameters using temperature programmed molecular dynamics, The Journal of Chemical Physics 145, 034104, 2016.

2. S Divi, A Chatterjee, Accelerating rare events while overcoming the low-barrier problem using a temperature program, The Journal of Chemical Physics 140 (18), 184116, 2014

3. A Chatterjee, Accelerating Rare Events and Building Kinetic Monte Carlo Models Using Temperature Programmed Molecular Dynamics, Journal of Materials Research, http://dx.doi.org/10.1557/jmr.2017.460

Symposium | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[SY-N6] Symposium N-6

Chair: Chad W Sinclair(Dept. of Materials Engineering, University of British Columbia, Canada)
Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room4

[SY-N6] **Modelling metals, alloys and cement paste across length and time scales**
○Laurent Karim Beland[1], Roger E Stoller[3], Yuri N Osetsky[3], Tingtao Zhou[2], Katerina Katerina Ioannidou[2], Franz-Josef Ulm[2], Roland Pellenq[2] (1.Queen's University, Canada, 2.Massachusetts Institute of Technology, United States of America, 3.Oak Ridge National Laboratory, United States of America)

[SY-N6] BCA-MD-KMC hybrid simulation for long time helium plasma irradiation inducing fuzzy nanostructure on tungsten
○Atsushi M Ito[1,2], Arimichi Takayama[1], Hiroaki Nakamura[1,3] (1.National Institute for Fusion Science, National Institutes of Natural Sciences, Japan, 2.The Graduate University for Advanced Studies, Japan, 3.Department of Electrical Engineering, Graduate School of Engineering, Nagoya University, Japan)

[SY-N6] Atomistic Modelling of Pipe Diffusion: a Direct Comparison of MD, KMC, aKMC and DMD
Frederic Houlle[1], Jutta Rogal[2], ○Erik Bitzek[1] (1.FAU Erlangen-Nuernberg, Germany, 2.ICAMS Ruhr University Bochum, Germany)

[SY-N6] Strategies for optimal construction of Markov chain representations of atomistic dynamics
○Danny Perez, Thomas Swinburne (Los Alamos National Laboratory, United States of America)

[SY-N6] Simulating the collective diffusion mechanism of amorphous solids at experimentally relevant time scales
○Yunjiang Wang[1,2], Shigenobu Ogata[3] (1.Institute of Mechanics, Chinese Academy of Sciences, China, 2.School of Engineering Science, University of Chinese Academy of Sciences, China, 3.Graduate School of Engineering Science, Osaka University, Japan)

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room4)

[SY-N6] Modelling metals, alloys and cement paste across length and time scales

Invited
○Laurent Karim Beland[1], Roger E Stoller[3], Yuri N Osetsky[3], Tingtao Zhou[2], Katerina Katerina Ioannidou[2], Franz-Josef Ulm[2], Roland Pellenq[2] (1.Queen's University, Canada, 2.Massachusetts Institute of Technology, United States of America, 3.Oak Ridge National Laboratory, United States of America）

Fundamentally, structural materials are bound by atomistic cohesive interactions, while our societies use these to design systems at scales of meters—or more. Likewise, the material's microstructural evolution takes place on scales as short as nanoseconds—e.g. diffusion of radiation-induced defects clusters in metallic alloys—all the way up to decades—e.g. creep of concrete under load.

This presentation will focus on applying multi-scale methods to address these challenges for two classes of systems: (1) metals and alloys under irradiation, and (2) calcium silicate hydrates (C-S-H), the main binding phase of cement paste.

In metals and alloys, the kinetics of collision cascade induced defects was modelled using adaptive kinetic Monte Carlo. Namely, the kinetic Activation Relaxation Technique —a self-learning, fully atomistic algorithm able to handle off-lattice defects and handle long-range elastic interactions—was used to capture the time-evolution of cascade debris after neutron or ion irradiation. Furthermore, a detailed investigation of point-defect diffusion in $Ni_xFe_{(1-x)}$ concentrated alloys revealed a non-monotonic dependence of diffusion coefficients as a function of Fe concentration. This was explained by coupling percolation effects with the composition dependence of point-defect vacancy migration energies.

In C-S-H, the adsorption of alkali ions—Na, K, and Cs—was studied, in the context of the alkali-silica reaction and spent fuel storage. By applying molecular dynamics, semi-grand canonical Monte Carlo, and the Activation Relaxation Technique *nouveau*, adsorption of alkali ions in the hydrated layer of C-S-H was characterized. The effect of alkali uptake on mesoscale mechanical properties was calculated using a coarse-grained model of C-S-H. While alkali uptake leads to significant expansion of individual C-S-H grains, it leads to modest—less than 5 MPa—mesoscopic expansive pressure, well within the elastic regime of concrete.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room4)

[SY-N6] BCA-MD-KMC hybrid simulation for long time helium plasma irradiation inducing fuzzy nanostructure on tungsten

○Atsushi M Ito[1,2], Arimichi Takayama[1], Hiroaki Nakamura[1,3] (1.National Institute for Fusion Science, National Institutes of Natural Sciences, Japan, 2.The Graduate University for Advanced Studies, Japan, 3.Department of Electrical Engineering, Graduate School of Engineering, Nagoya University, Japan）

In this paper, we developed the triple hybrid simulation method for plasma-material interaction (PMI). Although the present method is composed only of atomistic simulations, an elapse time achieved experimentally relevant time scale.

PMI occurs in the processing of semiconductors, thin film depositions, applications into nanomaterial formations, and the inside wall of magnetic confinement nuclear fusion reactors. In atomistic viewpoint, PMI is the surface reaction of a target material due to ion particles continuously injected from plasma. The PMI, which is not an exception, follows the multi-scale multi-physics mechanisms.

Moreover, an important factor in PMI is competition between an irradiation flux and the diffusion speed of the injected particles in the target material. The irradiation flux in laboratory experiments is 10^{20} to 10^{24} m^{-2}s^{-1}, and irradiation time is 10^2 s to 10^4 s. Although molecular dynamics (MD) is often used for PMI, the experimental irradiation time is too long for MD. Therefore, the irradiation flux was generally set 10^4 to 10^8 times of the experimental flux. However, since the diffusion speed in MD becomes realistic, the competition between the irradiation flux and the diffusion speed becomes unrealistic. Thus, the expansion of time scale is necessary for PMI simulation.

Here, the present target phenomenon is fuzzy nanostructure formation on the tungsten surface by exposure to helium plasma. Injected helium atoms agglomerated in the tungsten material, and the nanoscale helium bubbles are formed. After that, the fuzzy nanostructure of tungsten measuring several ten nanometers in width is grown on a surface. To represent the fuzzy nanostructure, we developed the BCA-MD-KMC hybrid simulation method. In this method, the injection process of helium ions is solved by binary collision approximation (BCA), the deformation process of a target material due to the pressure from the helium bubbles is solved by MD, and the diffusion process of the helium atoms in a tungsten material is solved by kinetic Monte-Carlo (KMC). In the hybrid simulation, the injection flux is kept at 10^{22} m^{-2}s^{-1} same as an experimental flux and then the irradiation time achieved 100 s. As a result, the fuzzy nanostructure growth was successfully represented.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room4)

[SY-N6] Atomistic Modelling of Pipe Diffusion: a Direct Comparison of MD, KMC, aKMC and DMD

Frederic Houlle[1], Jutta Rogal[2], ○Erik Bitzek[1] (1.FAU Erlangen-Nuernberg, Germany, 2.ICAMS Ruhr University Bochum, Germany)

Understanding and influencing self-diffusion in complex microstructures is of fundamental importance for improving the high-temperature mechanical properties of materials. Modelling diffusion in a quantitatively predictive way requires information about the underlying atomic-scale processes and corresponding activation energies. While various atomic-scale simulation approaches are routinely employed to study diffusion in homogeneous environments, the presence of strain gradients and defects still poses significant challenges to predictive atomic-scale models. In particular, currently only few detailed studies that compare the application of different simulation methods to diffusion at extended defects exist.

Here we present our recent atomistic simulations results of vacancy-mediated diffusion in the vicinity of an edge dislocations in aluminum modelled by an EAM potential. The direct high-temperature molecular dynamics (MD), adaptive kinetic Monte Carlo (aKMC) and diffusive molecular dynamics (DMD) simulations all use the identical atomistic starting configuration. The activation energies of all nearest-neighbor vacancy jumps in this configuration were determined by the nudged elastic band (NEB) method and used to build the

event catalogue for the kinetic Monte Carlo (KMC) simulations and to parametrize the DMD model. Significant differences between the direct MD simulations and the (a)KMC simulations are observed, which could be attributed to the coupling of the diffusive vacancy motion with the thermally-induced fluctuations of the dislocation.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room4)

[SY-N6] Strategies for optimal construction of Markov chain representations of atomistic dynamics

○Danny Perez, Thomas Swinburne （Los Alamos National Laboratory, United States of America）

A common way of representing the long-time dynamics of materials is in terms of a Markov chain that specifies the transition rates for transitions between metastable states. This chain can either be used to generate trajectories using kinetic Monte Carlo, or analyzed directly, e.g., in terms of first passage times between distant states. While a number of approaches have been proposed to infer such a representation from direct molecular dynamics (MD) simulations, challenges remain. For example, as chains inferred from a finite amount of MD will in general be incomplete, quantifying their completeness is extremely desirable. In addition, making the construction of the chain as computationally affordable as possible is paramount. In this work, we simultaneously address these two questions. We first quantify the local completeness of the chain in terms of Bayesian estimators of the yet-unobserved rate, and its global completeness in terms of the residence time of trajectories within the explored subspace. We then systematically reduce the cost of creating the chain by maximizing the increase in residence time against the distribution of states in which additional MD is carried out and the temperature at which these are respectively carried out. Using as example the behavior of vacancy and interstitial clusters in materials, we demonstrate that this is an efficient, fully automated, and massively-parallel scheme to efficiently explore the long-time behavior of materials.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room4)

[SY-N6] Simulating the collective diffusion mechanism of amorphous solids at experimentally relevant time scales

○Yunjiang Wang[1,2], Shigenobu Ogata[3] （1.Institute of Mechanics, Chinese Academy of Sciences, China, 2.School of Engineering Science, University of Chinese Academy of Sciences, China, 3.Graduate School of Engineering Science, Osaka University, Japan）

The nature of collective diffusion in amorphous solids is in strong contrast with diffusion in crystals. However, the atomic-scale mechanism and physics of collective motion remains elusive in disorder materials. Here the free energy landscape of collective diffusion triggered by single atom jump in a prototypical CuZr model metallic glass is explored with the recently advanced well-tempered metadynamics which significantly expands the observation time-scale of diffusion process at atomic-scale. Metadynamics samplings clarify a long-standing experimentally suggested collective diffusion mechanism in the deep glassy state. The collective nature is strongly temperature-dependent. It evolves from string-like motion with participation of only several atoms to be large size collective diffusion at high temperature, which would remarkably promote the atomic transport upon glass transition. The temperature and pressure dependence of collective diffusion are further quantified with big activation entropy and small activation volume of half atom volume, which

both agree quantitatively with experiments. Direct atomic-scale simulations of diffusion at laboratory time-scale brings several physical insights into the nature of collective diffusion in amorphous solids which is beyond the knowledge established in diffusion of crystals.

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K1] Symposium K-1

Chairs: Momoji Kubo(Institute for Materials Research, Tohoku University, Japan), Tomoaki Niiyama(Kanazawa Univ., Japan)

Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room5

[SY-K1] Supercomputer Post-K Project "Challenge of Basic Science - Exploring Extremes through Multi-Physics and Multi-Scale Simulations"

○Momoji Kubo （Tohoku Univ., Japan）

[SY-K1] Universal avalanche statistics across 16 decades in length: From nanocrystals (and neurons) to earthquakes and stars?

○Karin Dahmen （University of Illinois at Urbana Champaign, United States of America）

[SY-K1] Predicting avalanches and failure: wood and paper

○Mikko Alava, Juha Koivisto, Tero Mäkinen, Leevi Viitanen （Aalto University, Finland）

[SY-K1] System-spanning shear avalanches induced by thermal structural relaxation in metallic glasses

○Tomoaki Niiyama[1], Masato Wakeda[2], Tomotsugu Shimokawa[4], Shigenobu Ogata[3] （1.College of Science and Engineering, Kanazawa Univ., Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan, 3.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 4.Faculty of Mechanical Engineering, Kanazawa University, Japan）

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room5)

[SY-K1] Supercomputer Post-K Project "Challenge of Basic Science - Exploring Extremes through Multi-Physics and Multi-Scale Simulations"

○Momoji Kubo （Tohoku Univ., Japan）

Japanese government plans to construct a supercomputer Post-K at 2021, which is expected to have over 10^{18} flops. This calculation speed is 100 times faster than the present supercomputer K in Kobe, Japan. Japanese government started 13 projects (9 priority issues and 4 exploratory challenges) to develop original simulators for the supercomputer Post-K. Our Post-K project "Challenge of Basic Science - Exploring Extremes through Multi-Physics and Multi-Scale Simulations" (Leader: Prof. Momoji Kubo, Institute for Materials Research, Tohoku University) was selected as one of four exploratory challenges at June, 2016 and started at August, 2016. The summary of our Post-K project is as follows.

Supercomputer K significantly advanced individual sciences on exploring extremes such as fracture of materials, earthquake, atmospheric flow, ocean flow, volcanic eruption, magma, and extreme properties. On the basis of the above individual understanding obtained by supercomputer K, our Post-K project aims to solve multi-physics and multi-scale problems for exploring extremes by developing new calculation methods beyond the limits of calculation accuracy and possibility and by bridging the different physics and scales. Our Post-K project consists of four sub-challenges.

Sub-Challenge A: Fracture and Catastrophe

(Sub-Leader: Prof. Momoji Kubo, Tohoku University)

Sub-Challenge B: Phase Transitions and Flows

(Sub-Leader: Prof. Toshihiro Kawakatsu, Tohoku University)

Sub-Challenge C: Structures and Properties of Materials in Deep Earth and Planets

(Sub-Leader: Dr. Toshiaki Iitaka, RIKEN)

Sub-Challenge D: Fundamental Quantum Mechanics and Informatics

(Sub-Leader: Prof. Naoki Kawashima, The University of Tokyo)

In the supercomputer Post-K project, our group is focusing on the fracture and catastrophe of materials. Our recent outcomes on the following three topics will be presented in the conference.
Friction and wear processes of diamond-like carbon thin films.Stacking fault generation processes of polycrystalline ceramics.Sintering processes of Ni/YSZ electrode in solid oxide fuel cell.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room5)

[SY-K1] Universal avalanche statistics across 16 decades in length: From nanocrystals (and neurons) to earthquakes and stars?

Invited
○Karin Dahmen （University of Illinois at Urbana Champaign, United States of America）

Slowly-compressed nano-crystals, bulk metallic glasses, rocks, granular materials, and the earth all deform via intermittent slips or "quakes". We find that although these systems span 12 decades in length scale, they all show the same scaling behavior for their slip size distributions and other statistical properties. Remarkably, the size distributions follow the same power law multiplied with the same exponential cutoff. The cutoff grows with applied force for materials spanning length scales from nanometers to kilometers, indicating an underlying nonequilibrium phase transition. A simple mean field model for avalanches of slipping weak spots explains the agreement across scales. It predicts the observed slip-size distributions and the observed stress-dependent cutoff function. The analysis draws on tools from statistical physics and the renormalization group. The results enable extrapolations from one scale to another, and from one force to another, across different materials and structures, from nanocrystals to earthquakes. Connections to neuron avalanches in the brain and recent observations on stars will also be discussed, extending the range of scales to 16 decades in length.

References:

[1] J.T. Uhl, S. Pathak, D. Schorlemmer, X. Liu, R. Swindeman, B.A.W. Brinkman, M. LeBlanc, G. Tsekenis, N. Friedman, R. Behringer, D. Denisov, P. Schall, X. Gu, W.J. Wright, T. Hufnagel, A. Jennings, J.R. Greer, P.K. Liaw, T. Becker, G. Dresen, and K.A. Dahmen, Scientific Reports 5, 16493 (2015).
[2] N. Friedman, A. T. Jennings, G. Tsekenis, J.-Y. Kim, J. T. Uhl, J. R. Greer, and K. A. Dahmen, Phys. Rev. Lett. 109, 095507 (2012).
[3] J. Antonaglia, W.J. Wright, X. Gu, R.R. Byer, T.C. Hufnagel, M. LeBlanc, J.T. Uhl, and K.A. Dahmen, Physical Review Letters 112, 155501 (2014).
[4] J. Antonaglia, X.Xie, M. Wraith, J.Qiao, Y. Zhang, P.K. Liaw, J.T. Uhl, and K.A. Dahmen, Nature Scientific Reports 4, 4382 (2014).
[5] N. Friedman, S. Ito, B.A.W. Brinkman, L. DeVille, K. Dahmen, J. Beggs, and T. Butler, Phys. Rev. Lett. 108, 208102 (2012).
[6] M.A. Sheikh, R.L. Weaver, and K. A. Dahmen, Phys. Rev. Lett. 117, 261101 (2016).

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room5)

[SY-K1] Predicting avalanches and failure: wood and paper

○Mikko Alava, Juha Koivisto, Tero Mäkinen, Leevi Viitanen （Aalto University, Finland）

Natural and man-made structured materials like wood and paper exhibit complex response to external loading. We have demonstrated the presence of deformation avalanches in wood compression in analogy to other laboratory-scale experiments mimicking earthquakes. I will review this and the subsequent predictability of large events and discuss the relation of this to the wood microstructure, based on deformation analyses and tomographic studies [1-3]. Fiber networks - paper - exhibit a very complex creep response in, again, analogy to most other materials. The predictability of sample failure with or without an initial defect/notch depends on the presence of regularities in the rheological response, such as the localization of creep strain or the formation of a large Fracture Process Zone [4-6]. I will discuss the

experimental signatures that are of relevance for predictability, and what coarse-grained models teach us.

[1] T. Mäkinen et al., Phys. Rev. Lett. 115 (055501).
[2] L. Viitanen et al., J. Stat. Mech. 053401 (2017).
[3] T. Mäkinen et al., unpublished.
[4] J. Rosti et al., Phys. Rev. Lett. 105, 100601 (2010).
[5] J. Koivisto et al. Phys. Rev. E 94, 023002 (2016).
[6] L. Viitanen et al., submitted, Physical Review Applied.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room5)

[SY-K1] System-spanning shear avalanches induced by thermal structural relaxation in metallic glasses

○Tomoaki Niiyama[1], Masato Wakeda[2], Tomotsugu Shimokawa[4], Shigenobu Ogata[3]　(1.College of Science and Engineering, Kanazawa Univ., Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan, 3.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 4.Faculty of Mechanical Engineering, Kanazawa University, Japan)

Metallic glasses (MGs) are one of the most attractive materials because of their excellent properties [1]. However, brittle fractures are an obstacle for MGs to be applied as structural materials. This brittleness originating from shear band nucleation is determined by structural relaxation using thermal annealing [2]. Thus, the influence of structural relaxation upon the nucleation of shear banding that can induce catastrophic failure in MGs is a significant challenge in material science.
For this challenge, we focus on the avalanche behavior that provides sudden massive deformations and spatiotemporal correlation in solid plasticity [3]. Thus, this avalanche behavior is deeply connected to the localization of plastic deformation and catastrophic failure in MGs.
In this study [4], we investigate the geometry of the shear transformation avalanches that exhibit the power-law statistics using molecular dynamics simulations of shear deformation in two thermally processed MG models that are based on a less-relaxed glass and a well-relaxed glass. The simulation showed a shear-band like heterogeneous pattern in the well-relaxed glass model, whereas the less-relaxed model exhibits homogeneous deformation patterns. Considering the spatial correlation functions of the non-affine least square displacements of atoms during each each avalanche event, we reveal that the regions an avalanche developed in well-relaxed glasses tend to be anisotropic whereas those in less-relaxed glasses are isotropic. Moreover, a temporal clustering feature of the direction of avalanche propagations and a considerable correlation between the anisotropy and size of an avalanche in the well-relaxed glass model are demonstrated.

[1] A. L. Greer, Science 267, 1947 (1995).
[2] G. Kumar, et al., Acta Mater. 57, 3572 (2009).
[3] M. C. Miguel, et al., Nature 410, 667 (2001).
[4] T. Niiyama, et al., arXiv:1804.00852 (2108).

[SY-K2] Symposium K-2

Chairs: Ferenc Kun(University of Debrecen, Hungary), Ian Main(University of Edinburgh, UK)
Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room5

[SY-K2] Predictability of catastrophic failure in porous media

○Ian Main[1], Ferenc Kun[2], Jeremie Vasseur[3], Andrew Bell[1] （1.University of Edinburgh, UK, 2.University of Debrecen, Hungary, 3.Ludwig Maximilian University, Munich, Germany）

[SY-K2] Deciphering the dynamics of precursors to failure in quasi-brittle solids: an inspiration for understanding the statistics of earthquakes ?

○Laurent Ponson[1], Estelle Berthier[1], Vincent Démery[2] （1.Institut Jean le Rond d'Alembert, CNRS - Sorbonne University, Paris, France, 2.Gulliver, CNRS - ESPCI, Paris, France）

[SY-K2] Avalanche precursors and fracture strength in the limit of high disorder

○Ferenc Kun[1,2], Viktória Kádár[1] （1.Department of Theoretical Physics, University of Debrecen, Hungary, 2.Institute for Nuclear Research (Atomki), Debrecen, Hungary）

[SY-K2] Jump statistics of epicenters in thermally induced cracking of fiber bundles

○Naoki Yoshioka[1], Ferenc Kun[2], Nobuyasu Ito[1,3] （1.RIKEN Center for Computational Science, Japan, 2.Department of Theoretical Physics, University of Debrecen, Hungary, 3.Department of Applied Physics, Graduate Schoold of Engineering, The University of Tokyo, Japan）

[SY-K2] Time dependent fracture under unloading in a fiber bundle model

○Reka Korei, Ferenc Kun （Department of Theoretical Physics, University of Debrecen, Hungary）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room5)

[SY-K2] Predictability of catastrophic failure in porous media
Invited

○Ian Main[1], Ferenc Kun[2], Jeremie Vasseur[3], Andrew Bell[1] (1.University of Edinburgh, UK, 2.University of Debrecen, Hungary, 3.Ludwig Maximilian University, Munich, Germany)

Recent discrete element models for the processes leading up to material failure provide a very close match to experiment in the case of high porosity, highly disordered materials. On approach to catastrophic, system-sized failure the number of micro-cracks and their associated acoustic emissions (AE) increase at a rate marked by a smooth inverse power law, defining a failure time at the singularity in AE rate. This behaviour is reminiscent of a second-order phase transition. At the same time the deformation becomes progressively more localised on an incipient optimally oriented fault plane, and the scaling exponent b for the frequency-magnitude distribution of the acoustic emissions decreases to a minimum near the failure time. On the other hand, a simple elastic fracture mechanics for an ideal ordered, uniform solid with a single pre-existing crack provides no warning of incipient failure. In between these limits there are clear precursors, but failure occurs suddenly, and earlier than predicted by the inverse power-law model, more reminiscent of a first-order phase transition. We develop a mean field model for a population of cracks emanating from pores in an otherwise uniform medium to explain this systematic error in the predicted failure time. The correction depends non-linearly on the porosity, specifically the distance between pores in the starting model, and tends to zero in the limiting case of high-porosity materials. It provides a good match to aggregate data obtained from experiments on a range of materials, both natural and synthetic. We show the behaviour scales very well to a range of data from earthquakes prior to volcanic eruptions, including quasi-periodic 'drumbeat' long-period earthquake signals preceding a recent large vulcanian explosion at Tungurahua volcano, Ecuador. Unfortunately, such signals are not yet detectable prior to large earthquakes above a null hypothesis of conventional epidemic-type earthquake triggering models.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room5)

[SY-K2] Deciphering the dynamics of precursors to failure in quasi-brittle solids: an inspiration for understanding the statistics of earthquakes ?

○Laurent Ponson[1], Estelle Berthier[1], Vincent Démery[2] (1.Institut Jean le Rond d'Alembert, CNRS - Sorbonne University, Paris, France, 2.Gulliver, CNRS - ESPCI, Paris, France)

Quasi-brittle failure results from the evolution of a large number of interacting microcracks growing through the material microstructural disorder. Despite this complexity, quasi-brittle materials under slowly increasing compressive load exhibit a remarkably robust failure behavior: During a first stage, damage grows and accumulates through bursts of failure events that are localized both in space and time. This earthquake-like dynamic is characterized by scale free statistics with exponents that vary weakly with the type of materials and the loading conditions. Ultimately, the damage localizes into a macroscopic band that leads to the catastrophic failure of the specimen.
In this study, we investigate theoretically the physical mechanisms underlying intermittency and localization during quasi-brittle failure. Elasticity is shown to promote long-range interactions between the damaging elements constituting the specimen and to drive the collective response of the array of microcracks. To capture this cooperative dynamic, we encapsulate the interactions in an elastic kernel that derives from the

continuum mechanics of elasto-damageable solids. We then show how it can be used to (i) disentangle the statistical properties of precursors to failure and explain their scale-free statistics and (ii) predict the onset of localization and the emerging fracture pattern. Our theoretical predictions are critically compared to experimental and numerical observations made during the compressive failure of disordered quasi-brittle solids.

The relevance of this theoretical framework for unravelling the statistics of earthquakes is finally discussed.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room5)

[SY-K2] Avalanche precursors and fracture strength in the limit of high disorder

○Ferenc Kun[1,2], Viktória Kádár[1]　（1.Department of Theoretical Physics, University of Debrecen, Hungary, 2.Institute for Nuclear Research (Atomki), Debrecen, Hungary）

Most of the materials have an inherent disorder which appears at different length scales in the form of dislocations, flaws, microcracks, grain boundaries, or internal frictional interfaces. Under mechanical load, this quenched disorder plays a decisive role in the emerging fracture process: Increasing the extension of samples a size effect emerges, i.e. the ultimate strength of disordered materials is a decreasing function of their size. On the microscale the fracture process is composed of a large number of crack nucleation - propagation - arrest steps which generate a sequence of precursory cracking avalanches. This crackling noise is of ultimate importance to forecast natural catastrophes such as landslides and earthquakes, and the catastrophic failure of engineering constructions.

We investigate how the amount of microscale disorder affects the emerging fracture process focusing on the size scaling of the ultimate fracture strength and on the time series of avalanche precursors. We consider a fiber bundle model where the strength of fibers is described by a power law distribution. Tuning the amount of disorder by varying the power law exponent and the upper cutoff of fibers' strength, in the mean field limit an astonishing size effect is revealed: For small system sizes the bundle strength increases with the number of fibers and the usual decreasing size effect is only restored beyond a characteristic size. We show that the extreme order statistics of the micro-scale disorder is responsible for this peculiar behavior, which can be exploited for materials' design.

In the limit of very high disorder the avalanche activity does not show any acceleration so that no signatures of the imminent catastrophic failure can be identified. Limiting the disorder to a finite range an acceleration period emerges with precursors, however, the predictability of the catastrophic event depends on the details of the tail of the disorder distribution.

[1] V. Kádár, Zs. Danku, and F. Kun, Physical Review E **96**, 033001 (2017).
[2] Zs. Danku and F. Kun, J. Stat. Mech.: Theor. Exp. **2016**, 073211 (2016).

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room5)

[SY-K2] Jump statistics of epicenters in thermally induced cracking of fiber bundles

○Naoki Yoshioka[1], Ferenc Kun[2], Nobuyasu Ito[1,3]　（1.RIKEN Center for Computational Science, Japan, 2.Department of Theoretical Physics, University of Debrecen, Hungary, 3.Department of Applied Physics, Graduate Schoold of Engineering, The University of Tokyo, Japan）

Based on a fiber-bundle model we investigate epicenters of breaking events in thermally activated creep rupture. Breaking events are initiated by thermal fluctuation of load followed by load redistribution which leads to an avalanche of breakings. Using recently introduced kinetic Monte Carlo algorithm for a thermally activated fiber-bundle model, it is shown that jump distance between epicenters of consecutive breaking events has a power-law distribution with a non-trivial exponent. We also discuss relations between burst size and other quantities such as jump distance of epicenters and waiting time of breaking events.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room5)

[SY-K2] Time dependent fracture under unloading in a fiber bundle model

○Reka Korei, Ferenc Kun　（Department of Theoretical Physics, University of Debrecen, Hungary）

Failure of materials can also occur due to unloading from a previously applied stress level. Excavation during underground engineering rapidly releases stress which can result in rock bursts. Similar conditions may also occur on much larger length and time scales at the emergence of earthquakes: crustal unloading due to near-surface mass redistribution (water, ice or quarried material) can affect the subsurface stress field altering seismic activity and being also responsible for rupture activation and induced earthquakes. Fracture processes under unloading present a high degree of complexity which makes it difficult to achieve a general understanding.

To consider this problem, we investigate the process of sub-critical fracture which occurs when unloading from an initial load. We use a fiber bundle model of time dependent deformation and rupture which captures the slow damaging of loaded fibers and their immediate breaking when the local load exceeds the fibers' fracture strength. We focus on the case when a constant sub-critical load gives rise to failure in a finite time so that unloading may prevent the final breakdown. We show that the system has two phases: at rapid unloading only partial failure occurs and the sample has an infinite lifetime, however, slow unloading results in global failure in a finite time. We demonstrate that the transition between the phases of finite and infinite lifetime occurs as a continuous phase transition.

The unloading process is accompanied by breaking bursts of fibers with a varying rate. We show by computer simulations that in the regime of finite lifetime the initial relaxation is followed by a short acceleration period of bursting activity towards failure which is described by the Omori law. Based on the pattern of the time varying burst rate we propose a method to forecast the impending failure under unloading.

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K3] Symposium K-3

Chairs: Takahiro Hatano(University of Tokyo, Japan), Akio Nakahara(Nihon Univ., Japan)
Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room5

[SY-K3] Creep of strongly disordered materials: Plasticity, damage and approach to failure
○Michael Zaiser, David Fernandez Castellanos （Inst,. of Materials Simulation, Dept of Materials Science, FAU University of Erlangen-Nuremberg, Germany）

[SY-K3] **Creep rupture and Omori-Utsu law: Fiber bundle model approach**
○Takahiro Hatano[1], Subhadeep Roy[2] （1.University of Tokyo, Japan, 2.Norwegian University of Science and Technology, Norway）

[SY-K3] **Temperature dependent shear friction in metallic glass**
○Akio Ishii[1], Tomoaki Niiyama[2], Takahiro Hatano[3], Tomotsugu Shimokawa[2], Shigenobu Ogata[1] （1.Osaka Univ., Japan, 2.Kanazawa Univ., Japan, 3.Tokyo Univ., Japan）

[SY-K3] Mechanism of controlled crack formation induced by memory effect of clay paste
○Akio Nakahara[1], Rokuya Hayashi[1], Tomoki Hiraoka[1], Yousuke Matsuo[1], So Kitsunezaki[2] （1.Nihon Univ., Japan, 2.Nara Women's University, Japan）

[SY-K3] Effects of Shockwave-Induced Nanobubble Collapse on Precision Polishing : Molecular Dynamics Study
○yoshimasa aoyama[1], Jingxiang Xu[2], Yuske Ootani[1], Nobuki Ozawa[1], Momoji Kubo[1] （1.Dept. of Materials Science, Tohoku Univ., Japan, 2.Dept. of Mechanical Engineering, Shanghai Ocean Univ., China）

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room5)

[SY-K3] Creep of strongly disordered materials: Plasticity, damage and approach to failure

Invited

○Michael Zaiser, David Fernandez Castellanos （Inst,. of Materials Simulation, Dept of Materials Science, FAU University of Erlangen-Nuremberg, Germany）

Stochastic plasticity models have recently become popular for modelling the deformation behavior of structually disordered materials, from amorphous solids over crystals with disordered microstructure to geomaterials. We generalize such models to account for thermally activated creep processes in conjunction with structural damage. We show that the thus modified models exhibit three-stage creep curves where failure occurs as a finite-time singularity of the creep rate in conjunction with strong localization of deformation in a catastrophic shear band. Deformation occurs as a stochastic sequence of discrete avalanches with a rate that accelerates towards failure in the form of an inverse Omori law. Immediately before failure, the system switches to a regime of mechanical activation where the avalanche statistics exhibits universal features. We compare our findings with experimental data on failure of rock samples and discuss relations with other stochastic models of plasticity and fracture.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room5)

[SY-K3] Creep rupture and Omori-Utsu law: Fiber bundle model approach

○Takahiro Hatano[1], Subhadeep Roy[2] （1.University of Tokyo, Japan, 2.Norwegian University of Science and Technology, Norway）

We study the dynamical aspects of a statistical-mechanical model for fracture of heterogeneous media: the fiber bundle model with various interaction range. Although the model does not include any nontrivial elementary processes such as nonlinear rheology or stochasticity, the system exhibits creep-like behaviors under a constant load being slightly above the critical value. These creep-like behaviors comprise three stages: in the primary and tertiary stages, the strain rate exhibits power-law behaviors with time, which are well described by the Omori-Utsu and the inverse Omori laws, respectively, although the exponents are larger than those typically observed in experiments. A characteristic time that defines the onset of power-law behavior in the Omori-Utsu law is found to decrease with the strength of disorder in the system. The analytical solution, which agrees with the above numerical results, is obtained for the mean-field limit. Beyond the mean-field limit, the exponent for the Omori-Utsu law tends to be even larger but decreases with the disorder in the system. Increasing the spatial range of interactions, this exponent is found to be independent of disorder and to converge to the mean-field value. In contrast, the inverse Omori law remains independent of the spatial range of interaction and the disorder strength.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room5)

[SY-K3] Temperature dependent shear friction in metallic glass

○Akio Ishii[1], Tomoaki Niiyama[2], Takahiro Hatano[3], Tomotsugu Shimokawa[2], Shigenobu Ogata[1] （1.Osaka Univ., Japan, 2.Kanazawa Univ., Japan, 3.Tokyo Univ., Japan）

Sharp local sliding such as shear band is frequently observed in bulk metallic glass subject to mechanical loading, and it usually leads to a global mechanical instability and then a catastrophic failure of metallic glass. Although sliding induced frictional force is a key to understand the stability of metallic glass, the details has not been fully clarified yet. Using a micromechanics-based kinetic Monte Carlo tensile test simulation of metallic glass [1], we computed a temperature and velocity dependent shear frictional force in metallic glass in experimental time scale. We found a negative velocity dependency (velocity weakening) within certain temperature range and thus a velocity dependency transition from negative to positive (velocity hardening) at a transition temperature as the temperature increases. The similar trend has been observed in rock as well [2].

[1] P. Zhao, et al., International Journal of Plasticity, 40 pp.1-22 (2013).

[2] C H. Scholz, nature, 391 pp.37-42 (1998).

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room5)

[SY-K3] Mechanism of controlled crack formation induced by memory effect of clay paste

○Akio Nakahara[1], Rokuya Hayashi[1], Tomoki Hiraoka[1], Yousuke Matsuo[1], So Kitsunezaki[2] （1.Nihon Univ., Japan, 2.Nara Women's University, Japan）

Wet clay paste remembers the direction of vibration and flow it has experienced and, when the paste is dried, the direction of desiccation cracks strongly depends on the memory of such motions. To find out the mechanism of memory effect of vibration, we perform experiments to rewite memory in paste by applying additional vibration to the paste along different direction. Experimental results are found to be consistent with theoretical models which are based on residual stress theory.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room5)

[SY-K3] Effects of Shockwave-Induced Nanobubble Collapse on Precision Polishing : Molecular Dynamics Study

○yoshimasa aoyama[1], Jingxiang Xu[2], Yuske Ootani[1], Nobuki Ozawa[1], Momoji Kubo[1] （1.Dept. of Materials Science, Tohoku Univ., Japan, 2.Dept. of Mechanical Engineering, Shanghai Ocean Univ., China）

Chemical mechanical polishing (CMP) is used for the planarization of semiconductor materials. However, some of them are much hard. Therefore, the designing of efficient CMP process of hard materials is required. In order to achieve an efficient CMP process, we focused on a nanobubble. When the nanobubble collapses, the liquid around the bubble forms a jet which creates a water hammer shock. Therefore, we suggested that applying the jet increases the efficiency of CMP process. To establish the efficient CMP, revealing the effects of the nanobubble collapse on precise polishing is required. In order to reveal the effects of the nanobubble collapse on a solid surface, we performed nanobubble collapse simulation on a solid surface by molecular

dynamics method. First, we made the nanobubble in water solvent by removing the solvent molecules spherically. Next, we applied shockwave and performed nanobubble collapse simulation on the solid surface. In order to clarify the effects of one nanobubble collapse, we compared the nanobubble collapse simulations and only shockwave simulation. In the nanobubble collapse simulation, a jet was generated by the nanobubble collapse and the structural change in the solid surface was larger compared with the shockwave simulation. This suggests that a nanobubble would be useful to increase the removal rate of a solid surface. Next, in order to clarify the effects of different number of nanobubbles, we compared the nanobubble collapse simulations with one and two nanobubbles. We found that the structural change by the two nanobubbles simulation was larger than that by the one nanobubble simulation. When the jet passes the water solvent, the stream of the jet decays. However, when the generated jet passes another nanobubble, the stream of the jet does not decay, because there are no water molecules in the nanobubble. Therefore, increasing the number of nanobubbles would be useful to improve the removal rate.

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O9] Symposium O-9

Chairs: Yusuke Ootani(Tohoku University, Japan), Shuichi Uehara(Tohoku University, Japan)
Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room5

[SY-O9] **Combined experimental and computational study on the superlubricity mechanism of 2D Materials at the microscale**

○Tianbao Ma （Tsinghua University, China）

[SY-O9] **Quantum chemistry vs. rheology of some EMIM-based ionic liquids**

Szerena Kisztina Ujvari[1,2], Konstantinos Gkagkas[1], ○Andras Vernes[2,3] （1.Advanced Material Research Division, Toyota Motor Europe NV/SA, Technical Center, Hoge Wei 33B, 1930 Zaventem, Belgium, 2.AC2T research GmbH, Viktor-Kaplan-Str. 2/C, 2700 Wiener Neustadt, Austria, 3.Institute of Applied Physics, TU Wien, Wiedner Hauptstr. 8-10/134, 1040 Vienna, Austria）

[SY-O9] **Lubrication with a refrigerant : a challenge made possible thanks to fluid/surface chemistry**

Stéphane TROMP[1], Laurent JOLY[2], Manuel COBIAN[3], ○Nicolas FILLOT[1] （1.Univ Lyon, INSA-Lyon, , CNRS UMR5259, LaMCoS, F-69621 Villeurbanne, France, 2.Univ Lyon, Universite Claude Bernard Lyon 1, CNRS, Institut Lumiere Matiere, F-69622 Villeurbanne, France, 3.Univ Lyon, Ecole Centrale de Lyon, ENISE, ENTPE, CNRS UMR5513, Laboratory of Tribology and System Dynamics, F-69134 Ecully, France）

[SY-O9] **Meso-scale SPH simulation for friction and wear between elastic-plastic solids with various asperities**

○Natsuko Nakagawa Sugimura[1,2], Le Van Sang[2], Yuji Mihara[1], Hitoshi Washizu[2] （1.Dept. of Mechanical Engineering, Tokyo City Univ., Japan, 2.Grad. Sch. of Simulation Studies, Univ. of Hyogo,, Japan）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room5)

[SY-O9] Combined experimental and computational study on the superlubricity mechanism of 2D Materials at the microscale

Invited

○Tianbao Ma （Tsinghua University, China）

With chemical inertness, atomically flatness and interlayer van der Waals interaction, graphene and other 2D materials could act as potential ultra-thin protective coating to reduce adhesion, friction and wear.

Firstly, we predict a stable superlubricity state with vanishing friction between graphene and MoS_2 heterostructure. This is attributed to the perpetual interfacial incommensurability with the large intrinsic lattice mismatch, which leads to near-zero sliding-induced interfacial charge density fluctuation and ultrasmooth potential energy surface. Theoretical prediction has found preliminary evidence by the measurement of interlayer lateral force constant of 2D materials.

Secondly, we report a direct AFM measurement of sliding friction between graphene-coated microsphere (GMS) and graphene, and between GMS and hexagonal boron nitride (h-BN) hetero 2D layers. The exceptionally low and robust friction coefficient of 0.003 is obtained in ambient atmosphere, under high local contact pressure. This sustainable ultralow friction is attributed to the overall incommensurability of the multi-asperity contact covered with randomly oriented graphene nanograins. Furthermore, the local contact pressure fluctuations induced by the atomic roughness could be markedly suppressed by coating few-layer graphene (layer number >3) on the contacting asperities.

Thirdly, we report the preservation of ultra-low-friction state on graphene even under harsh chemical modifications. By proper alignment of graphene on a Ge(111) substrate, friction of graphene could be well preserved at an ultra-low level even after fluorination or oxidation. This behavior is experimentally found to be closely related to the suppression of molecular-level deformation of graphene within the moiré superlattice structure. Furthermore, friction modulation with dual-scale stick-slip behavior is observed on graphene/Ru(0001) substrate. The moiré superlattice-level slip instability could be attributed to the large sliding energy barrier, which arises from the morphological corrugation of graphene on Ru(0 0 0 1) surface.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room5)

[SY-O9] Quantum chemistry vs. rheology of some EMIM-based ionic liquids

Szerena Kisztina Ujvari[1,2], Konstantinos Gkagkas[1], ○Andras Vernes[2,3] （1.Advanced Material Research Division, Toyota Motor Europe NV/SA, Technical Center, Hoge Wei 33B, 1930 Zaventem, Belgium, 2.AC2T research GmbH, Viktor-Kaplan-Str. 2/C, 2700 Wiener Neustadt, Austria, 3.Institute of Applied Physics, TU Wien, Wiedner Hauptstr. 8-10/134, 1040 Vienna, Austria）

Ab-initio tribology is the part of computational tribology mainly dealing with tribological phenomena where electrons matter. In a previous work, [1] for example, the electronic contribution to the real contact area has been estimated by applying Bader's quantum theory of atoms in molecules (AIM). [2]

In this contribution, AIM is used in combination with the density-functional theory (DFT), i.e., for the accordingly determined ab-initio electronic charge density in case of some 1-ethyl-3-methyl-imidazolium-based ionic liquids (ILs) to topologically characterize the involved ions also when the selected EMIM-based ILs are confined. Considering the calculated Bader's manifolds for both the free-standing and confined

ions, and the separation area between the ions, an attempt will be made (i) to explain for ILs both experimentally [3] and computationally [4] observed layered structures, and (ii) to evaluate the relaxation time of ions. The latter will also be compared with that derived from the measured viscosities, and in addition the measured viscosities will be correlated with some DFT-determined quantum chemical indices [5].

1. M. Wolloch, G. Feldbauer, P. Mohn, J. Redinger, and A. Vernes, *Ab-initio calculation of the real contact area on the atomic scale*, Phys. Rev. B 91, 195436 (2015)

2. Richard F. W. Bader, *The density in density-functional theory*, J. Mol. Struc - TheoChem 943 (1-3), 2 (2010)

3. A. M. Smith, K. R. J. Lovelock, N. N. Gosvami, Peter Licence, A. Dolan, T. Welton, and S. Perkin, *Monolayer to bilayer structural transition in confined pyrrolidinium-based ionic liquids*, J. Phys. Chem. Lett. 4, 378 (2013)

4. K. Gkagkas, and V. Ponnuchamy, *The impact of coulombic interactions among polar molecules and metal substrates on flow and lubrication properties*, Model. Simul. Mater. Sci. Eng. 25 (6), 064004 (2017)

5. M. Karelson, V. S. Lobanov, and A. R. Katritzky, *Quantum chemical descriptors in QSAR/QSPR studies*, Chem. Rev. 96, 1017 (1996)

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room5)

[SY-O9] Lubrication with a refrigerant : a challenge made possible thanks to fluid/surface chemistry

Stéphane TROMP[1], Laurent JOLY[2], Manuel COBIAN[3], ○Nicolas FILLOT[1] (1.Univ Lyon, INSA-Lyon, , CNRS UMR5259, LaMCoS, F-69621 Villeurbanne, France, 2.Univ Lyon, Universite Claude Bernard Lyon 1, CNRS, Institut Lumiere Matiere, F-69622 Villeurbanne, France, 3.Univ Lyon, Ecole Centrale de Lyon, ENISE, ENTPE, CNRS UMR5513, Laboratory of Tribology and System Dynamics, F-69134 Ecully, France)

Lubrication is often seen as the major solution to avoid wear and high friction due to the relative motion of solids in contact. But this sometimes requires a heavy design (e.g. addition of lubricant pumps) while the actual trend goes for weight reduction of mechanical systems. The use of working fluids (e.g. refrigerant, gasoline) instead of classical lubricants (oil) allow to bypass this problem. Nonetheless, tribological contacts have to work with ultra low viscosity fluids (not designed to be good lubricants). The major consequence is that the film thickness separating the surfaces reaches the same order of magnitude as surface roughness. At this stage, a minimum quantity of fluid needs to be trapped between apserities to avoid direct contact. This is made possible if fluid molecules are adsorbed onto the surfaces.

The work presented here aims at explaining experimental observations of R-1233zd refrigerant ability to lubricate a highly loaded contact. Starting from a dedicated force field parametrization for the refrigerant-hematite interaction (from DFT calculations [1]), Large-Scale Molecular Dynamics simulations of extreme compression and shearing of R-1233zd show the resistance of the refrigerant adsorption, and its capability to undergo normal and tangential stresses.

[1] S. Tromp, L. Joly, M. Cobian, N. Fillot, Chemical Physics at Interfaces within a Refrigerant-Lubricated Contact: From Electronic Structure to Large-Scale Molecular Dynamics Simulations. J. Phys. Chem. C, 2018, DOI: 10.1021/acs.jpcc.7b11267

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room5)

[SY-O9] Meso-scale SPH simulation for friction and wear between elastic-plastic solids with various asperities

○Natsuko Nakagawa Sugimura[1,2], Le Van Sang[2], Yuji Mihara[1], Hitoshi Washizu[2] （1.Dept. of Mechanical Engineering, Tokyo City Univ., Japan, 2.Grad. Sch. of Simulation Studies, Univ. of Hyogo,, Japan）

We made the meso(micron-oder) scale model to simulate friction, wear and adsorption with heating between elastic-plasic bodies. Constitutive equation is based on the continuum equation and calculated with SPH(Smoothed Particle Hydrodynamics). SPH is one of particle methods to solve continuum equation with mesh free. SPH was initially developed for the hydrodynamics by Lucy et al., but it was applied to calculation of solids afterwards by Swegle et al. and has gained good results. In SPH, the physical variables of the particles are reconstructed by the adding the physical variables of the surrounding particles by an appropriate weighting called kernel. SPH particles are not truly particles like molecules but only physical fields. However, we regard the particles on the friction surfaces as also coarse grained molecules and add the interaction forces directly between such “particles”, which is mimicking the particle approach. That is, our model is what continuum calculation and particle calculation are mixed. It is just meso-scale that is situated in between the macro scale to demand continuum approach and the nano scale to demand particle approach. Although its physical discontinuity is not yet resolved, if the using both approaches confirm the reproducing valid frictional phenomena, the mechanism of its discontinuity may also be resolved. At this time, for the purpose to efficiently realize the calculation of the great amount of particles with parallel code, we use the FDPS open platform by Iwasawa &Makino et al. to create our simulation code.

We set the tens of micron system in which elastic-plastic bodies with various asperities are faced and one body is sliding under the vertical load to cause shear friction. So far, in the system with interface with regular asperities, the elasticity, plasticity, friction cure, heat generation and conduction were to some extent qualitatively expressed, although the frictional results depend on the several parameters and SPH boundary processing. Then, we will firstly show the characteristics of our model with regular asperity system in detail. Moreover, we will discuss the frictional properties changing the shape of asperities, i.e. with realistic asperities.

[SY-A9] Symposium A-9

Chair: Eliot Fried(Okinawa Institute of Science and Technology, Japan)
Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room6

[SY-A9] Group-theoretical construction for constitutive equation of the first strain gradient elasticity

◯Ryuichi Tarumi[1], Shunsuke Kobayashi[2], Yoji Shibutani[2] （1.Graduate School of Engineering Science, Osaka Univ., Japan, 2.Dept. of Mechanical Engineering, Osaka Univ., Japan）

[SY-A9] Physically based strain gradient plasticity model for length scale dependent yield strength

◯Peter Gudmundson （Department of Solid Mechanics, KTH Royal Institute of Technology, Sweden）

[SY-A9] **FTMP-based Seamless Description of Deformation-Fracture Transitions**

◯Tadashi Hasebe （Kobe Univ., Japan）

[SY-A9] On the crucial role played by instantaneous and hidden multifield features of lattice dynamics in their nonlocal pseudocontinuum modeling

◯Miguel Charlotte （University of Toulouse, Institute Clement Ader, CNRS -- UMR 5312 INSA/UPS/ISAE-SupAero/Mines Albi, France）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room6)

[SY-A9] Group-theoretical construction for constitutive equation of the first strain gradient elasticity

○Ryuichi Tarumi[1], Shunsuke Kobayashi[2], Yoji Shibutani[2] （1.Graduate School of Engineering Science, Osaka Univ., Japan, 2.Dept. of Mechanical Engineering, Osaka Univ., Japan）

Development of the theory of continuum mechanics is one of the central issues for quantitative understanding of multiscale phenomena. The first strain gradient elasticity (FSGE) is an attractive framework as it includes *non-locality* in the constitutive equation. Application of the theory for multiscale material modeling is however still limited due to the large number of independent strain gradient elastic constants. This study aims to overcome the difficulty by using the group theory. We conduct the irreducible decomposition for the 5th and 6th-rank strain gradient elastic constants, M and A, under general linear group GL(3). The decomposition is based on the Schur-Weyl duality principle and Young symmetrizer technique in Frobenius algebra. For the isotropic and centro-symmetric case, the 6th-rank tensor is decomposed into three sub-tensors, $A = A^{\{6\}}+A^{\{4,2\}}+A^{\{3,2,1\}}$, whereas the 5th-rank tensor M vanishes identically. Here, the one-dimensional sub-tensor $A^{\{6\}}$ is called the primitive symmetry class and satisfies the generalized Cauchy solid condition. The corresponding stress equilibrium equation yields a simplified 4th-order partial differential equation that is different from Aifantis' Laplacian-type gradient theory. Another one-dimensional sub-tensor $A^{\{3,2,1\}}$ denotes the elastic null-Lagrangian which is absent in the classical elasticity. The remaining three-dimensional sub-tensor $A^{\{4,2\}}$ has two characteristic length scales and one of which has an imaginary value. We also revealed that the combined sub-tensors, $A^{\{4,2\}}+A^{\{3,2,1\}}$, with a proper kinematic constrain condition, reduces the well-known couple stress elasticity. Implementation of the Cauchy-type FSGE for NURBS-based isogeometric analysis (IGA) demonstrates that stress field around a point defect is regularized due to the non-locality included in $A^{\{6\}}$.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room6)

[SY-A9] Physically based strain gradient plasticity model for length scale dependent yield strength

○Peter Gudmundson （Department of Solid Mechanics, KTH Royal Institute of Technology, Sweden）

Many experimental studies have shown a plastic strengthening effect for structural length scales approaching microstructural dimensions. Both increases in initial yield strength and strain hardening have been observed. Over the last 30 years different strain gradient plasticity (SGP) theories have been developed in order to capture these length scale dependences. However, up to now no generally accepted theory has emerged. In the present paper, focus is directed into a physically based SGP model for initiation of plastic deformation. The plastic behavior is governed by a dissipative part that primarily controls the hardening at moderate plastic strains and an energetic part that is of importance for the initiation of plastic flow. It is shown that a model based on the self-energies of dislocations can be translated into an internal free energy in terms of plastic strain gradients. In this way a physical connection is made between the SGP framework and dislocation mechanics. A microstructural length scale can then be defined as the Burgers vector divided by the strain for initiation of plastic deformation. When structural length scales approach this microstructural length scale, strengthening effects result. It the Taylor model is used for the dissipative part, the same microstructural length scale appears. The so developed three-dimensional SGP model is specialized to the simple load cases of tensile tension with a passivation layer that prohibits plastic deformation on surfaces as

well as pure bending with free and fixed boundary conditions for plastic strain. Simulations for varying thicknesses are compared to experimental observations reported in the literature. It is shown that the model in a good way can capture the length scale dependences. Suggestions for improvement of the dislocation theory based model for the internal free energy are discussed.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room6)

[SY-A9] FTMP-based Seamless Description of Deformation-Fracture Transitions

○Tadashi Hasebe （Kobe Univ., Japan）

This study attempts to tackle one of the ultimate problems in mechanics of materials based on FTMP (Field Theory of Multiscale Plasticity), i.e., modeling deformation-fracture transitions. Three typical fracture modes are targeted: (1) ductile fracture, (2) creep rupture and (3) fatigue crack initiation, whose evolutions are respectively triggered or promoted by deformation-induced substructures. For (1), critical conditions governing the outsets of macro/micro instabilities are extensively discussed, while (2) is concerned with localized recovery-induced rupture in packet models for lath martensite structures, in connection with the interaction fields. The mode (3), on the other hand, is successfully reproduced via evolving PSB ladder structure and attendant vacancy formation/diffusion processes. A noteworthy output here is that the use of the corresponding duality diagram representations enables us to "visualize" these complex processes, manifested as dynamic energy conversion between fluctuating elastic strain

---

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room6)

[SY-A9] On the crucial role played by instantaneous and hidden multifield features of lattice dynamics in their nonlocal pseudocontinuum modeling

○Miguel Charlotte （University of Toulouse, Institute Clement Ader, CNRS -- UMR 5312 INSA/UPS/ISAE-SupAero/Mines Albi, France）

In the past, a very large number of investigations has been interested in building various continuum descriptions of periodical mass-spring lattices which are capable of capturing at least some microscopically fast and microscopically localized phenomena that cannot be handled correctly by the classical continuum theories relying on a single displacement field. Very few of these works have however tried to illuminate some of the less well-known aspect of the concept of "action-at-a distance" involved in periodical mass-spring lattices, namely the "instantaneous propagation of disturbances",
and its nonlocal effects in finite material systems. These instantaneous features, that are developed in the present work, have notably been discussed formerly partly by Lord Rayleigh and T.H. Havelock for other dispersive media and more recently evoked by M. Charlotte and L. Truskinovsky. Such features have although been ignored or minimized up to now in most derivations of pseudocontinuum hamiltonian models of elasticity. In order to account for these features, the alternative viewpoint developed here uses on an implicit but somewhat standard multi-displacement

field description of the periodical mass-spring lattice motions and their (spatially nonlocal) pseudocontinuum wave mechanic representations which allow to deal in the same framework with both quasi-continuum (atomically diffuse) and anti-continuum (atomically localized) phenomena in finite material systems. In particular, the focus is put on the lattice motions of a simple finite particle chain with nearest neighbor interactions owing to its simplicity, complete analyticity, and physical clearness. The current analysis also explores an alternative standpoint, including both bulk- and boundary-dependent multi-field or multi-modal continuum descriptions, and that may constitute a new direction in which the continuum modeling theory could be fundamentally generalized. Thus, the outcome of the present multi-field approach is merely another non-classical quasi-continuum elastodynamics with both non-trivial nonlocal inertia and elasticity whose complexity depends naturally on the non-trivial interplay between the atomic bulk interactions and the boundary conditions.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A10] Symposium A-10
Chair: Steve Fitzgerald(University of Leeds, UK)
Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room6

[SY-A10] Interdiffusion and atomic mobilities in fcc Ag-Mg, Ag-Mn and Ag-Mg-Mn alloy
○Qianhui Min[1], Yuling Liu[1], Yong Du[1], Huixin Liu[1], Li Chen[1], Biao Hu[3], Changfa Du[2], Zhoushun Zheng[2] （1.Powder Metallurgy Research Institute,Central South University, China, 2.School of mathematics and statistics,Central South University, China, 3.School of Material Science and Engineering, Anhui University Of Science And Technology, China）

[SY-A10] Stacking and Multilayered Nature of Martensite in Copper Based Shape Memory Alloys
○Osman ADIGUZEL （Firat University , Turkey）

[SY-A10] Mesoscale understanding of ionic conduction in yttria stabilized zirconia
○Abhijit Chatterjee （Dept. of Chemical Engineering, Indian Institute of Technology Bombay, India）

[SY-A10] cancellation

[SY-A10] Accelerating stochastic simulations with path integrals
○Steve Fitzgerald （University of Leeds, UK）

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room6)

[SY-A10] Interdiffusion and atomic mobilities in fcc Ag-Mg, Ag-Mn and Ag-Mg-Mn alloy

○Qianhui Min[1], Yuling Liu[1], Yong Du[1], Huixin Liu[1], Li Chen[1], Biao Hu[3], Changfa Du[2], Zhoushun Zheng[2]
 （1.Powder Metallurgy Research Institute,Central South University, China, 2.School of mathematics and statistics,Central South University, China, 3.School of Material Science and Engineering, Anhui University Of Science And Technology, China）

On the basis of Ag/Ag-Mg, Ag/Ag-Mn, Ag-Mg/Ag-Mn, and Ag/Ag-Mg-Mn diffusion couples, the interdiffusion coefficients in face-centered cubic (fcc) phase of the Ag-Mg, Ag-Mn, and Ag-Mg-Mn alloys were messured at the temperature range between 873 and 1173 K by using semi-infinite diffusion couples together with the Sauere-Freise method. A reliable method was applied to evaluate the errors of the identified interdiffusivities in consideration of the propagation of errors. Based on available thermodynamic information, the atomic mobilities for the fcc Ag-Mg, Ag-Mn,and Ag-Mg-Mn syetems are obtained by using the DICTRA software package, and the computed results agree in general with experimental data.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room6)

[SY-A10] Stacking and Multilayered Nature of Martensite in Copper Based Shape Memory Alloys

○Osman ADIGUZEL （Firat University , Turkey）

Shape memory effect is characterized by the recoverability of two certain shapes of material at different temperatures. These materials are often called smart materials due to the functionality and their capacity of responding to changes in the environment. Shape memory is initiated by cooling and stressing material and processed by heating and cooling.

Shape memory effect is a result of successive thermal induced and stress induced martensitic transformations. Thermal induced martensitic transformation occurs as twinned martensite on cooling as martensite variants with cooperative movement of atoms by means of lattice invariant shears on {110} - type planes of austenite matrix. Twinned structures turn into detwinned martensite by means of stress induced martensitic transformation on stressing in martensitic state. Lattice invariant shears occurs in <110 >-type directions on the {110}-type basal planes.

Copper based alloys exhibit this property in metastable β-phase region, which has bcc-based structures at high temperature parent phase field. Twinning and lattice invariant shear is not uniform in these alloys and multilayered martensite with complex stacking structures, like 9R or 18R martensites occur by means of thermal induced martensitic transformation. All of these martensite phases are long-period stacking ordered structures that is the underlying lattice is formed by stacks of close-packed planes.

In the present contribution, x-ray diffraction and transmission electron microscopy studies were carried out on two copper based CuZnAl and CuAlMn alloys. X-ray diffraction profiles and electron diffraction patterns reveal that both alloys exhibit super lattice reflections inherited from parent phase due to the displacive character of martensitic transformation.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room6)

[SY-A10] Mesoscale understanding of ionic conduction in yttria stabilized zirconia

○Abhijit Chatterjee （Dept. of Chemical Engineering, Indian Institute of Technology Bombay, India）

Yttria-stabilized zirconia (YSZ) is widely used as an electrolyte in solid oxide fuel cells (SOFCs). Much of past research on ionic conductivity in YSZ has focused on understanding diffusion process atomistically, e.g., migration barriers for O^{2-} ion movement and vacancy trapping behavior, in an attempt to explain the bulk O^{2-} transport. How the mesoscale structure of YSZ, i.e., structures at length scales lying between the atomic/micro-scale and the macroscale, influences ionic conduction remains poorly understood. An improved understanding of mesoscale factors that affect ionic conduction in YSZ can potentially benefit our efforts to search for new SOFC electrolyte materials.

Two mesoscale aspects will be covered in this talk. The first part of the talk relates to the percolation network structure formed in YSZ. It is well known that Y3+ ions in the YSZ structure block the movement of O2- ions. Other parts of YSZ that locally do not contain the Y3+ ions form a fast ion conducting percolation network. The network topology is determined by the underlying cation arrangement. Insights into the percolation network composition, topology and O^{2-} ion conduction rates are provided using kinetic Monte Carlo simulations. A relationship between the ionic conductivity and the topological details of the network is derived.

The second part relates to free energy of finding O^{2-}-vacancy (O^{2-}-vac) pairs in a local environment, which again is a mesoscale property of the material. Higher probability of O^{2-}-vac pairs in some regions of YSZ can result in greater number of transitions in those regions. O^{2-} ion movement in bulk YSZ is studied using multiple independent short molecular dynamics (MD) trajectories. Analysis of the MD trajectories yields free energy of O^{2-}-vac pairs in 42 different local cation (Y^{3+}/Zr^{4+}) environments, as well as effective O^{2-} hopping rates and Arrhenius parameters. Based on the free energies we conclude that it is possible that ionic movement is hindered in some environments not just because of high migration barriers or vacancy trapping as believed earlier, but also because O^{2-}-vac pairs are destabilized by these environments. Increasing the temperature and/or decreasing the dopant composition stabilizes O^{2-}-vac pairs in these environments, which in turn affects the YSZ conductivity.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room6)

[SY-A10] cancellation

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room6)

[SY-A10] Accelerating stochastic simulations with path integrals

○Steve Fitzgerald （University of Leeds, UK）

Monte Carlo-type simulations can extend accessible timescales c.f. atomistic models by many orders of magnitude. However, their efficiency can be significantly reduced when some of the species being simulated have very low migration barriers. This can be addressed by coarse-graining the low-barrier migration into pseudo-free continuum diffusion and, and evolving the system by drawing timesteps and hop lengths from a first passage time distribution [1,2], but this neglects the effects of spatial variation in the potential landscape in which the particles move, i.e. drift. Existing extensions require every step of a random walk to be computed, or a Fokker-Planck equation to be solved numerically [3], thus increasing the computational cost.

In this work I will describe an alternative approach, beginning from the Langevin equation for a particle moving in a general smooth potential V(x). Assuming Gaussian white noise, the stochastic equation of motion can be recast as a path integral, which can be analysed using methods borrowed from quantum field theory. Closed-form solutions for the Green function / propagator P(x,t|0,0) in a general potential are possible when the noise strength (temperature) is less than the energy scale characterising the barriers the particle has to overcome (i.e. the same range of validity as the Arrhenius rate function exp(-E/kT).) Potential applications to material simulations will be discussed.

[1] Opplestrup, Tomas, et al. "First-passage Monte Carlo algorithm: diffusion without all the hops." *Physical review letters* 97.23 (2006): 230602.

[2] Muller, Mervin E. "Some continuous Monte Carlo methods for the Dirichlet problem." *The Annals of Mathematical Statistics*(1956): 569-589.

[3] Mauro, Ava J., et al. "A first-passage kinetic Monte Carlo method for reaction-drift-diffusion processes." *Journal of Computational Physics* 259 (2014): 536-567.

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I9] Symposium I-9

Chairs: Yuri Mishin(George Mason University, United States of America), Yang Xiang(Hong Kong University of Science and Technology, Hong Kong)
Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room7

[SY-I9] Grain Boundary Microstates Under Irradiation: A Moment in Time?

○Mitra L Taheri （Drexel University, Department of Materials Science &Engineering, United States of America）

[SY-I9] The Role of Grain Boundaries under Long-Time Radiation

○Jing Luo[1], Yichao Zhu[1], Xu Guo[1], Yang Xiang[3], Stephen Jonathan Chapman[2] （1.Dalian University of Technology, China, 2.Mathematical Institute, University of Oxford, UK, 3.Department of Mathematics, The Hong Kong University of Science and Technology, Hong Kong）

[SY-I9] Quantifying point defect fluxes to interfaces and the role of interface structure

○Shen J Dillon （University of Illinois , United States of America）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room7)

[SY-I9] Grain Boundary Microstates Under Irradiation: A Moment in Time?

Invited

○Mitra L Taheri （Drexel University, Department of Materials Science &Engineering, United States of America）

Understanding the sink efficiency of interfaces under irradiation is of paramount importance to tailoring materials for radiation tolerance. Using in situ irradiation coupled with precession electron diffraction analysis, defect absorption was tracked for increasing dose. Denuded zones were found to collapse, but in the absence of any detected changed in macroscopic degrees of freedom of the grain boundaries. Each grain boundary denuded zone experienced changes different doses, indicating a direct observation of the difference in grain boundary "immunity" to irradiation depending on character. Since a change in sink efficiency is likely due to a change in point defect absorption at the boundary, this indicates that something about the structure of these boundaries has changed. The grain boundary macroscopic character remains the same, however, leading to the conclusion that a change in microscopic character has occurred, possibly due to the formation of extrinsic defects on the boundary. To analyze this further, simulations were used to explore grain boundary microstates loaded with defects (mimicking a collision cascade) and assessed for vacancy formation energies. Overall, the results present a foundation for improving sink efficiency descriptions under irradiation, and take a step forward in understanding complex interfacial dependencies. Additionally, results will be shown for studies of grain boundary structure and stability, including faceting, in the context of grain boundaries acting as "phases." These advances present the possibility that the extent to which a grain boundary is at "equilibrium" controls many of its properties, and that its equilibrium is possible to be tuned.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room7)

[SY-I9] The Role of Grain Boundaries under Long-Time Radiation

○Jing Luo[1], Yichao Zhu[1], Xu Guo[1], Yang Xiang[3], Stephen Jonathan Chapman[2] （1.Dalian University of Technology, China, 2.Mathematical Institute, University of Oxford, UK, 3.Department of Mathematics, The Hong Kong University of Science and Technology, Hong Kong）

Materials containing a high proportion of grain boundaries offer significant potential for the development of radiation-resistent structural materials. However, a proper understanding of the connection between the radiation-induced microstructural grain boundary behaviour and its impact at long natural time scales is still missing. To bridge this gap in time scales, a rigorously coarse-grained formulation describing the coupled evolution of point defects and low-angle tilt grain boundaries is proposed. The derived formulation captures well the radiation-induced climb behaviour of grain boundary dislocations, which leads to asymmetry in grain shape evolution. It also reveals that the presence of point defect sources within a grain further accelerates its shrinking process, and radiation tends to elongate the twin boundary sections. Based on the proposed formulation, it is predicted for the first time that the minimum dimension of a polycrystalline aggregate needed for shielding the point defect concentration to a prescribed level scales with its grain boundary fraction at a sublinear rate.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room7)

[SY-I9] Quantifying point defect fluxes to interfaces and the role of interface structure

Invited

○Shen J Dillon （University of Illinois , United States of America）

Point defect fluxes to and from interfaces can dominate the response of materials exposed to irradiation, their equilibration after thermal perturbation, and their sintering. However, little is known experimentally about how non-equilibrium point defect concentrations equilibrate, how their concentration gradients develop in the lattice, and the role of interface structure in affecting sink efficiency. This talk describes experimental approaches to probing these phenomena using localized tracer diffusion measurements and irradiaiton induced creep in model sample geometries.

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I10] Symposium I-10
Chair: Saryu Fensin(Los Alamos National Lab, United States of America)
Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room7

[SY-I10] Structure and Mobility of Dissociated Cacancies at Twist Grain Boundaries and Screw Dislocations in Ionic Compounds

○Blas Pedro Uberuaga, Enrique Martinez, Kedarnath Kolluri, Xiang-Yang Liu （Los Alamos National Laboratory, United States of America）

[SY-I10] Reverse engineering the kinetics of grain growth

Mingyan Wang[1], Jules Dake[1], Søren Schmidt[2], ○Carl Krill[1] （1.Institute of Micro and Nanomaterials, Ulm University, Germany, 2.Dept. of Physics, Technical University of Denmark, Denmark）

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room7)

[SY-I10] Structure and Mobility of Dissociated Cacancies at Twist Grain Boundaries and Screw Dislocations in Ionic Compounds

Invited

○Blas Pedro Uberuaga, Enrique Martinez, Kedarnath Kolluri, Xiang-Yang Liu （Los Alamos National Laboratory, United States of America）

Interfaces, grain boundaries, and dislocations are known to have significant impact on the transport properties within materials. Even so, it is still not clear how the structure of interfaces influence the mobility and concentration of carriers that are responsible for transport. Using low angle twist grain boundaries in MgO as a model system for semi-coherent interfaces more generally, we examine the structural and kinetic properties of vacancies. These boundaries are characterized by a network of screw dislocations. Vacancies of both types, Mg and O, are strongly attracted to the dislocation network, residing preferentially at the misfit dislocation intersections (MDIs). However, the vacancies can lower their energy by splitting into two parts, which then repel each other along the dislocation line between two MDIs because of electrostatic repulsion, further lowering their energy.

This dissociated structure has important consequences for transport, as the free energy of the dissociated vacancies decreases with decreasing twist angle, leading to an increase in the net migration barrier for diffusion as revealed by molecular dynamics simulations. Similar behavior is observed in BaO and NaCl, highlighting the generality of the behavior. We analyze the structure of the dissociated vacancies as a pair of jogs on the dislocation and construct a model containing electrostatic and elastic contributions that qualitatively describe the energetics of the dissociated vacancy. Finally, we examine the nature of this mechanism in other ionic compounds without a rocksalt structure. Our results represent the first validation of a mechanism for vacancy dissociation on screw dislocations in ionic materials first discussed by Thomson and Balluffi in 1962.

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room7)

[SY-I10] Reverse engineering the kinetics of grain growth

Invited

Mingyan Wang[1], Jules Dake[1], Søren Schmidt[2], ○Carl Krill[1] （1.Institute of Micro and Nanomaterials, Ulm University, Germany, 2.Dept. of Physics, Technical University of Denmark, Denmark）

At first glance, the strategy for modeling grain growth seems obvious: simply combine an expression governing the physics of grain boundary (GB) migration with a treatment of the connectivity of the boundary network, such that shrinkage of one grain corresponds to growth of its neighbor. However, 70 years of analytic models and three decades' worth of computer simulations have left us with seemingly intractable discrepancies between theory and experiment—concerning, for example, the shape of the self-similar grain size distribution; the occurrence of growth stagnation at long annealing times; and, most strikingly, the emergence of a bimodal size distribution during instances of so-called "abnormal" grain growth.

In the world of industry, when repeated attempts to solve a technological challenge end in failure, employees

sometimes try to "reverse engineer" a competitor's product, dissecting the interplay between the device's internal parts to uncover its working principle. Afflicted with a similar sense of desperation, we applied this approach to the phenomenon of grain growth! Exploiting three-dimensional x-ray diffraction (3DXRD) microscopy, we investigated thermally induced coarsening in two different Al alloys. From microstructural snapshots interspersed between isothermal annealing steps, we were able to track the morphology, misorientation and migration of thousands of GBs over time, acquiring the basis for a robust statistical analysis of local growth kinetics. The results allow extracting dependencies of reduced mobility (the product of GB mobility and energy) on GB misorientation and inclination. In one specimen, the measured dependency is consistent with expectations for normal grain growth, but, in the other case, we find evidence for boundary kinetics that lie beyond the scope of standard models.

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I11] Symposium I-11

Chairs: Bob Svendsen(RWTH Aachen University, Germany), Jeremy K Mason(University of California, Davis, United States of America)
Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room7

[SY-I11] Recent advances in the Full-Field modeling of microstructural evolutions using a finite-element level set integrated framework.
ºDaniel Pino Munoz, Thomas Toulorge, Charbel Moussa, Nathalie Bozzolo, Marc Bernacki
（Mines ParisTech / PSL Research University, France）

[SY-I11] The effect of strong anisotropic grain boundary energy and mobility on microstructure formation and evolution: mesoscale modeling and simulation
ºBrandon Runnels[1], Josep Maria Gras Ribot[1], Ian Chesser[2] （1.University of Colorado Colorado Springs, United States of America, 2.Carnegie Mellon University, United States of America）

[SY-I11] A Machine Learning Exploration of Grain Boundary Mobility Mechanisms
Leila Khalili[1], Eric R Homer[2], ºSrikanth Patala[1] （1.North Carolina State University, United States of America, 2.Brigham Young University, United States of America）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room7)

[SY-I11] Recent advances in the Full-Field modeling of microstructural evolutions using a finite-element level set integrated framework.

Invited

○Daniel Pino Munoz, Thomas Toulorge, Charbel Moussa, Nathalie Bozzolo, Marc Bernacki （Mines ParisTech / PSL Research University, France）

Full field modeling of microstructure evolutions at polycrystalline scale is nowadays a very active field of research. Within this context we have been working in tight collaboration with industrial partners in order to be able to predict microstructural evolutions of metallic material due to recrystallization and grain growth phenomena. This collaboration had lead us to the development of a numerical framework based on the Level-Set method that allows to account fro complex microstructural evolution. These complex phenomena includes grain growth, Smith-Zener pinning and, in particular, static, dynamic and post-dynamic recrystallization. In this way the motion of the grain boundaries of microstructures is simulated accurately.

The general numerical framework will be presented along with recent developments that allowed us to significantly improve the performance of our approach. Our on-going developments aim at the enhancement of the existing capabilities of our numerical tools in order to account for high grain boundary energy and mobility. Different examples will the used to illustrate the robustness of the numerical approach as well as its capabilities to accurately simulate microstructural evolutions. Finally, some current challenges for the forthcoming years will be discussed.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room7)

[SY-I11] The effect of strong anisotropic grain boundary energy and mobility on microstructure formation and evolution: mesoscale modeling and simulation

Invited

○Brandon Runnels[1], Josep Maria Gras Ribot[1], Ian Chesser[2] （1.University of Colorado Colorado Springs, United States of America, 2.Carnegie Mellon University, United States of America）

Nanocrystalline materials have exceptional mechanical properties. Because of their small microstructural length scale, their macroscopic properties are dramatically influenced by grain boundaries (GBs). In this work we develop an algorithm for constructing the Allen-Cahn equation for grain boundary migration including an orientation-dependent, nonconvex, anisotropic boundary energy. The energy minimizing morphology for boundaries with nonconvex energy is faceted, but lacks a lengthscale, resulting in unstable solutions in phase field gradient flow. It is therefore necessary to include a second-order regularization to penalize corners To compute the variational derivative of this complex free energy, we simplify by transforming into the eigenbasis of the Hessian. This reduces the computation of principal curvatures to second derivatives with respect to the second and third principal axes, which preserves computational efficiency.To incorporate realistic boundary behavior, the lattice-matching model is used to calculate boundary energy for arbitrary orientations, on-the-fly. Simulations are conducted for microstructure evolution in a real-space implementation using adaptive mesh refinement. Finally, we propose a continuum understanding of GB motion as a shear transformation goverened by compatibility. Optimal boundary transformations are

determined using a systematic process for shear identification, and by computing the minimum energy barrier for each. Such transformations typically require an atomic "shuffle" meaning that they atoms do not transform in the Cauchy-Born sense. The resulting optimal transformation can then be incorporated at the mesoscale by modeling the elastic energy as a multiwell potential. This provides a continuum context for understanding disconnections and faceted boundary migration.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room7)

[SY-I11] A Machine Learning Exploration of Grain Boundary Mobility Mechanisms

Invited

Leila Khalili[1], Eric R Homer[2], ○Srikanth Patala[1] (1.North Carolina State University, United States of America, 2.Brigham Young University, United States of America)

The mobility of grain boundaries plays an important role in governing the kinetics of microstructural evolution in every class of polycrystalline materials. Of particular interest is the role of bicrystallography, characterized by the macroscopic crystallographic degrees of freedom, on the underlying atomistic mechanisms governing grain boundary mobility. In this talk, I will present an algorithm to automatically identify such mechanisms that give rise to mobility of an interface. We use machine-learning methods, inspired by recent work in disordered solids, to correlate local structure with the susceptibility for rearrangement of grain boundary atoms. We show that it is possible to automatically identify mobility mechanisms of grain boundaries with a diverse range of crystallographic character.

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I12] Symposium I-12

Chairs: Blas Pedro Uberuaga(Los Alamos National Laboratory, United States of America), Chris P Race(University of Manchester, UK)

Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room7

[SY-I12] **Formation and shrinkage of grain boundary loops in two-dimensional colloidal crystals**

Francois Lavergne, Arran Curran, Dirk Aarts, ○Roel Dullens （University of Oxford, UK)

[SY-I12] **Growth and characterization of two-dimensional poly(quasi)crystals**

○Petri Hirvonen[1], Gabriel Martine La Boissonière[2], Zheyong Fan[1], Cristian Achim[3], Nikolas Provatas[4], Ken R. Elder[5], Tapio Ala-Nissila[1,6] （1.Dept. of Applied Physics, Aalto Univ., Finland, 2.Dept. of Mathematics and Statistics, McGill Univ., Canada, 3.Dept. of Chemical Engineering, Univ. of Concepción, Chile, 4.Dept. of Physics, McGill Univ., Canada, 5.Dept. of Physics, Oakland Univ., United States of America)

[SY-I12] **A Parallel Algorithm for High Resolution 3D Phase Field Simulations of Polycrystalline Solidification**

○Pavel Strachota, Aleš Wodecki （Czech Technical University in Prague, Czech Republic)

[SY-I12] **Properties of β/ω phase interfaces in Ti and their implications on mechanical properties and ω morphology**

○Shuo Cao[1], Qing-Miao Hu[1], Rui Yang[1], Yong Jiang[2] （1.Institute of Metal Research, Chinese Academy of Science , China, 2.Central South University, China)

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room7)

[SY-I12] Formation and shrinkage of grain boundary loops in two-dimensional colloidal crystals

Invited

Francois Lavergne, Arran Curran, Dirk Aarts, °Roel Dullens （University of Oxford, UK）

Understanding the dynamics of grain boundaries in polycrystalline metals and alloys is crucial to enable tuning their mechanical properties. From an experimental point of view, grain boundaries in colloidal crystals are convenient model systems since imaging their dynamics requires only simple optical microscopy and they can be manipulated using optical tweezers. The formation and kinetics of grain boundaries are closely related to the topological constraints imposed on their complex dislocation structure. As such, loop-shaped grain boundaries are unique structures to establish such a link because their overall topological "charge" is zero due to their null net Burgers vector.

Here, we study the formation and shrinkage of such grain boundary loops by creating them on demand via a local rotational deformation of a two-dimensional colloidal crystal using an optical vortex. In particular, we observe that a grain boundary loop only forms if the product of its radius and misorientation exceeds a critical value. In this case, the deformation is plastic and the grain boundary loop spontaneously shrinks at a rate that solely depends on this product while otherwise, the deformation is elastically restored. We show that this elastic-to-plastic crossover is a direct consequence of the unique dislocation structure of grain boundary loops. Our results thus reveal a new general limit on the formation of grain boundary loops in two-dimensional crystals and elucidate the central role of defects in both the onset of plasticity and the kinetics of grain boundaries.

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room7)

[SY-I12] Growth and characterization of two-dimensional poly(quasi)crystals

°Petri Hirvonen[1], Gabriel Martine La Boissonière[2], Zheyong Fan[1], Cristian Achim[3], Nikolas Provatas[4], Ken R. Elder[5], Tapio Ala-Nissila[1,6] （1.Dept. of Applied Physics, Aalto Univ., Finland, 2.Dept. of Mathematics and Statistics, McGill Univ., Canada, 3.Dept. of Chemical Engineering, Univ. of Concepción, Chile, 4.Dept. of Physics, McGill Univ., Canada, 5.Dept. of Physics, Oakland Univ., United States of America）

We use a simple two-mode phase field crystal (PFC) model to simulate grain growth in realistic two-dimensional model systems of square and hexagonal, as well as of 10- and 12-fold symmetric quasicrystal lattice symmetries. Modeling the evolution of poly(quasi)crystals had remained a challenge until the arrival of PFC, giving access to long diffusive time scales. We characterize the model systems using a powerful new method for segmenting and analyzing grain structures. This method generalizes effortlessly to all lattice types of even-fold rotational symmetry. To our knowledge, our characterization method is the first of its kind so far for quasicrystals.

The grain structure segmentations produced by the characterization method are found to agree very well with the corresponding human-made segmentations. We observe power-law scaling of the average grain size as a function of the simulation time, and log-normal grain size distributions for all lattice types considered. Similarly, irrespective of the lattice type, grain misorientation distributions appear remarkably flat, indicative of little correlation in the lattice orientations between neighboring grains. Average number of neighboring

grains is between 5 and 6. We are currently working on improving our statistics to cut down the error margins and to verify or to refute the universality of these, and of further related, distributions.

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room7)

[SY-I12] A Parallel Algorithm for High Resolution 3D Phase Field Simulations of Polycrystalline Solidification

○Pavel Strachota, Aleš Wodecki (Czech Technical University in Prague, Czech Republic)

We deal with numerical solution of a three-dimensional phase field model of solidification in single component anisotropic materials. In this contribution, we extend the model by crystal orientation transformation. A robust algorithm is then developed to simulate the growth of multiple grains with an arbitrary number of random crystallographic orientations and a fully resolved 3D dendritic geometry. In the first part, the model and the hybrid parallel implementation of the algorithms are explained. The second part is devoted to demonstrating the effect of mesh-related numerical anisotropy, investigation of the parallel efficiency, and the simulations of complex polycrystalline solidification on very fine meshes.

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room7)

[SY-I12] Properties of β/ω phase interfaces in Ti and their implications on mechanical properties and ω morphology

○Shuo Cao[1], Qing-Miao Hu[1], Rui Yang[1], Yong Jiang[2] (1.Institute of Metal Research, Chinese Academy of Science , China, 2.Central South University, China)

The ω phase strengthens β-Ti alloys effectively as a precipitate phase but decreases the plasticity with increasing size dramatically. To understand the strengthening and embrittlement mechanism of ω phase in the β-Ti alloys, the property of the β/ω interface is demanded. In this regard, we calculated the interface energies (γ_{int}), cleavage energies (γ_{cl}), and generalized stacking faults energy surfaces of the β/ω interfaces with different orientations using a first-principles method based on density functional theory. The results indicate that the strong anisotropy of the interface energy explains the ellipsoid morphology of the ω phase with its major axis parallel to the $<111>_\beta$ direction. The calculated cleavage energies and unstable stacking fault energies γ_{us} are determined. By comparing the γ_{cl}/γ_{us} ratio of both interfaces and those of the bulk ω and β phases, we conclude that the interfaces are prone to crack initiation than the bulk and contribute to the ω-embrittlement of the β-Ti alloy.

[SY-D1] Symposium D-1
Chair: Daniel Urban(Fraunhofer IWM, Germany)
Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room8

[SY-D1] **Data-Driven Discovery of new materials**
○Isao Tanaka （Dept. Materials Science and Engineering, Kyoto Univ. , Japan）

[SY-D1] Machine Learning and Materials Discovery*
○Gus Hart （Brigham Young University, United States of America）

[SY-D1] Data-Driven Materials Design in an Industrial Environment
○Thomas Eckl, Lothar Kunz, Benedikt Ziebarth （Robert Bosch GmbH, Germany）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room8)

[SY-D1] Data-Driven Discovery of new materials
Invited

○Isao Tanaka （Dept. Materials Science and Engineering, Kyoto Univ. , Japan）

Challenges for accelerated discovery of materials with the aid of data science have been well demonstrated. One of the approaches uses materials database generated by density functional theory (DFT) calculations. A large number of DFT calculations with the accuracy comparable to experiments can be used for high throughput screening (real screening). Another approach called virtual screening uses machine-learning technique to select predictors for making a model to estimate the target property. The whole library can then be screened. Verification process is generally required to examine the predictive power of the model. Models and the quality of the screening can be improved iteratively through Bayesian optimization. The virtual screening is useful when real screening based upon the DFT data is not practical, i.e. when the computational cost for the descriptors is too high to cover the whole library within the practical time frame. This is the same if one needs to explore too large space to cover exhaustively. Discovery of new low lattice thermal conductivity crystals can be shown as an example of the application of the virtual screening technique [1]. Another approach relies only on inorganic crystal structure database (ICSD) that collects literature data obtained mostly by experiments. We have demonstrated that matrix- and tensor-based recommender systems are very powerful for discovery of currently unknown chemically relevant compositions (CRCs) of inorganic compounds from vast candidates [2]. A Tucker decomposition recommender system shows the best discovery rate of CRCs. For ternary and quaternary compositions, approximately 60 and 50 of the top 100 recommended compositions are found to be CRCs, respectively. The high discovery rate with neither DFT database nor other prior physical/chemical knowledge should be noteworthy.

[1] A. Seko et al, *Phys. Rev. Lett.* 115, 205901 **(2015)**.

[2] A. Seko et al, *Phys. Rev. Mater.* 2, 013805 **(2018)**.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room8)

[SY-D1] Machine Learning and Materials Discovery*
Invited

○Gus Hart （Brigham Young University, United States of America）

The relative accuracy and speed of density functional calculations have transformed computational materials science and enabled the creation of large databases of computed materials properties. But true "materials by design" or in-silico materials discovery has not yet been realized, though there are isolated success stories. It seems likely that into make computational discovery of new materials possible, or to discover materials engineering routes to improve already-deployed materials, a brute force approach will not be practical--- some other paradigm will be required. Machine learning, so successful in some other application areas, is an intriguing and promising idea, but there are hurdles to overcome. There are two important differences between the standard machine learning problems of image recognition, voice recognition, etc., and materials prediction. In the first instance, we cannot afford the typical accuracy tradeoff---materials predictions are not useful without meeting a high accuracy target; the energy difference of competing phases is often very small, requiring high fidelity in the models. The second difference is the amount of training data---we don't have

"big data". How do we move forward? In this talk I will review the state of the art in this emerging discipline and show some results from BYU's Materials Simulation Group efforts in this area.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room8)

[SY-D1] Data-Driven Materials Design in an Industrial Environment

○Thomas Eckl, Lothar Kunz, Benedikt Ziebarth （Robert Bosch GmbH, Germany）

We will present how a combination of an automated simulation workflow, including high-throughput DFT calculations, textmining, utilization of available data bases and machine learning can be used to design tailored materials with respect to cost efficiency and performance. We will discuss the necessary requirements from an industrial perspective and show first results in the field of battery materials and permanent magnets for electric engines. Possible extensions to go beyond the atomistic description and include the microstructure of materials are also briefly discussed.

Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D2] Symposium D-2
Chair: Tilmann Hickel(MPIE, Germany)
Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room8

[SY-D2] Using Machine-Learning to Create Predictive Material Property Models
○Chris Wolverton （Northwestern University, United States of America）

[SY-D2] Designing mesoscale structures of Li-ion battery electrode using FIB-SEM image via machine learning
○Yoichi Takagishi, Tatsuya Yamaue （Kobelco Research Institute Inc., Japan）

[SY-D2] **Stability Engineering of Halide Perovskite via Machine Learning**
○Wan-Jian YIN, Wanjian YIN （Soochow University, China）

[SY-D2] Systematic evaluation of ionization potentials of divalent cation binary oxides
○Yoyo Hinuma[1,2,3], Hiroyuki Hayashi[2,3], Yu Kumagai[4], Isao Tanaka[2,3], Fumiyasu Oba[2,5] （1.Center for Frontier Science, Chiba Univ., Japan, 2.Center for Materials Research by Information Integration, National Institute for Materials Science, Japan, 3.Department of Materials Science and Engineering, Kyoto Univ., Japan, 4.Materials Research Center for Element Strategy, Tokyo Institute of Technology, Japan, 5.Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology, Japan）

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room8)

[SY-D2] Using Machine-Learning to Create Predictive Material Property Models

Invited
○Chris Wolverton （Northwestern University, United States of America）

Rational, data-driven materials discovery has the potential to make research and development efforts far faster and cheaper. In such a paradigm, computer models trained to find patterns in massive chemical datasets would rapidly scan compositions and systematically identify attractive candidates. Here, we present several examples of our work on developing machine learning (ML) methods capable of creating predictive models using a diverse range of materials data. As input training data, we demonstrate ML on both large computational datasets of DFT calculations, as implemented in the Open Quantum Materials Database (oqmd.org), and also experimental databases of materials properties. We construct ML models using a large and chemically diverse list of attributes, which we demonstrate can be used as an effective tool to automatically learn intuitive design rules, predict diverse properties of crystalline and amorphous materials, such as formation energy, specific volume, band gap energy, and glass-forming ability, and accelerate combinatorial searches.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room8)

[SY-D2] Designing mesoscale structures of Li-ion battery electrode using FIB-SEM image via machine learning

○Yoichi Takagishi, Tatsuya Yamaue （Kobelco Research Institute Inc., Japan）

Optimizations of the mesoscale structure of Li-ion battery electrode have been demonstrated by using the advanced simulation method by single 2D slice image (Quasi-3D modeling) and machine learning. The mathematical model is based on the electrochemistry and physics model[1], and developed in order to calculate Li/Li+ concentration on the 2D plane, in consideration of virtual 3D structure. In this study, we firstly confirm the validity of the Quasi-3D model, and secondly optimize the electrode structure in mesoscale using Bayesian optimization, a method of machine learning.

In order to confirm the validity of our proposed model, full 3D discharge simulations with random packed active material particles have been performed and compared. By use of an appropriate value of "connection factor", quasi-3D model reproduce well a sliced Li/Li+ concentration calculated by the full 3D model in charge/discharge process, in addition that this model makes it possible to reduce computation time dramatically. Next, we have carried out optimizations of the mesoscale structure of the positive electrode $Li(Ni_{1/3}Mn_{1/3}Co_{1/3})O_2$ based on the actual FIB-SEM image via Bayesian optimization. As a result, statistical parameters of the optimized meso-scale structures, including the dispersion of active material size and location, remarkably differ depending on the objective functions for high rate charge/discharge performance or for long cycle performance.
1) M.Doyle et al. J. Electrochem.Soc. 1996, Vol.143, No.6, p.1890

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room8)

[SY-D2] Stability Engineering of Halide Perovskite via Machine Learning

○Wan-Jian YIN, Wanjian YIN （Soochow University, China）

Perovskite stability is of the core importance and difficulty in current research and application of perovskite solar cells. Nevertheless, over the past century, the formability and stability of perovskite still relied on simplified factor based on human knowledge, such as the commonly used tolerance factor *t*. Combining machine learning with first-principles density functional calculations, we proposed a strategy to firstly calculate the decomposition energies, considered to be closely related to thermodynamic stability, of 354 kinds halide perovskites, establish the machine learning relationship between decomposition energy and compositional ionic radius and investigate the stability of 14190 halide double perovskites. The ML-predicted results lead us to rediscover a series of stable rare earth metal halide perovskites (up to $\sim10^3$ kinds), indicating the generalization of this model and further provide elemental and concentration suggestion for improving the stability of mixed perovskite.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room8)

[SY-D2] Systematic evaluation of ionization potentials of divalent cation binary oxides

○Yoyo Hinuma[1,2,3], Hiroyuki Hayashi[2,3], Yu Kumagai[4], Isao Tanaka[2,3], Fumiyasu Oba[2,5] （1.Center for Frontier Science, Chiba Univ., Japan, 2.Center for Materials Research by Information Integration, National Institute for Materials Science, Japan, 3.Department of Materials Science and Engineering, Kyoto Univ., Japan, 4.Materials Research Center for Element Strategy, Tokyo Institute of Technology, Japan, 5.Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology, Japan）

Finding materials with suitable surface properties is unarguably important for applications including (photo)catalysis and crystal growth. Modeling of surface properties requires identification of surfaces that a given material will preferentially adopt. In a data-driven materials discovery and design approach, reasonable models of surfaces with various orientations and terminations must be obtained with minimum human intervention. Moreover, the surface energy as well as any relevant surface property, such as the ionization potential (IP), needs to be calculated systematically and results have to be stored in a database. Ultimately, reducing the number of costly first-principles calculations is desirable by using regression or some other means to estimate a certain surface property and eliminate sampling of the search space that is highly likely to have an unfavorable surface probability.

In this presentation we use first-principles calculations to systematically investigate the IPs of divalent cation binary oxides. The algorithm to make nonpolar and stoichiometric slab-and-vacuum models by Hinuma *et al*. [1] is used to construct such models. Identification of the drivers that affect the IP, which is a fundamental surface property, will be discussed. The insight obtained from this study would assist the search of descriptors that determine surface properties.

[1] Y. Hinuma, Y. Kumagai, F. Oba, I. Tanaka. Comp. Mater. Sci. **113**, 221 (2016).

[SY-D3] Symposium D-3

Chair: Daryl Chrzan(UC Berkeley, USA)
Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room8

[SY-D3] Finding the needle in the haystack: Materials discovery through high-throughput ab initio computing and data mining

○Geoffroy Hautier （Universite catholique de Louvain, Belgium）

[SY-D3] High-entropy alloys investigation using machine-learned potentials

○Tatiana Kostiuchenko, Alexander Shapeev （Dept. of Material Science and Engeneering , Skolkovo Institute of Science and Technology, Moscow, Russia）

[SY-D3] Stability evaluation of high-entropy alloys via accurate on-lattice model

○Evgenii Meshkov[1], Ivan Novoselov[1], Alexander Shapeev[2], Alexey Yanilkin[1] （1.All-Russian Research Institute of Automatics (VNIIA), Russia, 2.Skolkovo Institute of Science and Technology, Russia）

[SY-D3] Atomistically informed atomic mobility databases for continuum diffusion simulations

○Katrin Abrahams[1], Daniel Gaertner[2], Maximilian Grabowski[3], Irina Roslyakova[1], Oleg Shchyglo[1], Sergiy V. Divinski[2], Ingo Steinbach[1] （1.Scalebridging Thermodynamic and Kinetic Simulation (ICAMS), Ruhr-University Bochum, Germany, 2.Institute of Materials Physics, University of Münster, Germany, 3.Atomistic Modelling and Simulation (ICAMS), Ruhr-University Bochum, Germany）

[SY-D3] The European Materials Modelling Council: standardization, interoperability and data management tools for materials modelling

○Luca Bergamasco[1], Emanuele Ghedini[2], Gerhard Goldbeck[3], Eliodoro Chiavazzo[1], Pietro Asinari[1] （1.Politecnico di Torino, Italy, 2.Università di Bologna, Italy, 3.Goldbeck Consulting Ltd, UK）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room8)

[SY-D3] Finding the needle in the haystack: Materials discovery through high-throughput ab initio computing and data mining

Invited
○Geoffroy Hautier （Universite catholique de Louvain, Belgium）

Essential materials properties can now be assessed through ab initio methods. When coupled with the exponential rise in computational power, this predictive power provides an opportunity for large-scale computational searches for new materials. We can now screen thousands of materials by their computed properties even before the experiments. This computational paradigm allows experimentalists to focus on the most promising candidates, and enable researchers to efficiently and rapidly explores new chemical spaces.

In this talk, I will present the challenges as well as opportunities in materials discovery in high-throughput ab initio computing using examples from transparent conducting materials. I will especially highlight computational predictions which have been followed by experimental synthesis and characterization. In addition to allowing the ability to navigate through a large volume of materials data to identify promising compounds, high-throughput computing also offers unprecedented data mining opportunities to detect new relationships between chemistry, structures, and properties. I will illustrate examples of these relationships through our recent work in crystal structure descriptors and automatic local environment identification, which merge traditional solid-state chemistry and materials science concepts through modern informatics.

The impact of high-throughput computing is multiplied when the generated data is shared with free and easy access. I will finish my talk by presenting the Materials Project (http://www.materialproject.org), a collaborative project which precisely targets such a data dissemination.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room8)

[SY-D3] High-entropy alloys investigation using machine-learned potentials

○Tatiana Kostiuchenko, Alexander Shapeev （Dept. of Material Science and Engeneering , Skolkovo Institute of Science and Technology, Moscow, Russia）

High-entropy alloys (HEAs) are a class of materials promising for their potential durability and high heat-resistance. HEAs are defined as alloys consisting of at least four different components that form single-phase solid solutions due to high entropy of mixing.

It is rather difficult to find which components would form a HEA since solid solutions alloys tend to split into binary or mono-atomic alloys at low temperatures and can form metallic glasses at high temperatures. This makes it difficult to experimentally investigate HEAs. Hence there is a need in computational approaches to the design of HEAs.

In this work we propose a computational framework for predicting the temperature of the order-disorder (i.e., intermetallic-solid solution) transition for HEAs. We first construct a very computationally efficient machine-learning on-lattice model of interatomic interaction (an alternative to the cluster expansion model) [Shapeev A., 2017]. The model parameters are fitted to quantum-mechanical (DFT) data with accuracy of about

1meV/atom. Then we perform canonical Monte-Carlo simulations for b.c.c. (body-centered cubic), h.c.p. (hexagonal close-packed) and f.c.c. (face-centered cubic) lattices. We validate our results against the published works [Körmann F. et al, 2017][Huhn W.P. et al, 2013][Fernández-Caballero A. et al, 2017]. Particular approach in atomistic simulations significantly reduces calculation time, enables to increase explored atomic configurations range and preserves the accuracy level in comparison with *ab initio* calculations. In the case of successful development of the method of constructing phase diagrams using machine learning, human labor can be excluded from the routine process of studying phase diagrams. This will also reduce the computational costs consumed by conventional calculations from the first principles.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room8)

[SY-D3] Stability evaluation of high-entropy alloys via accurate on-lattice model

○Evgenii Meshkov[1], Ivan Novoselov[1], Alexander Shapeev[2], Alexey Yanilkin[1] （1.All-Russian Research Institute of Automatics (VNIIA), Russia, 2.Skolkovo Institute of Science and Technology, Russia）

High-entropy alloys (HEA) are a new promising class of metallic materials. Some of them demonstrate excellent mechanical properties at elevated temperatures, outstanding corrosion resistance, and high radiation tolerance. However, atomistic modeling of HEAs is hindered by their high chemical diversity. A novel approach is required to perform accurate and computationally feasible atomic-scale description of HEA.

In our approach, energy of the system is represented as a sum of contributions of local atomic environments. These contributions are parameterized by low-rank multidimensional tensors in order to reproduce DFT results [1]. This model is then embedded into kinetic Monte-Carlo to perform large-scale simulations. This approach gives an accurate description of alloys with a large number of elements.

We employ the proposed approach to evaluate thermodynamic stability of several multicomponent alloys, and to search for new single-phase compositions.
[1] Shapeev, A. (2017) Computational Materials Science, 139, 26-30

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room8)

[SY-D3] Atomistically informed atomic mobility databases for continuum diffusion simulations

○Katrin Abrahams[1], Daniel Gaertner[2], Maximilian Grabowski[3], Irina Roslyakova[1], Oleg Shchyglo[1], Sergiy V. Divinski[2], Ingo Steinbach[1] （1.Scalebridging Thermodynamic and Kinetic Simulation (ICAMS), Ruhr-University Bochum, Germany, 2.Institute of Materials Physics, University of Münster, Germany, 3.Atomistic Modelling and Simulation (ICAMS), Ruhr-University Bochum, Germany）

Diffusion is a key aspect for microstructural evolution and has to be solved in full-field models like the phase-field model. Many phase transformations are diffusion controlled that their kinetics depend crucially on mobilities of the diffusing elements as well as their thermodynamic factor. Both parameters, the Gibbs energies and the atomic mobilities are temperature, composition and pressure dependent. Parameters

representing these dependencies are stored in CALPHAD (CALculated PHAse Diagrams) type databases.

In this talk a new approach for the assessment of the temperature and composition dependence of the atomic mobility data using atomistic and experimental data is presented. The new model takes into account the physical meaning of three parameters on the basis of a mono-vacancy diffusion mechanism: the frequency factor, the vacancy formation energy and the migration energy. The temperature dependence is given by an Arrhenius equation, where the activation energy consists of the migration energy and the vacancy formation energy. The temperature dependence of both parameters is investigated using Kinetic Monte Carlo simulations. This information is used to deduce a general description of the temperature dependence of the activation energy based on these parameters. Additionally, the composition dependence of the pre-exponential factor and the activation energy is investigated separately using experimentally determined self-diffusion coefficients obtained from the tracer method and calculated self-diffusion coefficients based on kinetic Monte-Carlo simulations.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room8)

[SY-D3] The European Materials Modelling Council: standardization, interoperability and data management tools for materials modelling

○Luca Bergamasco[1], Emanuele Ghedini[2], Gerhard Goldbeck[3], Eliodoro Chiavazzo[1], Pietro Asinari[1]
（1.Politecnico di Torino, Italy, 2.Università di Bologna, Italy, 3.Goldbeck Consulting Ltd, UK）

The European Materials Modelling Council (EMMC) was established in 2014 as a new European network to coordinate and support the industrial uptake of materials modelling in Europe. The EMMC community consists of different types of stakeholders, namely: manufacturers (industrial end-users); software owners (academic and commercial software providers); Translators (skilled professionals able to translate industrial problems into modeling activities) and academic model developers (of electronic, atomistic, mesoscopic and continuum models). The main EMMC objectives are: to enhance the interaction and collaboration between all stakeholders; to identify materials model gaps in industry and to steer model development; to build strong foundations to ease model interoperability, integration and data management; to promote modelling in industry based on beneficial economic arguments. These activities rely on wide stakeholder consultation, with the ultimate goal to integrate materials modelling into the product life-cycle management, enhancing innovation and global competitiveness.

The aim of this talk is to present the EMMC activities, with particular regards to those related to standardization, interoperability and data management strategies for materials modelling. First, the Review of Materials Modelling (RoMM), edited by the European Commission, will be presented as the reference document for standardization. Based on this preamble, the CEN Workshop Agreement (CWA) for materials modelling terminology, the Modelling Data (MODA) sheets to document modelling in standard form, and the European Materials Modelling Ontology (EMMO) will be presented. Particular emphasis will be given to the discussion of physics-based vs data-based modelling approaches, showing how they fit into the abovementioned tools. Available results on the data-management regulation will be also shown and discussed. Finally, an outlook on how this framework will help materials discovery and design will be given.

723867

Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D4] Symposium D-4
Chair: Minoru Otani(AIST, Japan)
Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room8

[SY-D4] Exploration of large ab initio data spaces to design structural materials with superior mechanical properties
○Joerg Neugebauer, Jan Janssen, Tilmann Hickel, Blazej Gabowski （Max-Planck-Institut fuer Eisenforschung, Germany）

[SY-D4] Toward a machine learning aided interatomic potential for multi-element alloys: Application to binary compounds
○Doyl Dickel, David Francis, Christopher Barrett （Mississippi State University, United States of America）

[SY-D4] **Machine Learning potentials for modeling iradiation defects in iron and tungsten**
○Alexandra Goryaeva[1], Jean-Bernard Maillet[2], Mihai-Cosmin Marinica[1] （1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France, 2.CEA-DAM DIF, 91297 Arpajon Cedex, France）

[SY-D4] Effect of friction and ductility on relaxation dynamics and mechanical memory of crumpled materials
○Mehdi Habibi, Eric van Bruggen （Wageningen University, Netherlands）

[SY-D4] Big-data insights into solute-GB segregation
○Liam Huber, Blazej Grabowski, Joerg Neugebauer （MPIE, Germany）

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room8)

[SY-D4] Exploration of large ab initio data spaces to design structural materials with superior mechanical properties

Invited

○Joerg Neugebauer, Jan Janssen, Tilmann Hickel, Blazej Gabowski （Max-Planck-Institut fuer Eisenforschung, Germany）

Modern engineering materials have evolved from simple single phase materials to nano-composites that employ dynamic mechanisms down to the atomistic scale. The structural and thermodynamic complexity of this new generation of structural materials presents a challenge to their design since experimental trial-and-error approaches as successfully used in the past are often no longer feasible. Ab initio approaches provide perfect tools to new design routes but face serious challenges: Finite temperature free energies of the various phases are almost degenerate, requiring advanced theoretical formalisms that accurately capture all relevant entropic contributions. In addition, their hierarchical nature with respect to length and time makes it challenging to explore the large range of chemical compositions. We have therefore developed a python based framework *pyiron* that allows in a highly automated way to combine accurate finite temperature first principles calculations with big data analytics. The flexibility and the predictive power of these automated approaches will be discussed for examples ranging from the design of ductile Mg alloys to the discovery of general rules for interstitials in metals.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room8)

[SY-D4] Toward a machine learning aided interatomic potential for multi-element alloys: Application to binary compounds

○Doyl Dickel, David Francis, Christopher Barrett （Mississippi State University, United States of America）

As the chemical complexity of novel material systems continues to increase, the need for the rapid development of predictive, scalable interatomic potentials has grown as well. Machine learning, neural networks, and other data-driven techniques has shown promise in condensing large amounts of data from first principles and density functional theory calculation into classical dynamical equations with linear scaling, making them ideal for molecular dynamics simulation. A formalism for the development of a multi-species interatomic potential is presented and applied to binary metals. The resulting potential is then analyzed in terms of predictive power, validity, performance, and development time.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room8)

[SY-D4] Machine Learning potentials for modeling iradiation defects in iron and tungsten

○Alexandra Goryaeva[1], Jean-Bernard Maillet[2], Mihai-Cosmin Marinica[1] （1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France, 2.CEA-DAM DIF, 91297 Arpajon Cedex, France）

Prediction of condensed matter properties requires an accurate description of a material at the atomic scale. Ground state properties of a material are often described well within the Density Functional Theory (DFT) while studying irradiation-induced damage requires a length scale that is pushed beyond *ab initio* level of theory. Unachievable CPU cost of such calculations have fueled the search for alternatives, accounting for reasonable approximations, which has led to development of various empirical potentials, ranging from pairwise potentials to embedded atom model and tight binding. Although these potentials have been successful in making radiation damage feasible, inconsistency of the results from different potentials is a major shortcoming that hinders conclusive theoretical predictions for such important functional materials as Fe and W.

Here we present a new strategy to achieve machine learning interatomic potentials for metals that approach accuracy of DFT calculations and at the same time preserve a reasonable balance between precision and CPU cost. Targeting to model irradiation-induced defects and plasticity, the potentials are trained on the extensive DFT database that includes EOS, elastic deformation, planar defects (GSF), self-interstitial atoms (SIA), vacancies, and liquid state.
The new potentials for Fe and W are applied to investigate the complex energy landscape of defects under irradiation such as clusters of SIA. We aim to predict the relative stability of large SIA clusters up to nanometric-size, with a particular focus on to the relative stability of the conventional dislocation loops as well as the C15 clusters [1]. The present approach enables us to account for the effect of temperature [2]. Moreover, as a perspective development, the potential will be tested to reproduce high-pressure bcc-hcp transition in Fe.

[1] M.C. Marinica *et al.* (2012) *Phys Rev Lett* **108**, 025501

[2] T.D. Swinburne, M.C. Marinica (2018) *Phys Rev Lett* **120**, 135503

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room8)

[SY-D4] Effect of friction and ductility on relaxation dynamics and mechanical memory of crumpled materials

○Mehdi Habibi, Eric van Bruggen （Wageningen University, Netherlands）

Crumpled structures are ubiquitous in nature and technology. They combine low-density structures with surprising mechanical strength and the
ability to absorb mechanical energy. This combination of properties opens doors
to use them as mechanical metamaterials for a variety of applications.
However, in order to rationally design metamaterials, a thorough physical understanding of their unique features is needed. One remarkable physical property observed in crumpled structures is their slow mechanical relaxation
and their ability to carry a long lasting memory of previous mechanical states.
We experimentally investigate the role of material properties (ductility and friction) on relaxation dynamics of crumpled sheets by
comparing relaxation curves of different materials. We show that relaxation rates are not only dependent on material's elastoplastic properties, but also rely on friction and adhesion between surfaces.This is further explored by using a two-step compaction protocol, that allowed us to probe deeper into the material's relaxation behavior. We study the material dependency of the non-monotonic aging in a crumpled ball.

We show the normalized height of the non-monotonic aging peak depends
linearly on the time at which it arose with a slope that revealed a material property that
seemed to be correlated with the material dependent relaxation constant.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room8)

[SY-D4] Big-data insights into solute-GB segregation

○Liam Huber, Blazej Grabowski, Joerg Neugebauer （MPIE, Germany）

Solute-grain boundary (GB) interaction plays a critical role in the evolution and stabilization of grain structure and thus strongly impacts final material properties. Due to the large number of possible grain boundary configurations, there are a many inequivalent sites solutes can be incorporated at. Combined with the fact that there are many possible segregating chemical species in modern alloys, concepts to derive general trends in segregation are still missing. Using classical molecular statics, we perform high-throughput calculations of 1.4 million segregation energies for six solutes to 38 different boundaries in Al. The size of this data set is sufficient to apply machine learning techniques for building predictive models capable of predicting segregation energy to new GBs. It also provides useful insights into trends in the atomistic mechanisms controlling segregation behaviour. We show that the resulting segregation energy distributions can be interpreted analogously to electronic density of states and provides a useful perspective to consider solute concentration enrichment at the GB and GB embrittlement.

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H7] Symposium H-7

Chair: Patrick R. Onck(Univ. of Groningen, Netherlands)
Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room9

[SY-H7] Computational modeling approach for the rational design of DNA nanostructures

○Do-Nyun Kim, Jae Young Lee, Jae Gyung Lee, Young-Joo Kim, Kyung Soo Kim, Chanseok Lee （Department of Mechanical and Aerospace Engineering, Seoul National University, Korea）

[SY-H7] Quantitative Multiscale Modelling of Bionano Interface

○Vladimir Lobaskin[1], Stefano Poggio[1], David Power[1], Hender Lopez[2] （1.School of Physics, University College Dublin, Ireland, 2.Institute Laue-Langevin, Grenoble, France）

[SY-H7] Multiscale modelling of intrinsically-disordered proteins

Ankur Mishra, Henry De Vries, Hamid Jafarinia, Erik Van der Giessen, ○Patrick R. Onck （University of Groningen, Netherlands）

[SY-H7] Tracing the interplay of polymer topology and hydrodynamics

○Lisa B. Weiss[1], Arash Nikoubashman[2], Christos N. Likos[1] （1.University of Vienna, Austria, 2.Johannes Gutenberg University Mainz, Germany）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room9)

[SY-H7] Computational modeling approach for the rational design of DNA nanostructures

Invited
○Do-Nyun Kim, Jae Young Lee, Jae Gyung Lee, Young-Joo Kim, Kyung Soo Kim, Chanseok Lee （Department of Mechanical and Aerospace Engineering, Seoul National University, Korea）

Structural DNA nanotechnology has recently been advanced significantly enabling the construction of nanometer-scale structures with controllable three-dimensional shapes and properties. While overall mechanical properties of single and double DNA helices have been relatively well characterized both experimentally and computationally, those of various DNA motifs essential to build a DNA bundle structure are still hardly known due to experimental limits despite their importance for the rational design of DNA nanostructures. In this presentation, we introduce our computational modeling approach to establishing an efficient design process in order to achieve fine control over the geometrical shape and mechanical properties of self-assembling DNA nanostructures. Molecular dynamics simulations are highly utilized to extract the unknown mechanical properties of local DNA motifs that are fed into a more coarse-grained DNA model built on the finite element method. Then, this finite-element-based model of DNA nanostructure is used to predict its three-dimensional shape and mechanical properties, which provides designers structural feedback as quick as possible offering a chance to revise the design before actual synthesis. We expect our multiscale analysis framework facilitates the rational design of DNA nanostructures with a target shape and mechanical (or other derived) properties with precision.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room9)

[SY-H7] Quantitative Multiscale Modelling of Bionano Interface

○Vladimir Lobaskin[1], Stefano Poggio[1], David Power[1], Hender Lopez[2] （1.School of Physics, University College Dublin, Ireland, 2.Institute Laue-Langevin, Grenoble, France）

In biomedical and food technologies, the functionality of the engineered materials and potential hazards are triggered and controlled by molecular-level interactions at the biointerface, a nanoscale layer where biological fluids meet the foreign substances. The main concerns are related but not limited to the emerging risks for human health. The questions of biocompatibility of materials arise naturally in respect to medical appliances such as stents, dental and cardiac implants, or prosthetic joints as they can cause immediate hazard upon introduction into the human body. These interactions are often non-specific and unintended. Quantitative understanding of biointerface structure is therefore crucial for achieving a better control over the surface activity biomaterials and reducing the associated health risks.

In this work, we propose a systematic multiscale bottom-up method to coarse-grain the interactions of foreign materials with biological fluids of arbitrary composition. Biomolecules (lipids, proteins and carbohydrates) are coarse-grained by mapping their main chemical fragments onto single beads, and their interaction with the substrate surface is characterised by potentials of mean force (PMF) from atomistic

simulations [1]. The substrate is represented by a two-layer model where the surface interacts with the molecule beads via those PMFs, while the core interacts with via van der Waals forces calculated using Lifshitz theory. The united-atom model for biomaterial-biomolecule segment interaction is used to evaluate the adsorption free energy of arbitrary biomolecules on a specified foreign surface. This mesoscale representation is used to build a united-block model, which can address competitive adsorption of entire proteins and lipids onto the adsorbent and predict the content of biomolecular corona.

The main outcome of our work is a framework for comparative characterisation of nano- and biomaterials in terms of descriptors of bionano interface such as protein binding affinity and content of the corona, which forms a basis for construction of nanoinformatic data-driven models for predicting material functionality.

[1] H. Lopez, V. Lobaskin, J. Chem. Phys. 143, 243138 (2015)

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room9)

[SY-H7] Multiscale modelling of intrinsically-disordered proteins

Ankur Mishra, Henry De Vries, Hamid Jafarinia, Erik Van der Giessen, ○Patrick R. Onck （University of Groningen, Netherlands）

Proteins are often called the work-horse molecules of life because they are involved in almost any structure and activity in living systems. It has long been thought that proteins inherit their function from the secondary and tertiary structure in which they are folded. However, more and more evidence is appearing that show that also unfolded, intrinsically-disordered proteins (IDPs) play an important biological role, in both health and disease. In this work we focus on two of these biological roles, i.e., (i) in mediating transport through the nuclear pore complex (NPC) and (ii) in the formation of pathological protein aggregates in neurodegenerative diseases. IDPs are long chains of amino acids with conformations that are primarily dictated by the non-covalent interactions between the individual amino acids. Due to the large size of the protein complexes of interest, high-resolution (all-atom) molecular-dynamics simulations are restricted to study only a few IDPs. Here, we use a coarse-grained, one-bead-per-amino-acid model that is fine enough to capture the exact amino-acid sequence, but coarse enough to account for the collective interaction of hundreds of IDPs. In this presentation, recent results are presented on the collective behavior of IDPs in forming the selective permeability barrier of the NPC and on the phase-separation of pathological IDPs in the neurodegenerative disease ALS. For both studies the relation between amino-acid sequence and collective/aggregation behavior will be emphasized and discussed.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room9)

[SY-H7] Tracing the interplay of polymer topology and hydrodynamics

○Lisa B. Weiss[1], Arash Nikoubashman[2], Christos N. Likos[1] （1.University of Vienna, Austria, 2.Johannes Gutenberg University Mainz, Germany）

Polymers exhibit a variety of topologies ranging from linear to cyclic and various knot types, which are of importance in biology, rheology and material science. Macromolecules of distinct topology consist of the same type and number of monomers making it challenging to separate them using chemical approaches. Nevertheless, topology influences strongly their response to flow fields in concentrated [1] and dilute solutions [2]. Exploiting these differences for future separation strategies requires a detailed understanding of the interplay of hydrodynamic interactions and topology. Due to the inherent separation of time scales of macromolecules and solvent, here the Multi-Particle Collision Dynamics algorithm is employed to couple an explicit coarse-grained solvent to polymers treated with Molecular Dynamics.

We investigated the transport of topologically-distinct polymers in microfluidic slit channels. We find that in bare channels and in dilute solutions there is only minor difference in the migration behavior, which is not sufficient for separation. In contrast, decorating the channel walls with attractive spots arranged on a track parallel to the flow results in a reliable and novel strategy for separation of linear and ring polymers that takes full advantage of the different topologies [3]. Those spots effectively capture and immobilize linear chains, while forcing ring polymers to change their preferred orientation close to the walls. In doing so, ring polymers are enabled to roll along the spots with a finite velocity. Furthermore, investigation of the migration in semi-dilute linear and ring polymer mixtures exhibits an astonishing difference. Finally, we extend our studies to knotted polymers to construct knot-sensitive filters.

References

[1] Kapnistos, M.; Lang, M.; Vlassopoulos, D.; Pyckhout-Hintzen, W.; Richter, D.; Cho, D.; Chang, T.; Rubinstein, M. Nat. Mater. 2008, 7, 997-1002.
[2] Hsiao, K.-W. W.; Schroeder, C. M.; Sing, C. E. Macromolecules 2016, 49, 1961-1971.
[3] Weiss, L. B.; Nikoubashman, A.; Likos, C. N. ACS Macro Letters 2017, 6, 1426-1431.

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H8] Symposium H-8

Chair: Patrick R. Onck(Univ. of Groningen, Netherlands)

Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room9

[SY-H8] Modeling and Simulation of DNA Foldback Intercoil Structure

○Moon Ki Kim, Byung Ho Lee, Soojin Jo （School of Mechanical Engineering, Sungkyunkwan University, Korea）

[SY-H8] DNA-particle vitrimer systems

○francesco sciortino （Sapienza Universita' di Roma, Italy）

[SY-H8] Relation between Macroscopic Flows in a Contraction-Expansion Channel and Dynamics of Well-Entangled Polymer Chains

○Takeshi Sato, Takashi Taniguchi （Dept. of Chemical Engineering, Kyoto Univ., Japan）

[SY-H8] Origin of large scale spatial organization of DNA-polymer in bacterial chromosomes.

○Apratim Chatterji[1], Tejal Agarwal[2], Manjunath G.P.[3], Farhat Habib[4] （1.IISER-Pune, India 411008, India, 2.IISER-Pune, India, 411008, India, 3.NYU, USA, United States of America, 4.Inmobi, Bangalore, India 560103., India）

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room9)

[SY-H8] Modeling and Simulation of DNA Foldback Intercoil Structure

Invited

○Moon Ki Kim, Byung Ho Lee, Soojin Jo （School of Mechanical Engineering, Sungkyunkwan University, Korea）

The stem-loop foldback intercoil (FBI) DNA is one of unique four-stranded DNA structures. Its intercoil stem region is constructed by interwinding DNA duplexes in their major groove. Although the FBI DNA is closely related with DNA homologous recombination, inversion, and deletion process, its structural and dynamic characteristics have not been yet revealed. In this study, we create a 3D FBI computer model based on homologous and palindromic DNA base sequences and its structural validity is confirmed by a variety of topological comparison with B-DNA including its diameter and helicity such as 22 angstrom and 10.5 base pairs per turn, respectively. Then, its dynamic features are investigated by normal mode analysis (NMA). NMA results show that the stem part has more rigidity compared to the other parts during the major bending and twisting motions. It is also cross-validated by the AFM experiment in which the height different of stem part is apparently measured. In addition, the DNA homologous recombination phenomenon is observed by using molecular dynamics simulation (MD) in atomic details. MD results imply that homologous recombination of the DNA FBI structure is triggered by base flipping of the stem region resulting in B-Z DNA junctions at the interface between stem and loop. Consequently, this computational modelling and simulation study enables us to better understand both structural and biological features of the FBI DNA.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room9)

[SY-H8] DNA-particle vitrimer systems

○francesco sciortino （Sapienza Universita' di Roma, Italy）

Vitrimers are a new class of polymeric materials in which the network nodes, despite the covalent bonding, can change their bonded partners via reversible exchange reactions with unreacted sites. The ability to dynamically rearrange the network structure and the external control (for example, via temperature) of the rate of exchange opens up the possibility to spontaneously heal internal fractures, recycle the material shape, and release applied stresses.

Along the lines of using DNA as a material, we have proposed an innovative design of a vitrimer system entirely made of DNA sequences [1]. In this DNA gel, bonds can switch without breaking, providing a mechanism for changing the network structure under an external driving force, retaining at all times the same number of bonds. To implement the bond switching mechanism, we use toehold-mediated displacement, one of the basic processes underlying dynamic DNA nanotechnology.

Beside discussing how a DNA vitrimer can be designed in silico and in the lab, I will discuss some other examples of particle vitrimer systems[2] in which the bond-swithching dynamics is modeled numerically with a three-body potential[3]. Preliminay application of this method show how the self and collective dynamics of these particles sensitively depend on microscopic swaps. Finally, I will discuss the origin of the observed non-dispersive (in wavevector) collective relaxation mode[4].

[1]Flavio Romano and Francesco Sciortino
Switching Bonds in a DNA Gel: An All-DNA Vitrimer

Phys. Rev. Letts. 114, 078104 (2015)

[2] Lorenzo Rovigatti, Giovanni Nava, Tommaso Bellini and Francesco Sciortino
Self-Dynamics and Collective Swap-Driven Dynamics in a Particle Model for Vitrimers
Macromolecules, 51 ,1232-1241 (2018).

[3] Francesco Sciortino, *Three-body potential for simulating bond swaps in molecular dynamics*
Eur. Phys. J. E (2017) 40: 3 DOI 10.1140/epje/i2017-11496-5

[4] Giovanni Nava, Marina Rossi, Silvia Biffi, Francesco Sciortino, and Tommaso Bellini
Fluctuating Elasticity Mode in Transient Molecular Networks
Phys. Rev. Lett. 119, 078002 (2017).

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room9)

[SY-H8] Relation between Macroscopic Flows in a Contraction-Expansion Channel and Dynamics of Well-Entangled Polymer Chains

○Takeshi Sato, Takashi Taniguchi （Dept. of Chemical Engineering, Kyoto Univ., Japan）

We have successfully applied a multiscale simulation (MSS) method [T. Murashima and T. Taniguchi, *Europhys. Lett.*, **96**, 18002 (2011)] to flows of a monodispersed linear entangled polymer melt in a contraction-expansion channel. In our MSS method, a macroscopic model based on the Lagrangian picture is coupled with a microscopic polymer model through the velocity gradient tensor and the stress tensor. The smoothed particle hydrodynamics (SPH) method is employed as the macroscopic model, and the slip-link model [M. Doi and J. Takimoto, *Phil. Trans. R. Soc. Lond A*, **361**, 641 (2003)] is employed as the microscopic model. Two-dimensional flows of a well-entangled polymer melt in a 4:1:4 contraction-expansion channel are examined using our MSS method. From our MSSs, we have investigated both macroscopic and microscopic information. As for the macroscopic information, we have focused on the spatial-dependent Weissenberg number (Wi). As for the microscopic information, we have evaluated the local orientation of polymer chains, the spatial distribution of the average number of entanglements and the number density of entanglements along a polymer chain. The states of the polymer chains are altered mainly in the region corresponding to Wi >1. In this region, we have confirmed that the polymer chains are strongly oriented, the average number of entanglements decreases and the number density of entanglements decreases in the center part on the polymer chain and has peaks near the tails. Furthermore, we have examined the number density of entanglements along a polymer chain in detail. From an analysis of the number density of entanglements, we have found that an effective advection and a hooking event play an important role in forming the number density of entanglements. Microscopic information obtained by our MSSs will provide us with new insights for the molecular design of a polymer chain.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room9)

[SY-H8] Origin of large scale spatial organization of DNA-polymer in

bacterial chromosomes.

○Apratim Chatterji[1], Tejal Agarwal[2], Manjunath G.P.[3], Farhat Habib[4] （1.IISER-Pune, India 411008, India, 2.IISER-Pune, India, 411008, India, 3.NYU, USA, United States of America, 4.Inmobi, Bangalore, India 560103., India）

Using data from contact maps of the DNA-polymer of bacteria E. Coli (at kilo base pair resolution) as an input to our model, we introduce cross-links between monomers in a bead-spring model of a flexible ring polymer at very specific points along the chain. By suitable Monte Carlo Simulations we show that the presence of these cross-links lead to a specific architecture and organization of the chain at large (micron) length scales of the DNA. We also investigate the structure of a ring polymer with an equal number of cross-links at random positions along the chain. We find that though the polymer does get organized at the large length scales, the nature of organization is quite different from the organization observed with cross links at specific biologically determined positions. We used the contact map of E. Coli bacteria which has around 4642 kilo base pairs in a single chromosome. In our coarse grained flexible ring polymer model we used 4642 monomer beads and observe that around 82 cross links are enough to induce large scale organization of the molecule accounting for statistical fluctuations induced by thermal energy. The length of a DNA chain of a even simple bacterial cell such as E. Coli is much longer than typical proteins, hence we avoided methods used to tackle protein folding problems. We define new suitable quantities to identify large scale structure of a polymer chain with a few cross-links. We have carried out similar studies with the DNA-bacteria of C.Crecentus with cross-links at specific points relevant to the DNA of C.Crecentus, and obtain identical conclusions. This assures us about the robustness of our results.

Published in :
1. Tejal Agarwal *et al J. Phys.: Condens. Matter* **30** 034003 (2018).
2. Tejal Agarwal, Tejal Agarwal *et al EPL* **121** 18004 (2018).

[SY-H9] Symposium H-9

Chair: Kees Storm(Eindhoven University of Technology, Netherlands)
Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room9

[SY-H9] Micromechanics and instabilities in soft composite materials

○Stephan Rudykh （University of Wisconsin - Madison, United States of America）

[SY-H9] Deformation analysis of UV curing 3d printed materials by combined molecular dynamics-finite element method

Jiwon Jung, Chanwook Park, ○Gunjin Yun （Seoul National University, Korea）

[SY-H9] Modelling and 3D Printing Kelvin Cell Acoustic Metamaterial

○Huina MAO[1], Peter Göransson[1], John Kennedy[2], Henry Rice[2], Umberto Iemma[3] （1.Dept. of Aeronautical and Vehicle Engineering, KTH Royal Institute of Technology, Sweden, 2.Dept. of Mechanical and Manufacturing Engineering, Trinity College Dublin, Ireland, 3.Engineering Department, Roma Tre University, Italy）

[SY-H9] Theoretical approach for EUV resist fabrication: DFT-MD-FDM study

○Muyoung Kim[1], Junghwan Moon[1], Joonmyung Choi[3], Sungwoo Park[1], Byunghoon Lee[3], Changyoung Jeong[3], Maenghyo Cho[2,1] （1.Divison of Multiscale Mechanical Design, School of Mechanical and Aerospace Engineering, Seoul National University, Korea, 2.Institute of Advanced Machines and Design, Seoul National University, Korea, 3.SAMSUNG ELECTRONICS CO., LTD, Korea）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room9)

[SY-H9] Micromechanics and instabilities in soft composite materials

Invited

○Stephan Rudykh （University of Wisconsin - Madison, United States of America）

Soft microstructured materials enable modifications of material properties and functionalities through applied deformations, or other external stimuli, for example, electric, or magnetic fields [1]. The deformation induced tunability is mainly due to controllable changes of the microstructural arrangements, on par with material nonlinearities [2]. Moreover, the microstructures can be designed to be prone to elastic instabilities giving rise to dramatic microstructure transformations, and switchable functionalities such as cancelling certain frequency ranges of elastic waves (through induced band gaps). In the presentation, we will show our numerical and theoretical results for multiphase deformable composite materials including deformable layered materials, bio-inspired nacre-like structures [3], periodic 3D fibre composites, and periodically structured particulate materials. These numerical and theoretical results will be illustrated by the experimental observations on 3D printed multiphase composites subjected to finite deformations. Finally, the ways of material properties modifications via application of external magnetic and electric fields will be explored. In particular, magnetorheological elastomers (MRE) [1] and soft dielectric elastomers (DE) with periodic microstructures will be examined, and the coupled magneto- and electro-mechanical stability of these active architectured materials will be analysed.

References

[1] Goshkoderia, A., Rudykh, S. 2017. Stability of magnetoactive composites with periodic microstructures undergoing finite strains in the presence of a magnetic field. *Composites Part B* **128**: 19-29.

[2] Galich, P.I., Fang, N.X., Boyce, M.C., Rudykh, S. 2017. Elastic wave propagation in finitely deformed layered materials. *Journal of the Mechanics and Physics of Solids* **98**, 390-410.

[3] Slesarenko, V., Kazarinov, N., Rudykh, S. 2017. Distinct failure modes in bio-inspired 3D-printed staggered composites under non-aligned loading. *Smart Materials and Structures* **26**, 035053.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room9)

[SY-H9] Deformation analysis of UV curing 3d printed materials by combined molecular dynamics-finite element method

Jiwon Jung, Chanwook Park, ○Gunjin Yun （Seoul National University, Korea）

3d printing technology with UV cured polymer has been applied to diverse industrial areas since it has advantages of reducing time and costs for producing complex structures. Especially in aerospace industries where parts with complex geometries are needed, 3d printing is said to be a suitable manufacturing technique for such elaborate components. However, there has been little research on the polymerization-induced deformation such as microscopic porosity and cure shrinkage strain in the 3d printing technology to our knowledge.

In this work, molecular dynamics (MD) simulation is adopted for modeling UV induced polymerization process to derive cure shrinkage strain. Based on the finite element method, the strain of the polymer from MD simulation is then applied to the structure modeled by Abaqus software, to predict macroscopic deformation. This prediction methodology is verified with experiment results observed from deformation of 3d printed structures in reality.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room9)

[SY-H9] Modelling and 3D Printing Kelvin Cell Acoustic Metamaterial

○Huina MAO[1], Peter Göransson[1], John Kennedy[2], Henry Rice[2], Umberto Iemma[3] （1.Dept. of Aeronautical and Vehicle Engineering, KTH Royal Institute of Technology, Sweden, 2.Dept. of Mechanical and Manufacturing Engineering, Trinity College Dublin, Ireland, 3.Engineering Department, Roma Tre University, Italy）

Anisotropic metamaterial properties could be reached from design geometric structures. It can consist of functionality unit cells including microscale complex geometries to control the wave propagation. Structures based on regular Kelvin cells were selected and aims for design innovative devices to mitigate the civil aviation noise.

Inspired by the ultrahigh resolution 3D printer technology, manually controlled cell geometry would be possible. Polymer material was used in 3D printer. Samples with 0.1 mm diameter beam element kelvin cell model was printed in our lab and shows certain acoustic properties to reduce noise.

To understand the fully anisotropic metamaterial behavior, inverse estimation method was applied to get the 21 stiffness parameters in Hooke's matrix. Optimization method was developed to design Kelvin cell structure to target noise reduction functions. It consists in numerically fitting a solid anisotropic model on a set of transfer functions extracted from Kelvin model. The estimated stiffness matrix is updated after each iteration until converge to an optimal solution. Feedbacks from modelling were used to control the geometry and material parameters in design. It would also be used to investigate modified noise scattering patterns in acoustic metamaterial. 3D printed samples would also be tested in wind tunnel to verify the numerical analysis.

Additional sub-elements, e.g., polymer microparticles could also be imbedded in the cells to increase viscous/damping loss and widen frequency bands. The frequency band could be adjusted according to the application by changing the geometry. Most of the sound could be decreased in the selected frequencies. If titanium was used in 3D printer, the cell size of the metamaterial would be much smaller that would increase acoustic properties too. The sound absorbing capacity of the titanium metamaterials, together with their strength and weather resistance, would also make them attractive candidates in noise and vibration control of aircrafts.

This work is a part of European project AERIALIST (AdvancEd aiRcraft-noIse-AlLeviation devIceS using meTamaterials), which aims at the disclosure of the potential of metamaterials to envisage innovative devices for the mitigation of the civil aviation noise (https://www.aerialist-project.eu).

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room9)

[SY-H9] Theoretical approach for EUV resist fabrication: DFT-MD-FDM study

○Muyoung Kim[1], Junghwan Moon[1], Joonmyung Choi[3], Sungwoo Park[1], Byunghoon Lee[3], Changyoung Jeong[3], Maenghyo Cho[2,1] (1.Divison of Multiscale Mechanical Design, School of Mechanical and Aerospace Engineering, Seoul National University, Korea, 2.Institute of Advanced Machines and Design, Seoul National University, Korea, 3.SAMSUNG ELECTRONICS CO., LTD, Korea）

Size of wafer has been reduced for improving performance and productivity in semiconductor manufacturing industry, and Extreme Ultraviolet (EUV) light source is state of the art strategy to achieve the goal. Fabrication of photoresist pattern is one of the main procedures in EUV lithography, and critical problems (pattern bridging or pinching) deteriorate as downsizing its size. Even though experimental- and theoretical approaches have been reported to provide physical mechanism and solution of performance degradation, technical huddles originating from complex photochemistry (chemical reaction by electron attachment or diffusion of reactant) hinder the rigorous investigation. From this point of view, we constructed multiscale model having sequential theoretical framework of density functional theory (DFT)-molecular dynamics (MD)-finite difference method (FDM). Our newly-developed model provides full description of photo-triggered chemical reaction (acid activation by electron attachment and acid diffusion-deprotection evolution) and also quantification of sub-10 nm photoresist morphology in atomistic level. This achievement will be the cornerstone of theoretical research which facilitates fundamental understanding on important factors for EUV performance and rational design of the next-generation PR.

[SY-H10] Symposium H-10

Chair: Kees Storm(Eindhoven University of Technology, Netherlands)
Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room9

[SY-H10] In silico design of self-assembly nanostructured polymer systems by multiscale molecular modelling

○Maurizio Fermeglia （University of Trieste , Italy）

[SY-H10] Dynamical properties of suspensions of star block-copolymers in shear flow.

○Diego Felipe Jaramillo - Cano[1], Manuel Camargo[2], Christos N. Likos[1] （1.Faculty of Physics, University of Vienna, Austria, 2.CICBA, Universidad Antonio Nariño - Campus Farallones, Colombia）

[SY-H10] Heterogeneous flow and internal friction in amorphous carbon

○Richard Jana[1], Lars Pastewka[1], Daniele Savio[2], Volker L Dehringer[3], Gábor Csányi[3], Julian von Lautz[2], Michael Moseler[2], Peter Gumbsch[2,4] （1.Albert Ludwigs Universitaet Freiburg, Germany, 2.Fraunhofer-Institut für Werkstoffmechanik IWM, Germany, 3.University of Cambridge, UK, 4.Institue for Applied Materials, Karlsruhe Institute of Technology, Germany）

[SY-H10] **Increasing the thermal conductivity of polymer nanocomposites filled with carbon nanotubes via molecular dynamics simulation**

○Yangyang Gao[1], Liqun Zhang[1], Florian Müller-Plathe[2] （1.Beijing University of Chemical Technology, China, 2.Technische Universität Darmstadt, Germany）

[SY-H10] **Thermal transport in polymer-based nanocomposite materials across multiple scales**

Rajat Srivastava, ○Matteo Fasano, Shahin Mohammadnejad, Hernan Chavez Thielemann, Eliodoro Chiavazzo, Pietro Asinari （Energy Department, Politecnico di Torino, Italy）

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room9)

[SY-H10] In silico design of self-assembly nanostructured polymer systems by multiscale molecular modelling

Invited

○Maurizio Fermeglia （University of Trieste , Italy）

One of the major goals of computational material science is the rapid and accurate prediction of properties of new materials. In order to develop new materials and compositions with designed new properties, it is essential that these properties can be predicted before preparation, processing, and characterization. Despite the tremendous advances made in the modeling of structural, thermal, mechanical and transport properties of materials at the macroscopic level (finite element (FE) analysis of complicated structures), there remains a tremendous uncertainty about how to predict many critical properties related to performance, which strongly depends on nanostructure. It is then essential analyze the structure at molecular level, with all the chemical and physical implication. Currently, atomistic level simulations such as molecular dynamics (MD) or Monte Carlo (MC) techniques allows to predict the structure and properties for systems of considerably large number of atoms and time scales of the order of microseconds. Although this can lead to many relevant results in material design, many critical issues in materials design still require time and length scales far too large for practical MD/MC simulations. This requires developing techniques useful to design engineers, by incorporating the methods and results of the lower scales (e.g., MD) to mesoscale simulations. In this work, we present applications of multiscale modeling procedures for predicting macroscopic properties strongly depending of interactions at nanoscale scale. Several different polymer systems of interest in the area of materials sciences and life sciences will be considered. including (i) functionalized nanoparticles in nanostructured polymer matrices (localization of gold nanoparticles in di-block copolymers and selective placement of magnetic nanoparticles in diblock copolymer films, (ii) functionalized nanoparticles in un structured polymer matrices (effect of chain length and grafting density) and (iii) self-assembly organization for biomedical applications (on nanoparticles and multivalent self-assembly building blocks in nanoparticles.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room9)

[SY-H10] Dynamical properties of suspensions of star block-copolymers in shear flow.

○Diego Felipe Jaramillo - Cano[1], Manuel Camargo[2], Christos N. Likos[1] （1.Faculty of Physics, University of Vienna, Austria, 2.CICBA, Universidad Antonio Nariño - Campus Farallones, Colombia）

Star block-copolymers (SBCs) are versatile building blocks with specific softness, functionalization, shape, and flexibility. They self-organize into a large variety of soft patchy nanoparticles, whose conformations and patchiness can be tuned and modified by different chemical-physical parameters. The static equilibrium properties of concentrated suspensions of SBCs have been an object of several studies because of the rich variety of assembly scenarios that can be achieved. In this work, we took a step forward in the study of non-equilibrium properties of suspensions of SBCs. By means of a particle-based, multiscale simulation approach, which combines standard molecular dynamics (MD) for the star monomers and multiparticle collision dynamics (MPCD) for the solvent particles, we investigated the behavior of dilute suspensions of SBCs under lineal shear flow for a wide range of parameters of the system; the latter include the functionality, the polymerization degree and the amphiphilicity degree of the star, the monomer packing fraction, the solvent

quality, and the shear rate. Our analysis focus on the dynamical behavior of the at-equilibrium-formed network structures as a consequence of the patches reorganization induced by the shear flow. The obtained results have interesting implications on the system's rheological properties and viscoelastic responses in dilute bulk phases because the SBCs are able to form a variety of different intermolecular transient bonds involving rather weak ones between individual arms and much stronger ones between multiarm patches.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room9)

[SY-H10] Heterogeneous flow and internal friction in amorphous carbon

○Richard Jana[1], Lars Pastewka[1], Daniele Savio[2], Volker L Dehringer[3], Gábor Csányi[3], Julian von Lautz[2], Michael Moseler[2], Peter Gumbsch[2,4]   (1.Albert Ludwigs Universitaet Freiburg, Germany, 2.Fraunhofer-Institut für Werkstoffmechanik IWM, Germany, 3.University of Cambridge, UK, 4.Institue for Applied Materials, Karlsruhe Institute of Technology, Germany)

We use molecular dynamics simulations to probe the plastic response of representative bulk volumes of amorphous carbon at densities from 2.0 g cm^{-3} to 3.3 g cm^{-3} in simple and biaxial shear. We compare multiple interatomic potential expressions, in particular classical empirical bond-order potentials (screened Tersoff and REBO2), the modified embedded atom method (MEAM) and machine learning approaches, in particular the Gaussian approximation potential (GAP). After an initial elastic response, the samples yield without any strain hardening or softening. Individual plastic events are strikingly similar to those observed for bulk metallic glasses: Like in other amorphous materials, we find that plasticity is carried by fundamental rearrangements of regions of ˜100 atoms, the shear transformation zone. We find that STZs coalesce to forms a shear band and that the relationship between stress and pressure during flow is well described by a Drucker-Prager law. Amorphous carbon is a prototypical single-component network material and its pair distribution function vanishes between first and second neighbor. This allows definition of an unambiguous nearest neighbor relationship and a mean coordination number. Stress correlates well with mean coordination, suggesting a simple constitutive model for this material. This relationship breaks down at low coordination numbers. We explain this with Thorpe's constraint counting theory, which predicts that networks become floppy below a certain value of mean coordination.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room9)

[SY-H10] Increasing the thermal conductivity of polymer nanocomposites filled with carbon nanotubes via molecular dynamics simulation

○Yangyang Gao[1], Liqun Zhang[1], Florian Müller-Plathe[2]   (1.Beijing University of Chemical Technology, China, 2.Technische Universität Darmstadt, Germany)

It is very important to improve the thermal conductivity of polymer nanocomposites (PNCs) to widen their application. In this work, by employing reverse nonequilibrium molecular dynamics simulations in a full atomistic resolution, we systematically investigated the effect of the chemical grafting of carbon nanotube (CNT) on the thermal conductivity of PNCs. First, the interfacial thermal conductivity is proportional to the grafting density, while it first increases and then saturates with the grafting length. Meanwhile, the intrinsic in-plane thermal conductivity of CNT drops sharply as the grafting density increases. Combined with effective

medium approximation, the maximum overall thermal conductivity of PNCs appears at an intermediate grafting density because of these two competing effects. In addition, two empirical formulas are suggested, which quantitatively account for the effects of grafting length and density on the interfacial and parallel thermal conductivity. Secondly, the thermal resistance between the CNTs gradually decreases with the increase of the grafting density and grafting length, which can be well described by an empirical equation. The heat transfer process from one CNT to another can be well described by a thermal circuit model between the CNTs. Thirdly, a stronger enhancement of the thermal conductivity is realized when chains are grafted at the end atoms of CNTs. Under deformation, the orientation of both the chains and the CNTs improves the thermal conductivity parallel to the tensile direction, but reduces the thermal conductivity perpendicular to it. We have quantified the contribution of the polymer alignment and the CNT alignment to the anisotropy of thermal conductivity. In general, computer simulation is shown to have the capability to obtain some fundamental understanding of PNCs, in hopes of providing some design principles for fabricating high performance PNCs.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room9)

[SY-H10] Thermal transport in polymer-based nanocomposite materials across multiple scales

Rajat Srivastava, ○Matteo Fasano, Shahin Mohammadnejad, Hernan Chavez Thielemann, Eliodoro Chiavazzo, Pietro Asinari （Energy Department, Politecnico di Torino, Italy）

The improved physical properties of composite materials are revolutionizing many fields, from automotive to biomedical industries, from electronics to space applications. Composites are typically made of polymeric matrices reinforced with macroscopic fillers, e.g. carbon fibres. Nowadays, scientists are investigating the possibility of introducing nanostructured fillers as wells, to further enhance the effective properties of composites. Carbon nanostructures such as carbon nanotubes or graphene are particularly suitable for that, because of their outstanding mechanical, electrical and thermal properties. However, the resulting nanocomposites are characterised by properties at scales spanning from nano to macro and, therefore, should be simulated by sophisticated multi-scale approaches.

In this work, an original multi-scale approach to the thermal transport in polymer-based materials reinforced with carbon nanotubes or graphene sheets is presented and experimentally validated. First, molecular dynamics simulations are adopted to compute the thermal boundary resistance at the polymer-nanofiller and nanofiller-nanofiller interfaces, according to the different structural and chemical characteristics of the nanocomposite. The thermal conductivities of nanofillers and polymer matrix are computed as well, with molecular precision. Second, these nanoscale transport properties are used to estimate the effective thermal conductivity of nanocomposite, thanks to a mesoscopic simulation approach based on Dijkstra algorithm. The accuracy of the code is verified against a finite element model. After that, sensitivity analyses are carried out to investigate the impact of different fillers on the effective thermal conductivity of nanocomposite. Modelling results are then validated by experiments, and the most severe bottlenecks in the thermal conductivity enhancement of nanocomposites are finally identified.

Our work provides guidelines towards the technical-economical optimization of novel nanostructured materials with tunable thermal properties, with the aim to transfer them from lab experiments to industrial exploitation.

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B5] Symposium B-5
Chair: Jean-Paul Crocombette(CEA, Univ. Paris-Saclay, France)
Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room10

[SY-B5] He impurities in boron carbide : structure, kinetics, and Raman signatures
○Guido Roma, Kevin Gillet, Anton Schneider, Jean-Paul Crocombette （CEA, Univ. Paris-Saclay, France）

[SY-B5] Irradiation damage in nuclear graphite at the atomic scale
○Alain Chartier[1], Laurent Van Brutzel[1], Justin Pageot[2] （1.DEN, Service de la Corrosion et du Comportement des Materiaux dans leur Environment, CEA Saclay, France, 2.DEN, Service d'Etudes des Materiaux Irradies, CEA Saclay, France）

[SY-B5] Using computational modeling to understand radiation damage tolerance in complex oxides both from the bottom-up and the top-down
○Blas Pedro Uberuaga （Los Alamos National Laboratory, United States of America）

[SY-B5] Development of defect mechanics-based multi-scale simulation techniques for reliability study of high performance electronic devices in radiation environments
○Yukeun Eugene Pak[1], Youjung Seo[2], Dhaneshwar Mishra[1], Keonwook Kang[3], Jihyun Kim[4] （1.Advanced Institutes Convergence Technology, Korea, 2.Seoul National University, Korea, 3.Yonsei University, Korea, 4.Korea University , Korea）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room10)

[SY-B5] He impurities in boron carbide : structure, kinetics, and Raman signatures

Invited

○Guido Roma, Kevin Gillet, Anton Schneider, Jean-Paul Crocombette （CEA, Univ. Paris-Saclay, France）

Helium impurities, produced by nuclear reactions in the neutron absorber boron carbide, are a matter of concern because they form bubbles and eventually affect the mechanical properties of the absorbing elements in fast breeder sodium reactors. In order to shed light on the mechanisms of bubble formation we have investigated, using first principles methods, the insertion of He in boron carbide (with stoichiometry B_4C) and the possible migration mechanisms. Whereas in absence of preexisting damage, at equilibrium, He is expected to occupy interstitial sites and diffuse via an interstitial mechanism [1], we show that, under irradiation where a supersaturation of vacancies is expected, He atoms can be trapped at vacancies and diffusion might be slowed down.

How to probe such kind of impurities? Raman spectroscopy is increasingly used to quantify damage in irradiated materials, including boron carbide. In order to help the interpretation of such experiments we calculated from first principles the first order Raman spectrum of B_4C containing defects ; to circumvent the size effect we devised an inclusion procedure allowing us to obtain the dynamical matrix and the Raman tensor of a supercell containing a defect at a dilution lower than 0.1 atomic %. The results show that interstitial He impurities do not significantly perturb the spectrum, while substitutional ones do.

[1] A. Schneider, G. Roma, J.-P. Crocombette, V. Motte, D. Gosset, J. Nucl. Mater. **496**, 157 (2017).

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room10)

[SY-B5] Irradiation damage in nuclear graphite at the atomic scale

○Alain Chartier[1], Laurent Van Brutzel[1], Justin Pageot[2] （1.DEN, Service de la Corrosion et du Comportement des Materiaux dans leur Environment, CEA Saclay, France, 2.DEN, Service d’Etudes des Materiaux Irradies, CEA Saclay, France）

Radiation response and microstructure evolution of nuclear graphite are investigated by combination of both Molecular Dynamics (MD) simulations and experimental observations with mainly High Resolution Transmission Electron Microscopy images (HRTEM) and X-ray diffraction patterns (XRD). Radiation response of single crystal graphite is examined using MD with point defects accumulation method. Results reveal that graphite structure undergoes three stages before amorphisation: (i) an increase of the number of point defects; (ii) a wrinkling of graphene layers pinned by small amorphous pockets; and (iii) a full amorphisation of the structure via percolation of the small amorphous pockets [1]. Each stage can be related to the swelling along the c-axis and the shrinking in the basal plane. In particular rippling contributes significantly to the strain. One filler particle - composed of almost aligned crystallites separated by Mrozowski cracks - is also generated to provide insights on a more realistic microstructure of an-irradiated nuclear graphite.

Subsequently, simulated XRD pattern and HRTEM images have been generated from the MD simulations and are compared with experimental observations [2]. Simulated HRTEM images show many features observed in experimental images in both virgin and irradiated nuclear graphite. Some of these features can be linked unequivocally to defined atomistic configurations. Basal grain boundaries (GBs), Mrozowski cracks, graphene

sheets and their folding belong to this category. Conversely, some patterns in simulated HRTEM cannot be related to a unique atomistic configuration and might eventually give rise to misleading interpretation. This is evidenced for edge dislocations in virgin nuclear graphite as well as for residues of graphene layers in highly damaged graphite.

These findings confirm that univocal identification of atomic scales structures in graphite from HRTEM images only is uneasy.

[1] A. Chartier, L. Van Brutzel, B. Pannier, and Ph. Baranek, Carbon 91 (2015) 395.
[2] A. Chartier, L. Van Brutzel, and J. Pageot, Carbon 133 (2018) 224.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room10)

[SY-B5] Using computational modeling to understand radiation damage tolerance in complex oxides both from the bottom-up and the top-down

○Blas Pedro Uberuaga （Los Alamos National Laboratory, United States of America）

Meeting the ever-increasing demand for energy is a key challenge for the 21st century. Nuclear energy is a proven and green energy source that will be a key component of the world's energy profile. However, maximizing the efficiency of nuclear energy systems requires materials that have significantly increased tolerance against radiation damage. Computational modeling has an important role in understanding and discovering new materials for next-generation nuclear energy systems.

In this talk, we will describe research efforts that apply computational modeling to understand the response of materials to radiation damage. We will focus on a class of complex oxides, pyrochlores, that have been proposed for nuclear waste encapsulation. Pyrochlores, with the chemical formula $A_2B_2O_7$, are related to the simpler fluorite structure, with the added complication of having two cation species and oxygen structural vacancies. Past work by numerous groups has shown that the radiation tolerance of these materials is sensitive to the nature of the A and B cations and, in particular, their propensity to disorder. However, these observations are empirical at best and there is still a lack of understanding on the factors that govern the radiation response of these materials.

We have tackled this problem from two different perspectives. First, using accelerated molecular dynamics, we have studied how cation disorder, often created during radiation damage, impacts defect kinetics and thus the transport mechanisms that dictate damage recovery. This bottom-up approach has revealed that a percolation transition occurs as disorder is introduced that leads to higher defect mobilities, which in turn promotes self-healing of the damage. On the other hand, we have used materials informatics to analyze the role of pyrochlore chemistry on radiation tolerance. In this case, divorced from the complexities of making true predictions of performance, we instead use machine learning to take a top-down perspective and discover heuristic relationships between the material composition and the susceptibility of the material to amorphization. While neither study provides a complete understanding of radiation damage in these materials, together they provide a more complete picture of the factors that dictate their response to

irradiation.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room10)

[SY-B5] Development of defect mechanics-based multi-scale simulation techniques for reliability study of high performance electronic devices in radiation environments

○Yukeun Eugene Pak[1], Youjung Seo[2], Dhaneshwar Mishra[1], Keonwook Kang[3], Jihyun Kim[4]　(1.Advanced Institutes Convergence Technology, Korea, 2.Seoul National University, Korea, 3.Yonsei University, Korea, 4.Korea University , Korea)

GaN-based electronic devices are very attractive for space applications since their radiation hardness characteristics are superior to the Si-based devices. For space missions requiring very conservative design margins, the presence of fabrication-induced defects as well as the radiation-induced defects limit the utilization of space-borne electronics. Therefore, prediction models to understand the defect generation mechanisms and the radiation effects on GaN devices are needed to properly engineer the reliability of these devices for the radiation environment.

To this end, we developed the quantitative linear elasticity models that can predict the stresses and piezoelectric fields induced in multilayer quantum wells in the presence of lattice defects such as dislocations. These electroelastic field calculations are coupled with the quantum mechanical formulation to predict the electronic and optical behavior of GaN-based devices such as LEDs and high-electronic-mobility transistors(HEMTs). To characterize the radiation effects, molecular dynamics (MD) simulations were performed to study the formation mechanisms of point defects caused by the energy transfer from irradiated particles. The required parameters for MD simulations were obtained by the Monte Carlo (MC) simulation code, GEANT4, and the results are compared with the irradiation test results.

[SY-B6] Symposium B-6

Chair: Jaime Marian(University of California Los Angeles, United States of America)
Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room10

[SY-B6] Ion Irradiation as a Surrogate for Reactor Irradiation: The Expected and the Surprises
○Gary S Was[1], Zhijie Jiao[1], David Woodley[1], Stephen Taller[1], Gerrit Vancoevering[1], Anthony Monterrosa[1], Elizabeth Getto[4], Brian Wirth[2], Arthur Motta[3] （1.University of Michigan, United States of America, 2.University of Tennessee, United States of America, 3.Pennsylvania State University, United States of America, 4.United Stated Naval Academy, United States of America）

[SY-B6] **Dose Effect on the Irradiation Induced Loop Density and Burgers Vector in Ion-Irradiated Ferritic/Martensitic Steel HT9 Through In-Situ TEM**
Ce Zheng[1], Stuart Maloy[2], ○Djamel Kaoumi[1] （1.North Carolina State University, United States of America, 2.Los Alamos National Laboratory, United States of America）

[SY-B6] **Novel Deformation Mechanism of Helium Irradiated Copper**
○WEIZHONG HAN （Xi'an Jiaotong University, China）

[SY-B6] Isotope effect on quantum diffusion of interstitial hydrogen in face-centered cubic metals
○Hajime Kimizuka[1], Shigenobu Ogata[1,2], Motoyuki Shiga[3] （1.Osaka University, Japan, 2.Kyoto University, Japan, 3.Japan Atomic Energy Agency, Japan）

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room10)

[SY-B6] Ion Irradiation as a Surrogate for Reactor Irradiation: The Expected and the Surprises

Invited

○Gary S Was[1], Zhijie Jiao[1], David Woodley[1], Stephen Taller[1], Gerrit Vancoevering[1], Anthony Monterrosa[1], Elizabeth Getto[4], Brian Wirth[2], Arthur Motta[3]　(1.University of Michigan, United States of America, 2.University of Tennessee, United States of America, 3.Pennsylvania State University, United States of America, 4.United Stated Naval Academy, United States of America)

Reactor core materials in both fast reactors and LWRs granted life extension must withstand irradiation to high doses at high temperature. Ferritic-martensitic (F-M) alloys are attractive candidates for structural components of fast and thermal reactors, and high chromium and high nickel-containing austenitic steels are potential replacement alloys for LWR core materials. Both require high dpa, for which ion irradiation is ideally suited. To simulate the reactor radiation environment, self-ion irradiation and He injection are conducted simultaneously into both F-M and austenitic alloys. Reactor irradiations of the same alloys have been, or are being conducted in the BOR-60 fast reactor to assess the capability of ion irradiation to emulate the evolution of reactor generated microstructures and mechanical properties. Computational models for defect cluster evolution are being developed and benchmarked against experimental data to ultimately provide predictive capability for the response of both microstructure (loops, voids, precipitates, etc.), and mechanical properties (hardening, ductility, slip behavior) to irradiation. To date, agreement is quite promising with many outcomes ocurring as expected. However, there are a number of observations or results that are unexpected. Results will be presented on the microstructure and mechanical property evolution in ion and reactor irradiation integrated with computational modelling in an effort to understand the extent to which ion irradiation can be used as a surrogate for reactor irradiation, and to illuminate processes that are not well understood.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room10)

[SY-B6] Dose Effect on the Irradiation Induced Loop Density and Burgers Vector in Ion-Irradiated Ferritic/Martensitic Steel HT9 Through In-Situ TEM

Ce Zheng[1], Stuart Maloy[2], ○Djamel Kaoumi[1]　(1.North Carolina State University, United States of America, 2.Los Alamos National Laboratory, United States of America)

TEM samples of F/M steel HT9 were irradiated to 20 dpa at 420˚C, 440˚C and 470˚C in a TEM with 1 MeV Kr ions so that the microstructure evolution could be followed in situ and characterized as a function of dose. Dynamic observations of irradiation induced defect formation and evolution were done at the different temperatures. The irradiation-induced loops were characterized in terms of their burgers vector, size and density as a function of dose and similar observations and trends were found at the three temperatures: (i) both **a**/2 <111> and **a** <100> loops are observed; (ii) in the early stage of irradiation, the density of irradiation induced loops increases with dose (0-4 dpa) and then decreases at higher doses (above 4 dpa), (iii) the dislocation line density shows an inverse trend to the loop density with increasing dose: in the early stages of irradiation the pre-existing dislocation lines are lost by climb to the surfaces while at higher doses (above 4 dpa), the build-up of new dislocation networks is observed along with the loss of the radiation-

induced dislocation loops to dislocation networks; (iv) at higher doses, the decrease of number of loops affects more the $a/2 <111>$ loop population; the possible loss mechanisms of the $a/2 <111>$ loops are discussed. Also, the ratio of $a <100>$ to $a/2 <111>$ loops is found to be similar to cases of bulk irradiation of the same alloy using 5 MeV Fe^{2+} ions to similar doses of 20 dpa at similar temperatures.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room10)

[SY-B6] Novel Deformation Mechanism of Helium Irradiated Copper

○WEIZHONG HAN （Xi'an Jiaotong University, China）

The workability and ductility of metals usually degrade with exposure to irradiation, hence the phrase "radiation damage". Here, we found that Helium (He) radiation can actually enhance the room-temperature deformability of submicron-sized copper. In particular, Cu single crystals with diameter of 100 nm to 300 nm and containing numerous pressurized sub-10 nm He bubbles, become stronger, more stable in plastic flow and ductile in tension, compared to fully dense samples of the same dimensions that tend to display plastic instability (strain bursts). The sub-10 nm He bubbles are seen to be dislocation sources as well as shearable obstacles, which promote dislocation storage and reduce dislocation mean free path, thus contributing to more homogeneous and stable plasticity. Failure happens abruptly only after significant bubble coalescence. Furthermore, we discover that the helium bubble not only can coalesce with adjacent bubbles, but also can split into several nanoscale bubbles under tension. Alignment of the splittings along a slip line can create a bubble-free-channel, which appears softer, promotes shear localization, and accelerates the failure in shearing-off mode. Detailed analyses unveil that the unexpected bubble fragmentation is mediated by the combination of dislocation cutting and internal surface diffusion, which is an alternative micro-damage mechanism of helium irradiated copper besides the bubble coalescence. These results shed light on plasticity and damage developments in metals. Ref. PRL 117 (2016) 515501, Nano Lett.16 (2016)4118 and Nano Lett. 17 (2017) 3725.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room10)

[SY-B6] Isotope effect on quantum diffusion of interstitial hydrogen in face-centered cubic metals

○Hajime Kimizuka[1], Shigenobu Ogata[1,2], Motoyuki Shiga[3] （1.Osaka University, Japan, 2.Kyoto University, Japan, 3.Japan Atomic Energy Agency, Japan）

Safe control of tritium is one of the technological challenges in the development of next-generation deuterium-tritium fusion reactors where tritium is used as nuclear fuel. From a scientific viewpoint, measuring the rate of diffusion of hydrogen isotopes in metals is important for understanding the isotope effect on the kinetics of hydrogen transport and hydrogen-induced deterioration of materials. However, a consensus on the physical mechanisms and numerical values of diffusivities of hydrogen isotopes in metals is still lacking. In this study, we clarified the site preference and diffusion rate of interstitial hydrogen and tritium in several face-centered cubic (fcc) metals, such as palladium, aluminum, and copper, by performing *ab initio* path-integral molecular dynamics (PIMD) modeling in the framework of density functional theory. This was necessary as the hydrogen atom has sufficiently low mass that it exhibits significant nuclear quantum delocalization and zero-point motion even at ambient temperature. The nuclear quantum effect on the

activation free energies for hydrogen migration was characterized according to the PIMD-based free energy profiles obtained from the thermodynamic integration of the centroid force along the migration path at 75-1200 K. We found that the nuclear quantum effects significantly affected the activation barrier for hydrogen migration and the difference between the energies of the hydrogen atom at the octahedral and tetrahedral interstitial sites even at ambient temperature. Consequently, we revealed the role of quantum fluctuations on the *reversed* isotope dependence for hydrogen diffusion in certain fcc metals.

[SY-B7] Symposium B-7

Chair: Marjorie Bertolus(CEA/DEN/DEC, Centre CEA de Cadarache, France)
Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room10

[SY-B7] Thermal properties of fluorite-type metal dioxides: CeO_2, ThO_2, UO_2, NpO_2, PuO_2 and AmO_2

○Masato Kato （Japan Atomic Energy Agency, Japan）

[SY-B7] **SCIANTIX: A new inert gas behaviour module ready for use**

○Davide Pizzocri, Tommaso Barani, Lelio Luzzi （Politecnico di Milano, Italy）

[SY-B7] Modeling swelling in U_3Si_2 nuclear fuel using a multi-scale computational approach

○Larry Aagesen[1], Karim Ahmed[2], Benjamin Beeler[1], Daniel Schwen[1], Yongfeng Zhang[1] （1.Idaho National Laboratory, United States of America, 2.Texas A&M University, United States of America）

[SY-B7] Why Multiscale Modeling of Nuclear Fuel is Absolutely Essential and Why it is so Challenging

○Michael R Tonks[1], Yongfeng Zhang[2], David Andersson[3], Simon Phillpot[1], Christopher Stanek[3] （1.University of Florida, United States of America, 2.Idaho National Laboratory, United States of America, 3.Los Alamos National Laboratory, United States of America）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room10)

[SY-B7] Thermal properties of fluorite-type metal dioxides: CeO_2, ThO_2, UO_2, NpO_2, PuO_2 and AmO_2

Invited

$^{\bigcirc}$Masato Kato （Japan Atomic Energy Agency, Japan）

Actinide dioxide having a fluorite structure is one of prospective candidates as a fuel of advanced reactors. Thermal property of nuclear fuels is essential data to evaluate fuel performance. Therefore, great efforts to measure properties and understand their mechanism have been made so far. It is well-known that thermal properties of actinide oxides changes significantly depending on temperature, and their mechanism is complicated. Author's research group has studied on thermal properties of CeO_2, UO_2, PuO_2 and their solid solution. In this work, basic properties of various fluorite-type dioxides were summarized, and temperature dependence of thermal properties were evaluated.

In fluorite-type oxides of CeO_2, ThO_2, UO_2, NpO_2, PuO_2 and AmO_2, mechanical property, Debye temperature, Grunisen constant, thermal expansion, oxygen potential, heat capacity C_p and thermal conductivity were reviewed, and the data were compared. Heat capacity at volume constant C_v and thermal expansion term C_d were considered from their data in heat capacity evaluation. The calculation result of (C_v+C_d) was in good agreement with experimental data in CeO_2 and ThO_2, but the calculated data of other actinide dioxides underestimated the experimental data by 10-20 J/molK. The extra C_p from (C_v+C_d) was considered as a Schottky term C_{sch} which related to 5f electrons. In fact, 5 f electrons do not exist in CeO_2 and ThO_2. Experimental data of UO_2, NpO_2, PuO_2 and AmO_2 were described with the calculated $(C_v+C_d+C_{sch})$. The extra C_p was described assuming two level energy model.

Thermal conductivity of the dioxides was evaluated by phonon conduction mechanism using Slack's equation. Phonon conduction of pure oxide can be represented by 1/(BT). Thermal conductivity of CeO_2 and ThO_2 was represented by Slack's equation very well. But, other conduction mechanism is needed to evaluate thermal conductivity of UO_2, NpO_2, PuO_2 and AmO_2.

It is reported that excited term at high temperatures which is contributed with Frenckel defect, electron and so on exists in heat capacity and thermal conductivity. The experimental data at high temperatures are lacked to evaluate the excited terms. In addition of experimental data in high temperature region, computational approach is expected to understand deeply mechanism in property change.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room10)

[SY-B7] SCIANTIX: A new inert gas behaviour module ready for use

$^{\bigcirc}$Davide Pizzocri, Tommaso Barani, Lelio Luzzi （Politecnico di Milano, Italy）

Being able to bridge lower length-scale calculations with the engineering-scale simulations of fuel performance codes requires the development of dedicated intermediate-scale codes. In this work, we present SCIANTIX, a recently developed code which aims to fill this gap. SCIANTIX is a 0D stand-alone computer code under development at Politecnico di Milano since 2016. It is designed to be included as a module in existing fuel performance codes (e.g., TRANSURANUS). It contains models describing inert gas behaviour at the scale of a fuel grain, represented as a point (i.e., 0D). Since it is 0D, no spatial discretization

is required, and all variables are treated as average in space. Nevertheless, the models available in SCIANTIX (covering intra- and inter-granular inert gas behaviour, and high burnup structure formation and evolution as well) are physics-based and not correlation-based. The main characteristic of SCIANTIX is thus the simplicity of the models (i.e., low computational burden, in line with the requirements of fuel performance codes), paired with the possibility to inform them with parameters from lower length-scale calculations. SCIANTIX is validated against hundreds of experimental data describing inert gas behaviour at the scale of fuel grains. The validation is supported by uncertainty analyses on the main model parameters. Moreover, sensitivity analyses are performed to prioritize further research activities. Showcases of validation, uncertainty and sensitivity analyses are presented in this work (e.g., concerning gas concentrations, evolution of intra- and inter-granular bubble populations, swelling, high burnup structure formation). As for the numerical treatment of the model equations, SCIANTIX is developed with full numerical consistency and entirely verified with the method of manufactured solutions (verification of different numerical solvers is also showcased in this work). The open source release of the code is planned soon.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room10)

[SY-B7] Modeling swelling in U_3Si_2 nuclear fuel using a multi-scale computational approach

○Larry Aagesen[1], Karim Ahmed[2], Benjamin Beeler[1], Daniel Schwen[1], Yongfeng Zhang[1]　(1.Idaho National Laboratory, United States of America, 2.Texas A&M University, United States of America)

U_3Si_2 is a leading candidate for application as an accident-tolerant fuel for commercial nuclear power generation. Due to U_3Si_2' s high thermal conductivity relative to conventional UO_2 fuel, it is believed to have a wider margin to melting/relocation in accident scenarios. However, based on limited experimental data, it is believed that U_3Si_2 undergoes much more significant swelling. To predict the swelling of U3Si2, a multi-scale computational approach has been developed. A phase-field model of fission gas bubble was developed, which tracks vacancies on the U lattice sites and Xe atoms as defect species. The proportional swelling of the fuel was assumed to be equal to the volume fraction of the bubble phase. The phase-field model was parameterized using density functional theory and molecular dynamics calculations. The incorporation of the swelling predictions to engineering-scale fuel performance models will be discussed.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room10)

[SY-B7] Why Multiscale Modeling of Nuclear Fuel is Absolutely Essential and Why it is so Challenging

Invited

○Michael R Tonks[1], Yongfeng Zhang[2], David Andersson[3], Simon Phillpot[1], Christopher Stanek[3]　(1.University of Florida, United States of America, 2.Idaho National Laboratory, United States of America, 3.Los Alamos National Laboratory, United States of America)

The performance of reactor fuel is historically determined using codes that rely on empirical fits to experimental data. However, as reactor operation becomes more variable and as we consider changes to the fuel and cladding system to increase accident tolerance, these empirical models become insufficient to meet our needs. The US Nuclear Engineering Advanced Modeling and Simulation (NEAMS) program is beginning to

implement an alternative approach to fuel performance materials models that relies on representing the evolving state of the fuel microstructure using state variables that impact the material properties. However, developing the required models for this approach using only experimental data would be extremely difficult, time consuming, and expensive. Hierarchical multiscale modeling and simulation, ranging from density functional theory to mesoscale simulation approaches, provides a powerful means to obtain additional data to inform the development of these new materials models. However, applying this multiscale approach to reactor fuel has a number of challenges. In this presentation I will summarize this multiscale approach being taken in the US and discuss a number of the issues that make it difficult.

[SY-B8] Symposium B-8

Chair: Guang-Hong Lu(Beihang University, China)
Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room10

[SY-B8] Kinetic Monte Carlo study of tungsten fuzz formation under low energy helium irradiation

○Zhangcan Yang, Yingzhao He, Quansong Peng （School of Energy and Power Engineering, Huazhong University of Science and Technology, China）

[SY-B8] Constrained thermodynamic model for multi-component alloys under irradiation: A matrix formulation from first-principles Hamiltonian

○Duc Nguyen-Manh[1], J.S Wrobel[2], A. Fernandez_Caballero[3], S.L. Dudarev[1] （1.Materials Science and Scientific Computing Department, Culham Centre for Fusion Energy, UKAEA, UK, 2.Faculty of Materials Science and Engineering, Warsaw University of Technology, Poland, 3.School of Mechanical Aerospace and Civil Engineering, University of Manchester , UK）

[SY-B8] Kinetic Monte-Carlo Simulations of Radiation Damage in W(Re,Os) Alloys

○Matthew James Lloyd[1,2], David Armstrong[1], Enrique Martinez Saez[3], Duc Nguyen-Manh[2] （1.Department of Materials, University of Oxford, UK, 2.Culham Centre for Fusion Energy, UK, 3.Los Alamos National Laboratory, United States of America）

[SY-B8] Modeling Re-precipitate hardening in neutron irradiated W and W-Re alloys: from point defects to macroscopic hardening

Chen-Hsi Huang[1], Leili Gharaee[2], Paul Erhart[2], ○Jaime Marian[1] （1.University of California Los Angeles, United States of America, 2.Chalmers University, Sweden）

[SY-B8] In-situ TEM of Formation Processes of Defects in Tungsten under Irradiation: Comparison between Electron and Self-ion Irradiations

○Kazuto Arakawa （Shimane University, Japan）

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room10)

[SY-B8] Kinetic Monte Carlo study of tungsten fuzz formation under low energy helium irradiation

○Zhangcan Yang, Yingzhao He, Quansong Peng （School of Energy and Power Engineering, Huazhong University of Science and Technology, China）

Tungsten has been considered as the primary candidate for the plasma-facing materials of fusion reactors. However, the formation of fuzz-like nanostructures on tungsten surfaces under low-energy helium plasma irradiation has raised big concerns since these fuzzy structures have been shown to be detrimental to the performance of the materials and the stability of plasma. Unfortunately, the mechanism of fuzz formation is still under debate. Here we present an Object Kinetic Monte Carlo study that links the nucleation and growth of helium bubbles with the evolution of surface morphology. The key difference of our model compared with a previous model by Lasa's[1] is that the motion of the punched dislocation loops and the diffusion of surface ad-atoms are modeled in detailed in our model. As a result, our model is able to produce real fuzz-like structures rather than the glassy structures in Ref [1]. We first study the sub-surface helium clustering behavior in tungsten as a function of temperature, helium implantation rate, and concentration of pre-existing defects [2]. The key parameters that affect helium clustering behavior have been identified. We then investigate the possible processes that may contribute to the surface evolution and quantitatively analyze their relative contribution. We find that the motion of dislocation loops and the surface diffusion are the two key processes to the surface evolution. Bubble rupture only affects the initial surface roughness, but plays a negligible role in the growth of fuzz structures.

Reference:

[1] A. Lasa et al 2014, EPL, 105(2), 25002.

[2] Z. Yang et al 2017, Fusion Science and Technology, 71(1), 60.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room10)

[SY-B8] Constrained thermodynamic model for multi-component alloys under irradiation: A matrix formulation from first-principles Hamiltonian

○Duc Nguyen-Manh[1], J.S Wrobel[2], A. Fernandez_Caballero[3], S.L. Dudarev[1] （1.Materials Science and Scientific Computing Department, Culham Centre for Fusion Energy, UKAEA, UK, 2.Faculty of Materials Science and Engineering, Warsaw University of Technology, Poland, 3.School of Mechanical Aerospace and Civil Engineering, University of Manchester , UK）

Understanding the behaviour of multi-component alloys under irradiation is one of the great challenges for the development of materials for nuclear applications. Recent experimental investigations revealed that micro-structural evolution of multi-component metallic alloys formed by transmulation under neutron irradiation can be very complicated since they may undergo spinodal decomposition and radiation-induced precipitation due to the strong coupling between defects and local chemical environment. Very recently, it was shown that concentrated solute solution alloys including high-entropy alloys (HEAs) may exhibit significantly improved performance under irradiation that depends strongly on the number of alloying elements and local alloy composition.

In this work, a revisited constrained thermodynamic model, initially proposed by Georges Martin, has been developed to model multi-component alloys under irradiation. The model is based on ab initio calculations in combination with a cluster-expansion Hamiltonian generalized for systems containing vacancy (V) and interstitial (I) defects. It is found that this formalism can be mathematically represented in terms of a matrix formulation for any N-component system via cluster correlation functions, which in turn can be deduced consistently from Monte-Carlo simulations. Analytical expressions for local short-range order parameters for alloy components and configurational entropies as functions of temperature and composition have been derived explicitly from this matrix representation. In the first nearest-neighbour approximation, the new approach reproduces the ABVI Ising model for a binary system as well as the thermodynamic limit of the Cluster Variation Method. We apply this formalism to anomalous precipitation in W(Re,Os,Ta) alloys under neutron irradiation as well as in low activation bcc and high-radiation resistance fcc HEAs and their derivatives.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room10)

[SY-B8] Kinetic Monte-Carlo Simulations of Radiation Damage in W(Re,Os) Alloys

○Matthew James Lloyd[1,2], David Armstrong[1], Enrique Martinez Saez[3], Duc Nguyen-Manh[2]   (1.Department of Materials, University of Oxford, UK, 2.Culham Centre for Fusion Energy, UK, 3.Los Alamos National Laboratory, United States of America)

The realisation of fusion energy is dependant on the development of high performance materials that can withstand the extreme conditions that they will be subjected to. The plasma facing components of a fusion reactor will experience a combination of high thermal loading ($\sim$10MWm^{-2}) and an intense flux of both 14MeV neutrons and high energy He/H ions ($\sim$5-20dpa/yr), meaning they will have to operate at very high temperatures ($\sim$1300 K). Tungsten is currently the leading candidate material due to its high melting temperature ($\sim$3695K); good thermal conductivity ($\sim$150Wm^{-1}K^{-1}) and resistance to sputtering (Eth=200eV). But at such a high neutron flux, transmutation of W in a fusion reactor is significant, resulting in several at.% Re, Os and Ta over the lifetime of the reactor. Precipitation of Re and Os has been observed well below their solubility limit in W, resulting in embrittlement, hardening, and a reduction in thermal conductivity.

The research presented examines irradiated W-(Re,Os,Ta) alloy systems, using a combination of DFT parametrised, multicomponent atomistic kinetic Monte-Carlo (AKMC) modelling, and high resolution nanoscale characterisation techniques such as atom probe tomography (APT). The role of interstitial defects in W-Re and W-Os is thought to play an important role in precipitation, because of the low rotation energy of the W-Re/W-Os mixed dumbbell. This enables the 3D transport of solute atoms, that would otherwise be confined to the <111> direction. We present a multicomponent kinetic Monte Carlo model, incorporating both vacancy and interstitial defects, and solute concentration dependant interactions. The predictions made by our model are supported by APT data of W-Re and W-Os alloys irradiated at high temperature, using W ions.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room10)

[SY-B8] Modeling Re-precipitate hardening in neutron irradiated W and W-Re alloys: from point defects to macroscopic hardening

Chen-Hsi Huang[1], Leili Gharaee[2], Paul Erhart[2], ○Jaime Marian[1]　(1.University of California Los Angeles, United States of America, 2.Chalmers University, Sweden）

High-temperature, high-dose, neutron irradiation of W results in the formation of Re-rich clusters at concentrations one order of magnitude lower than the thermodynamic solubility limit. These clusters may eventually transform into brittle W-Re intermetallic phases, leading to severe embrittlement and loss of thermal conductivity. Standard theories of radiation-enhanced diffusion and precipitation cannot explain the formation of these precipitates and so understanding the mechanism by which nonequilibrium clusters form under irradiation is crucial to predict material degradation and devise mitigation strategies. In this work, we integrate neutronics, primary damage calculations, molecular dynamics results, Re transmutation calculations, and stochastic cluster dynamics simulations to study neutron damage in single-crystal tungsten to mimic divertor materials. We study the material response under experimental conditions at the JOYO fast reactor and the High Flux Isotope Reactor, for which measurements of cluster densities and hardening levels exist. We then provide calculations under expected DEMO fusion conditions. Several key mechanisms involving Re atoms and defect clusters are found to govern the accumulation of irradiation damage in each case. We use established correlations to translate damage accumulation into hardening increases and compare our results to the experimental measurements. We find hardening increases in excess of 5000 MPa in all cases, which calls into question the performance of these materials under service conditions in fusion reactors.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room10)

[SY-B8] In-situ TEM of Formation Processes of Defects in Tungsten under Irradiation: Comparison between Electron and Self-ion Irradiations

Invited
○Kazuto Arakawa　(Shimane University, Japan）

Nuclear-fission and fusion materials are degraded primarily due to the accumulation of radiation-produced lattice defects, such as point defects (self-interstitial-atoms (SIAs) and vacancies) and point-defect clusters (dislocation loops and cavities). In order to precisely predict the lifetimes of nuclear materials, accurate understanding of the origins of the defect accumulation—generation of defects and their subsequent dynamics—is crucial.

In-situ transmission electron microscopy (TEM) is a powerful technique for probing defect dynamics, in response to external stimuli such as irradiation under heating or cooling. As the irradiation sources for the in-situ TEM, electrons and ions are available. In the electron irradiation, only point defects are generated as the primary damage via knock-on displacement. In contrast, in the ion irradiation, point-defect clusters are also generated as the primary damage, which is called "collision cascade", like neutron irradiation.

In this presentation, we focus on the formation process of dislocation loops in tungsten under irradiation. Firstly we show our results on dynamic properties of SIAs [1] and SIA dislocation loops, which have been

mainly obtained with high-voltage electron microscopes in Osaka University and Nagoya University in Japan. And, we provide our results on the formation processes of dislocation loops under self-ion irradiation, which have been obtained with an ion-accelerators combined microscope in the JANNuS-Orsay facility in France. Through the comparison between these results, we try to extract the effects of collision cascade on the formation processes of dislocation loops.

References

[1] T. Amino, K. Arakawa, and H. Mori, *Scientific Reports* 6 (2016) 26099.

Plenary Talk | Plenary Talk

[PL6] Plenary Talk 6

Integrated earthquake simulation enhanced with high performance computing

Chair: Karin Dahmen(University of Illinois at Urbana Champaign, USA)

Fri. Nov 2, 2018 8:30 AM - 9:20 AM Room1

Muneo Hori

[PL6] Plenary Talk 6

○Muneo Hori （Earthquake Research Institute, The University of Tokyo, Japan）

(Fri. Nov 2, 2018 8:30 AM - 9:20 AM Room1)

[PL6] Plenary Talk 6

Integrated earthquake simulation enhanced with high performance computing

○Muneo Hori （Earthquake Research Institute, The University of Tokyo, Japan）

Integrated earthquake simulation (IES) is a seamless simulation of earthquake hazard, disaster and disaster response for an urban area. A set of numerical analysis of Earth Science, earthquake engineering and social sciences are used to carry out this simulation, together with analysis models of the target area that are automatically constructed by using available data of undergrounds, structures, and social activities. High performance computing is essential for the simulation with higher spatial and temporal resolution and for the evaluation of uncertainties related to a possible earthquake scenario, state of structures and social activities; capability computing is used to solve a large-scale model of an urban area, and capability computing is used to solve numerous cases and analysis models for the uncertainties. This lecture presents the current state of IES that uses K computer and other supercomputers. The following topics are focused: 1) key numerical techniques that are implemented into finite element method for scalable parallel computation; 2) particle simulation for fluid and human being; ad 3) the automated model construction that take advantage of various distinct data sources. Several examples of IES that are made for actual cities in Japan are presented. Discussions are made for the future use of higher fidelity models of structures in order to make more reliable seismic response analysis.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C13] Symposium C-13
Chair: Jaafar A. El-Awady(Johns Hopkins University, United States of America)
Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room1

[SY-C13] Mesoscopic studies of slip and twinning processes in hcp polycrystalline materials
○Irene Beyerlein[1], Marat Latypov[1], Jason Mayeur, Wyatt Witzen[1], Mitra Taheri[2], Tresa Pollock[1]
（1.University of California at Santa Barbara, United States of America, 2.Drexel University, United States of America）

[SY-C13] Crystal plasticity formulation involving volume fraction-based deformation twinning model
○Yuichi Tadano （Department of Mechanical Engineering, Saga University, Japan）

[SY-C13] An Elastic-Viscoplastic Crystal Plasticity Modeling for Plane Strain Deformation of Pure Magnesium
○Weidong Song, Liansong Dai （Beijing Institute of Technology, China）

[SY-C13] The Minimum Energy Pathways Identifications of Twinning Dislocation Loop Nucleation of Extension Twinning in Magnesium
○Xiao-Zhi Tang[1], Qun Zu[2], Lixin Sun[4], Yue Fan[3], Ya-Fang Guo[1] （1.Inst. of Mechanics, Beijing Jiaotong Univ., China, 2.Schl. of Mechanical Engineering, Hebei Univ. of Tech., China, 3.Dept. of Mechanical Engineering, Univ. of Michigan, United States of America, 4.Dept. of Nuclear Science and Engineering, MIT, United States of America）

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room1)

[SY-C13] Mesoscopic studies of slip and twinning processes in hcp polycrystalline materials

Invited

○Irene Beyerlein[1], Marat Latypov[1], Jason Mayeur, Wyatt Witzen[1], Mitra Taheri[2], Tresa Pollock[1] （1.University of California at Santa Barbara, United States of America, 2.Drexel University, United States of America）

Under deformation, strain and lattice orientation gradients can develop near crystalline heterogeneities, such as grain boundaries, deformation twins, and voids. These important effects have been studied intensely most often in materials that deform by a single slip mode. In this presentation, we discuss multiscale crystal plasticity modeling efforts to understand the development of lattice orientation gradients induced near and at the boundaries of microstructural defects within crystals of materials with either a BCC or HCP crystal structure. These two material classes commonly deform by multiple slip modes and this distinction is taken into account in the modeling. The results presented in this talk will highlight the effects of microscopic differences in the strengths of these slip modes on the evolution of dislocation density.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room1)

[SY-C13] Crystal plasticity formulation involving volume fraction-based deformation twinning model

○Yuichi Tadano （Department of Mechanical Engineering, Saga University, Japan）

Deformation twinning is an important deformation mechanism of metallic materials as well as slip deformation, especially in hexagonal closed-packed (HCP) metals such as magnesium and titanium. Therefore, understanding twinning behavior is essential to improve mechanical properties of HCP metals. HCP metals generally have a strong anisotropy in crystalline scale. For example, in case of magnesium, plastic deformation due to slip along the c-axis is hard to occur because of much higher critical resolved shear stress of pyramidal slip system, and deformation twinning occur to enhance plastic deformation along the c-axis. The most dominant twinning in magnesium is {10-12}<11-20> tensile twinning system, the number of which is six. As several experimental results showed that untwinned and twinned regions can simultaneously exist in a grain, the author proposed a crystal plasticity model considering the volume fraction of deformation twinning. In the practical problems, multiple twinning systems may be simultaneously activated in a grain because of inhomogeneity of deformation. Therefore, the deformation twinning model has been extended to incorporate the volume fraction of multiple twinning systems. To represent the polycrystalline behaviors of materials, the homogenization-based finite element method is adopted, so that the mechanical behaviors of polycrystalline magnesium can appropriately be reproduced. Numerical investigation using the proposed model is performed, and the adequacy of the model is validated.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room1)

[SY-C13] An Elastic-Viscoplastic Crystal Plasticity Modeling for Plane Strain Deformation of Pure Magnesium

○Weidong Song, Liansong Dai （Beijing Institute of Technology, China）

A rate-dependent elastic-viscoplastic constitutive model is proposed. The model of plane deformation of single crystal magnesium is established by considering seven orientations with different loading directions. The basal, prismatic and pyramidal slip systems in the parent grain, compressive twinning (CT) and tensile twinning (TT) are incorporated in the model. The constitutive descriptions of CT and TT are distinguished to better characterize their effects on the overall hardening of magnesium. The contributions of different deformation modes to the macroscopic plastic deformation of magnesium single crystals in the seven cases are presented. These computational predictions are compared with their corresponding macroscopic experimental observations (stress-strain responses) and other numerical results. These results prove that it is necessary to distinguish different twinning systems and their associated hardening laws for the plastic deformation of magnesium and its alloy.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room1)

[SY-C13] The Minimum Energy Pathways Identifications of Twinning Dislocation Loop Nucleation of Extension Twinning in Magnesium

○Xiao-Zhi Tang[1], Qun Zu[2], Lixin Sun[4], Yue Fan[3], Ya-Fang Guo[1] （1.Inst. of Mechanics, Beijing Jiaotong Univ., China, 2.Schl. of Mechanical Engineering, Hebei Univ. of Tech., China, 3.Dept. of Mechanical Engineering, Univ. of Michigan, United States of America, 4.Dept. of Nuclear Science and Engineering, MIT, United States of America）

The twinning dislocation loop nucleation on the coherent twin boundary in magnesium is investigated by potential energy approaches, and also the dynamic simulations at various temperatures and strain rates.

Based on our numerical results of extension twinning, the single lattice transformation within the coherent twin boundary migration is identified to be the elementary migration process, and its stress-free potential energy barrier is lower than the thermal energy at room temperature. The migration can be triggered thermally once the shear stress makes the transformed lattice at a low energy state. Both the nucleation energy and the critical radius of a twinning dislocation loop are calculated. We believe our discoveries pursue a better understanding of the plasticity of hexagonal close-packed metals.

[SY-E13] Symposium E-13

Chairs: Erik Bitzek(FAU Erlangen-Nuernberg, Germany), Kisaragi Yashiro(Gifu University, Japan)
Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room2

[SY-E13] 3D Aspects of Fracture in Crack - Obstacle Interactions and Effects of Crack Front Curvature

○Erik Bitzek[1], Polina Baranova[1], Johannes J. Möller[2] （1.FAU Erlangen-Nuernberg, Germany, 2.Fraunhofer IWM, Germany）

[SY-E13] Vortex instabilities in the deformation of Cu|Au nanolaminates

Adrien Gola[1,2], Peter Gumbsch[2,3], ○Lars Pastewka[1,3,2] （1.University of Freiburg, Germany, 2.Karlsruhe Institute of Technology, Germany, 3.Fraunhofer IWM, Germany）

[SY-E13] **Molecular dynamics simulation of the interaction between grain boundary and point defects**

○Liang Zhang[1], Yasushi Shibuta[1], Cheng Lu[2] （1.The University of Tokyo, Japan, 2.University of Wollongong, Australia）

[SY-E13] Deformation mode analysis by the eigenvectors of the atomic elastic stiffness

○Kisaragi Yashiro （Gifu University, Japan）

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room2)

[SY-E13] 3D Aspects of Fracture in Crack - Obstacle Interactions and Effects of Crack Front Curvature

Invited

○Erik Bitzek[1], Polina Baranova[1], Johannes J. Möller[2] (1.FAU Erlangen-Nuernberg, Germany, 2.Fraunhofer IWM, Germany)

Traditionally, fracture mechanics mainly considers 2D problems in which the crack front is approximated by a straight line. At the nanoscale, cracks can, however, be strongly curved, e.g., in the case of crack nuclei or as a result of the interaction of a propagating crack with obstacles. Nanoscale crack front curvature can significantly influence the fracture behavior of semi-brittle materials that show a brittle-to-ductile transition with increasing temperature, like refractory metals, intermetallics or semiconductors. Their fracture behavior is ultimately determined by the competition between the dynamics of the atomic bond-breaking processes and dislocation activity in the direct vicinity of the crack. The relative orientation of the local crack front to possible dislocation slip systems can therefore have a major impact on crack tip processes.

Here we present the results of our atomistic simulations of straight cracks in W, Fe and NiAl interacting with various obstacles. Cracks interacting with individual pre-existing lattice dislocations showed stimulated dislocation nucleation and new crack tip blunting mechanisms. Voids were shown to efficiently stop propagating cracks by impeding the re-nucleation of a sharp crack and by facilitating dislocation emission. Fully-3D simulations of penny-shaped cracks revealed an increased tendency for crack tip plasticity compared to straight cracks due to the availability of more slip systems and the resulting dislocation - crack interactions. The results are discussed in the context of the development of predictive multiscale models for fracture toughness.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room2)

[SY-E13] Vortex instabilities in the deformation of Cu|Au nanolaminates

Adrien Gola[1,2], Peter Gumbsch[2,3], ○Lars Pastewka[1,3,2] (1.University of Freiburg, Germany, 2.Karlsruhe Institute of Technology, Germany, 3.Fraunhofer IWM, Germany)

Vortex-instabilities are typically associated with fluid-type flow patterns, such as the well-known Kelvin-Helmholtz instability that can be directly observed in cloud patterns. Recently, Vortex-type instabilities have been observed during the deformation of multilayered materials, both with nano- [1] and micrometer-sized [2] layers. We here use molecular dynamics simulation to investigate Vortex formation in Cu|Au nanolaminates. Our simulations reveal an instability that leads to corotation of neighboring regions of the nanolaminate, giving rise to deformation pattern reminiscent of Kelvin-Helmholtz instabilities. Contrary to the latter instabilities, the plastic Vortex formation occurs at strains below 2 which appears compatible with strains experienced during frictional loading [1]. We compare our molecular dynamics results with deformation patterns generated through ideal plastic and fluid mechanical models.

[1] Luo, Z.-P., Zhang, G.-P. &Schwaiger, R. Microstructural vortex formation during cyclic sliding of Cu/Au multilayers. *Scr. Mater.* **107,** 67-70 (2015).
[2] Pouryazdan, M., Kaus, B. J. P., Rack, A., Ershov, A. &Hahn, H. Mixing instabilities during shearing of metals. *Nat. Commun.* **8,** 1611 (2017).

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room2)

[SY-E13] Molecular dynamics simulation of the interaction between grain boundary and point defects

○Liang Zhang[1], Yasushi Shibuta[1], Cheng Lu[2]　(1.The University of Tokyo, Japan, 2.University of Wollongong, Australia)

Molecular dynamics simulations were carried out to investigate the dynamic interaction between different grain boundaries (GBs) and two types of point defects, namely the stacking fault tetrahedron (SFT) and the void. The GB can migrate itself under the shear strain and can serve as a sink to remove SFT and void. The sink efficiency of GBs is sensitive to their structural characteristics, the size of point defects, and temperature. The high-angle GBs can show a great ability to remove the point defects even at a low temperature, while the increase of temperature can facilitate the annihilation of the point defects at the low-angle GBs. The simulation reveals a new possible GB-mediated damage healing mechanism of irradiated materials. In particular, the nanotwinned metals are generally anticipated to be less effective in the alleviation of radiation damage because they contain mostly coherent twin boundaries, which are low-energy boundaries and are inefficient defect sinks in irradiated metallic materials. However, recent *in situ* studies have indicated that some nanotwinned metals exhibit unprecedented radiation tolerance, and the unexpected self-healing of twin boundaries in response to radiation was observed. In this work, we proposed two possible self-healing mechanisms of twin boundaries by considering the defective coherent twin boundary structures which contained incoherent twin segments or self-interstitial atoms. The mechanisms were confirmed and atomistic evidence was provided by carrying out the long-time molecular dynamics simulations.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room2)

[SY-E13] Deformation mode analysis by the eigenvectors of the atomic elastic stiffness

○Kisaragi Yashiro　(Gifu University, Japan）

Inspired by the Wang's stability criteria based on the "elastic stiffness" coefficients, we have proposed to evaluate the local stability by the atomic elastic stiffness matrix and discuss the onset of local deformation such as dislocation nucleation, crack propagation, etc, with the positive definiteness of the matrix. The 6x6 matrix of the elastic stiffness correlates the stress and strain in the 6 dimensional strain space; thus the loss of the positiveness means the emergence of the unstable deformation path. The stiffness matrix is *not* identical to the "elastic coefficients" or usually named as "elastic constants" except in the no-load equilibrium or in the linear elasticity. In the thermodynamics of crystal lattices, the stress and the elastic coefficients are defined as the 1st and 2nd order derivatives of the internal energy per unit volume, respectively, and the stiffness in the nonlinear region is expressed with the elastic coefficients *plus* the stress contribution. In the atomic simulations based on the interatomic potential function, the internal energy is the sum of each atom contribution so that we can define the atomic stress and atomic elastic coefficients, then evaluate 6x6 stiffness matrix and its eigenvalue for each atom. The negative eigenvalue can be found on the surface and various lattice defects as already reported, then we advanced our instability analysis with the corresponding eigenvector of the atoms with negative eigenvalue. That is, the principal strain axes of the 3x3

strain tensor are evaluated as unstable deformation path for the atoms with negative eigenvalue and corresponding eigenvector of 6 strain components. In the case of crack initiation from the surface at the equator line of circular hole in the bcc-Fe under [110] tension, the deformation mode at the crack tip is normal to the (010) cleavage plane although the resulting crack opening occurs in the (110) planes. Another example is the dislocation emission from same circular hole under [111] tension, the deformation modes at the dislocation core are not only parallel to the [112] slip plane but also large normal mode corresponding to the Peierls barriers. In the presentation, we demonstrate various application of our deformation analysis to bcc-Fe, hcp-Mg, and 3C-SiC etc.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E14] Symposium E-14

Chairs: Thierry Auger(CNRS, France), Jamila Rahmoun(LAMIH-ENSIAME, Valenciennes University, France)
Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room2

[SY-E14] Stability Controlled Crack Evolution in Staggered Laminate Bio-material
○Yi Yan, Akihiro Nakatani （Dept. of Adaptive Machine Systems, Osaka University, Japan）

[SY-E14] A brittle to ductile transition modeling for liquid metal embrittlement
○Thierry Auger （CNRS, France）

[SY-E14] Buckling delamination of ductile thin films on rigid substrates
○Nadia Ben Dahmane, Guillaume Parry, Rafael Estevez （Univ. Grenoble Alpes, SIMAP, F-38000 Grenoble, France）

[SY-E14] An analytical model of the peeling forces at edges of multilayers subjected to temperature variations
○Chengyin Zhang[2], Neng-Hui Zhang[1,2] （1.Department of Mechanics, College of Sciences, Shanghai University, China, 2.Shanghai Key Laboratory of Mechanics in Energy Engineering, Shanghai Institute of Applied Mathematics and Mechanics, Shanghai University, China）

[SY-E14] **Characterization and multi-scale modeling of the mechanical response of the human humerus under dynamic loading**
○Jamila Rahmoun[1], Hakim Naceur[1], Pascal Drazetic[2], Christian Fontaine[3] （1.LAMIH-ENSIAME, Valenciennes University, France, 2.LAMIH-IUT, Valenciennes University, France, 3.Lab. d'anatomie, Lille University, France）

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room2)

[SY-E14] Stability Controlled Crack Evolution in Staggered Laminate Bio-material

○Yi Yan, Akihiro Nakatani （Dept. of Adaptive Machine Systems, Osaka University, Japan）

Nacre that is a bio-material with a staggered laminate micro-structure of hard and soft constituents shows a good performance of strength, stiffness, and toughness. The toughness of nacre with 95% hard and brittle phase and less than 5% soft collagen phase remarkably increases with cracking. Recent research shows that cracking in the bio-material is a stable process in macroscopic point of view, in which the fracture process zone widely spreads and in space, rather than the unstable process in many brittle/quasi-brittle materials, and that the high performance of the material is achieved by a shear ligament toughening mechanism. In this study, we solve a problem on cracking process under tensile test of model specimen with staggered micro-structure by using FEM and a simplified model, and discuss the relationship between the macroscopic behaviour and the fundamental properties of micro-structure. We find that the crack initiation in such staggered micro-structure originates from the loss of macroscopic stability and the following strain concentration. Coupling the normal debonding and shear sliding at interface of hard phases, a stable behaviour is achieved globally before a globally unstable point in stress-strain space, in which locally unstable domains do not contribute to the macroscopic instability. This mechanism can be considered as a stability enhancement, i.e. a kind of toughening. The cracking behaviour of our model shows size effect. The macroscopic stable stage is significantly affected by both the model and grain size of hard phase. Our research offers a different angle of view in exploring the microscopic mechanism of cracking process of staggered laminate bio-material.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room2)

[SY-E14] A brittle to ductile transition modeling for liquid metal embrittlement

○Thierry Auger （CNRS, France）

Liquid metal embrittlement is a surface adsorption induced fracture phenomenon that is currently not easily amenable to modeling. A strategy framed in terms of a competition between dislocation emission and Griffith fracture at the crack tip will be presented within the standard brittle to ductile transition realm. The goal is to be able to qualitatively predict the sensitivity to LME by coupling atomic scale modeling with a semi-continuous approach. The brittle to ductile transition description of an elastically loaded crack tip has been adapted to LME that relies on solid-liquid surface energy modeling at the atomic scale by AbInitio molecular dynamics and generalized stacking faults modeled at the atomic scale within the Peirls-Nabarro framework. We will present preliminary results on a model system for LME and a comparison with experimental results in terms of sensitivity.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room2)

[SY-E14] Buckling delamination of ductile thin films on rigid substrates

○Nadia Ben Dahmane, Guillaume Parry, Rafael Estevez （Univ. Grenoble Alpes, SIMAP, F-38000 Grenoble, France）

Thin film coatings submitted to high compressive stresses may experience a simultaneous buckling and delamination phenomenon called "blistering". The mechanism of formation and propagation of blisters in the form of straight wrinkles and circular blisters has been extensively studied in the literature considering a linear elastic behaviour of the film[1,2]. The recent developments in numerical calculations allowed a better understanding of the mechanism of formation and propagation of complex buckling geometries including wavy buckles. In particular, the relationship between the mode mixity dependent interfacial toughness and the morphology of the wavy buckles has been elucidated[3].

However, up-to-date, the response of ductile thin films deposited on rigid substrates remains an open issue. For instance, it has been evidenced experimentally[4] that circular blisters in ductile thin films exhibit larger folding angles at their base compared to the elastic model predictions. In addition, recent experimental observations of 400nm gold films deposited on silicon wafers showed straight buckles with higher deflections compared to the elastic model. These differences in morphology are thought to originate from the elastic-plastic response of the film but the governing features need to be clarified.

In this work, we are interested in the observation and characterization of buckling structures observed on gold films deposited on silicon substrates. In this context, we carried out a Finite Elements simulations with a model that accounts for isotropic yielding and the non-linearity of the film. A mode mixity dependent cohesive zone model is used to describe the thin film/substrate interface. This model allowed us to highlight the effect of plasticity on the equilibrium profiles resulting from elastic-plastic blistering, for both straight and circular blisters morphologies. In particular, a stabilizing effect of the circular blister form, which has been observed experimentally, has been demonstrated through calculation.

[1] Hutchinson et al., Adv. in Appl. Mech. 29 (1992) 63.
[2] Hutchinson et al. Acta Metallurgica Materialia, 40 (1992) 295
[3] Faou et al., J. Mech. Phys. Sol., 75 (2015) 93.
[4] Coupeau et al., Thin Solid Films 469 (2004) 221.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room2)

[SY-E14] An analytical model of the peeling forces at edges of multilayers subjected to temperature variations

○Chengyin Zhang[2], Neng-Hui Zhang[1,2] （1.Department of Mechanics, College of Sciences, Shanghai University, China, 2.Shanghai Key Laboratory of Mechanics in Energy Engineering, Shanghai Institute of Applied Mathematics and Mechanics, Shanghai University, China）

Due to different mechanical properties of various materials in a multilayered beam or plate, there is a thermal mismatch between layers when the structural temperature changes. The interfacial peeling stresses and interfacial shear stresses caused by the thermal mismatch can result in a delamination between layers, especially in the edge regions, and this can lead to the damage of a layered structures. Because of the complexity of the boundary stresses, it is difficult to obtain exact a closed-form solution for these interfacial thermal stresses in the edge regions. Therefore, instead of the precise stress field, we divert to the interfacial

peeling moment integrated by the localized interfacial normal stress and the interfacial shear force integrated by the localized interfacial shear stresses. The in-plane stresses in terms of Zhang's two-variables are integrated across the cross section in the far-field region in order to formulate the interfacial peeling moment and interfacial shear force in the edge regions for the multilayered beam system. To verify the applicability of the analytical model of the peeling forces (including interfacial peeling moment and shear force), an aluminum-silicon bimaterial beam in electronic devices is taken as a calculating sample. The influence of the thickness and Young's modulus of the film on the peeling forces are discussed. And the analytical predictions have a good agreement with the results from a finite-element analysis.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room2)

[SY-E14] Characterization and multi-scale modeling of the mechanical response of the human humerus under dynamic loading

○Jamila Rahmoun[1], Hakim Naceur[1], Pascal Drazetic[2], Christian Fontaine[3] （1.LAMIH-ENSIAME, Valenciennes University, France, 2.LAMIH-IUT, Valenciennes University, France, 3.Lab. d'anatomie, Lille University, France）

The relevance and biofidelity level of the human numerical models are key issues in car accidents related trauma research. To limit the risk of injuries of upper extremities and plan the preventive intervention, the humerus biomechanical properties must be correctly assessed. However, the constitutive laws used are largely derived from experimental characterizations carried out at the macroscopic scale without taking into account the bone architecture. A multi-scale approach coupled with nanoindentation experiments revealed to be more appropriate when the robustness of computation and accuracy of results are of interest.

In this study, we propose a multi-scale approach for the accurate characterization and modeling of the mechanical behavior of the human humerus under dynamic loading. The present model is based on the coupling between the Mori-Tanaka homogenization scheme, and an isotropic elastic damage model in the thermodynamic framework. In order to consider the strain rate effect on the humerus behavior, the standard model of Johnson-Cook is adopted. The obtained model is implemented using a User Material routine within the code LS-DYNA. The validity of the resulting FE model has been validated by comparing numerical predictions with experimental observations from characterization tests at different length-scales. To this end, a first experimental campaign was undertaken by means of nanoindentation tests on prismatic samples extracted directly from the same humerus diaphysis in order to determine its microscopic elastic properties. Then, local measurements of the damage effects were performed using several tension/compression and bending tests on small humerus specimens. Once the humerus material parameters were determined, a set of global validation bending impact tests composed of nine humeri were carried out using a drop tower for the determination of the mechanical response and the damage growth until complete humerus fracture.

The outcome of the proposed multi-scale model appears to correctly predict the general trends observed experimentally via the good estimation of the humerus ultimate impact load. The fracture patterns predicted by the proposed damage model are consistent with the physical humerus rupture even if this model is limited only to the estimation of the failure initiation.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F13] Symposium F-13

Chair: Takayuki Aoki(Tokyo Institute of Technology, Japan)
Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room3

[SY-F13] Advanced analysis tools for atomistic microstructure modeling
○Alexander Stukowski （Dept. of Materials Science, Darmstadt University of Technology, Germany）

[SY-F13] Studing thermo-oxidative degradation of polyimide in oxygen enviorment using MD simulations
○Ashwani Kumar Sengar, Sumit Basu （IIT Kanpur, India）

[SY-F13] In-plane characterization of structural and thermodynamic properties for steps at faceted chemically heterogeneous solid/liquid interfaces
○Hongtao Liang[1], Brian B. Laird[2], Mark Asta[3], Yang Yang[1] （1.Physics Department and State Key Laboratory of Precision Spectroscopy, School of Physical and Material Science, East China Normal Universit, China, 2.Department of Chemistry, University of Kansas, United States of America, 3.Department of Materials Science and Engineering, UC Berkeley, United States of America）

[SY-F13] Design of neural network for thermodynamics data of non-equilibrium multiphase field model
○Hiroshi Wakameda[1], Sukeharu Nomoto[1], Akinori Yamanaka[3], Toshiyuki Koyama[2] （1.ITOCHU Techno-Solutions Corporation, Japan, 2.Materials Design Innovation Engineering, Nagoya Univ., Japan, 3.Department of Mechanical Systems Engineering, Tokyo University of Agriculture and Technology, Japan）

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room3)

[SY-F13] Advanced analysis tools for atomistic microstructure modeling

Invited

○Alexander Stukowski （Dept. of Materials Science, Darmstadt University of Technology, Germany）

Direct molecular dynamics (MD) simulations of materials microstructures become feasible thanks to fast growing computing capacities and can deliver a wealth of important observations on fundamental mechanisms. Such simulations are cross-scale rather than multi-scale, i.e. simultaneously large enough to represent meso- and macroscopic structures and processes and yet fully resolved, tracing every "jiggle" of atomic motion. Our recent MD simulations of dislocation-based crystal plasticity will be presented as an example [Nature 550, 492-495 (2017)].

To deal with the overwhelming complexity of processes on these scales, we develop advanced computational methods and tools to recast the massive transient trajectory data generated in large-scale MD simulations into a human comprehensible and analyzable form using methods of "in-situ computational microscopy". These algorithms automatically identify grain boundaries, surfaces and interfaces, dislocations, other defects, structural phases and deformation fields and can track their evolution. The data reduction and transformation of the underlying MD model into high-level microstructure representations make insightful visualization, quantitative analyses and linking with higher-scale materials models possible.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room3)

[SY-F13] Studing thermo-oxidative degradation of polyimide in oxygen enviorment using MD simulations

○Ashwani Kumar Sengar, Sumit Basu （IIT Kanpur, India）

Polyimides are important class of high-temperature polymers. These polyimides finds applications in diverse fields such as aerospace, electronics and automobiles. PMR-15 is one these polyimide which is extensively used as matrices for composite in the aerospace industry due to its high glass transition temperature, mechanical strength with high modulus of elasticity. However diffusion of oxygen in polymer and subsequent reaction with polymer leads to formation of oxidized layer. This layer drastically changes the mechanical properties of the polymer. Since these polyimide's founds application in aircraft design, so thermo-oxidative degradation of polymer may prove fatal and catastrophic in oxygen rich environment. Crack initiation and damage growth also follows due to thermo-oxidative degradation. We will be studying thermo oxidative degradation of PMR-15 polymer through molecular dynamics(MD) simulation. Molecular simulations has been become quite popular tool to predict macroscopic properties of polymer through statistical study at atomistic level. However getting correct force field parameter to simulate an exact material is challenging and of utmost importance. We attempt to study PMR-15 polymer with its full atomistic details intact and predicting it micromechanical properties through MD simulation. Due to some computational and forcefield limitations, coarse grained model of polyimide had been previously studied. In our analysis, we don't make any pre-assumption of course graining during sample preparation. We prepare our sample of PMR-15 with correct cross linking strategy such that we get density close to experimental value of 1.324. We will quantifies mechanical properties such as elastic constant and phenomenogical quantities such as diffusion constant and tries to predict the life of polymer due to thermo-oxidative degradation. We want challenge the time and scale limitations of MD simulation by attempting to simulate full scale atomistic model of the polymer PMR-

15. This study will give more insight about capabilities of MD simulations and also provides reasons where it fails to give us valid results. This study will provide an alternative path to study the systems where experimental analysis is difficult to setup or too expensive and cumbersome.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room3)

[SY-F13] In-plane characterization of structural and thermodynamic properties for steps at faceted chemically heterogeneous solid/liquid interfaces

○Hongtao Liang[1], Brian B. Laird[2], Mark Asta[3], Yang Yang[1]　(1.Physics Department and State Key Laboratory of Precision Spectroscopy, School of Physical and Material Science, East China Normal Universit, China, 2.Department of Chemistry, University of Kansas, United States of America, 3.Department of Materials Science and Engineering, UC Berkeley, United States of America)

We present a methodology for studying steps at faceted chemically heterogeneous solid/liquid interfaces based on molecular-dynamics simulations. The methodology is applied to a faceted Al(111)/Pb(liquid) interface yielding a direct calculation of step free energy and extensive atomic-scale characterization for the interfacial layer containing the step. We characterized the step by calculating the in-plane density, potential energy, pressure components and stresses profiles. Main findings include: i) Calculated step free energy is in good agreement with TEM experimental measurement. ii) The step is connecting the interface liquid under tension and the interface solid under compression. iii) Fundamental properties of interface solid and interface liquid show orders of magnitudes difference in comparing with those predicted from the bulk Al-Pb alloy phase diagram. It is hoped that the methodology is extendable to the exploration of complexion equilibria/transitions at grain boundaries.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room3)

[SY-F13] Design of neural network for thermodynamics data of non-equilibrium multiphase field model

○Hiroshi Wakameda[1], Sukeharu Nomoto[1], Akinori Yamanaka[3], Toshiyuki Koyama[2]　(1.ITOCHU Techno-Solutions Corporation, Japan, 2.Materials Design Innovation Engineering, Nagoya Univ., Japan, 3.Department of Mechanical Systems Engineering, Tokyo University of Agriculture and Technology, Japan)

We construct neural network which estimates Gibbs free energy and chemical potential from temperature and composition of system for non-equilibrium multiphase field model. The mini-batch gradient descent method is selected for training of which data is led from calculation of non-equilibrium multiphase field model using Thermo-Calc thermodynamic database. We achieve highly precision neural network enough to use in non-equilibrium multiphase field model by introducing minimum and maximum data to the mini-batch method.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F14] Symposium F-14

Chair: Markus Kuehbach(Max-Planck-Institut fur Eisenforschung GmbH, Germany)

Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room3

[SY-F14] Large-scale multiphase flow simulations on a GPU supercomputer

○Takayuki Aoki （Tokyo Institute of Technology, Japan）

[SY-F14] **Transport Properties Of Fluid Mixtures In Micro- And Mesoporous Kerogen Membranes**

○Patrick Alain Bonnaud[1], Romain Vermorel[1], Julien Collell[2], Guillaume Galliéro[1] （1.University of Pau and Adour Countries, France, 2.Total E&P, France）

[SY-F14] Numerical simulation of ionic transport through deformable porous media: application to cortical bone tissue modeling

○Jana Turjanicova[1,2], Eduard Rohan[1,2], Vladimír Lukeš[2] （1.Dept. of Mechanis, Univ. of West Bohemia in Pilsen, Czech Republic, 2.NTIS - New technologies for information society, Czech Republic）

[SY-F14] Hydrogen Transport and Thermal Desorption in Multiphase Steels

○Andrej Turk[1], Pedro E.J. Rivera-Díaz-del-Castillo[2], Enrique Galindo-Nava[1] （1.University of Cambridge, UK, 2.Lancaster University, UK）

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room3)

[SY-F14] Large-scale multiphase flow simulations on a GPU supercomputer

Invited

○Takayuki Aoki （Tokyo Institute of Technology, Japan）

GPU (Graphics Processing Unit) was originally designed for graphics rendering and has been widely used for supercomputers in the world, since it has high computational performance and wide memory bandwidth and suitable for scientific computing. We have developed stencil codes written in CUDA and executed them on a GPU supercomputer TSUBAME. Several simulations of gas-liquid and gas-solid two-phase flows are demonstrated with the numerical methods and the algorithms such as AMR (Adaptive Mesh Refinement) and dynamic load balance for efficient large-scale simulations.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room3)

[SY-F14] Transport Properties Of Fluid Mixtures In Micro- And Mesoporous Kerogen Membranes

○Patrick Alain Bonnaud[1], Romain Vermorel[1], Julien Collell[2], Guillaume Galliéro[1] （1.University of Pau and Adour Countries, France, 2.Total E&P, France）

With the exhaustion of conventional resources, the production of gas from organic-rich shales has encountered a rising interest over the last 15 years. In such resources, gas is trapped in nodules of organic matter scattered in an inorganic matrix mostly constituted of quartz, clays, and calcite. Nodules represent only few percentages of the total volume of shales and result from a maturation process during the burial stage. These nodules of organic matter contain mostly kerogen that acts as a source, but also as a container of hydrocarbons. Various forms were reported differentiating to each other by their origin, their maturity, and sediment history, which affects, for example, their chemical composition, their density, and the porosity. A common feature of kerogens is their multi-scale porous network with pore sizes ranging from micropores (<2 nm) to macropores (>50 nm). Structure and connectivity of pores greatly affect the materials permeability. In porous structures where the flow is limited by micropores (e.g., pore throats), very low permeabilities are observed.

Despite the important development of shales, fluid flow mechanisms within kerogen matrix remains poorly understood. While experimental characterization remains difficult, molecular dynamics simulations were proven very useful to characterize transport mechanisms within kerogen membranes. The aforementioned studies staid limited to microporous systems, while mass transfer originating from small pores and transiting to larger pores, fractures, and production wells is a multi-scale mechanism. In this work, we designed and developed molecular simulation tools to capture both microporosity and mesoporosity of kerogen through the aggregation and the spatial arrangement of smaller basic units in order to generate representative molecular structures. From those models, we investigated by molecular dynamics simulations how the nature (i.e., maturity and sediment origin) and the chemical composition influence both the porous network and the related physical and transport properties of fluid mixtures (e.g., selectivity, phase coexistence, diffusivity) in kerogen.

This method and findings underscore the importance of accounting for both micro- and mesoporosity to

accurately model fluid transport in kerogen.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room3)

[SY-F14] Numerical simulation of ionic transport through deformable porous media: application to cortical bone tissue modeling

○Jana Turjanicova[1,2], Eduard Rohan[1,2], Vladimír Lukeš[2] (1.Dept. of Mechanis, Univ. of West Bohemia in Pilsen, Czech Republic, 2.NTIS - New technologies for information society, Czech Republic)

Cortical bone tissue is known to have a strictly hierarchical porous structure on multiple scales. On the canalicular-lacunar scale, it consist of two phases: deformable collagen-apatite matrix charged by a small electric charge and bone fluid filling the pore space created by network of small interconnected channels. Bone fluid is considered an electrolyte solution of two species of charged monovalent ions of opposite polarizations. Due to the potential differences, the electrical double layer occurs in the proximity of the solid-fluid interface. Considering its effect, the transport of such electrolyte through a network of small channels with charged surface is controlled by coupling between the electric field , Stokes flow, the migration-diffusion process and deformation of solid matrix.

In order to describe cortical bone effective properties on the macroscopic scale, the unfolding homogenization method is applied on the model of ionic transport through deformable porous media. The microstructure on canalicular-lacunar scale is simplified by assumption of its periodicity and is represented by so-called representative periodic cell. The characteristic responses on this cell are used to compute the effective coefficients describing cortical bone behavior on the macroscopic scale (scale of one osteon). Macroscopic model behavior was tested on the simple boundary value problem. Implementation of upscaling process as well as numerical simulation on the macroscopic model was made in in-house developed python based FEM software SfePy.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room3)

[SY-F14] Hydrogen Transport and Thermal Desorption in Multiphase Steels

○Andrej Turk[1], Pedro E.J. Rivera-Díaz-del-Castillo[2], Enrique Galindo-Nava[1] (1.University of Cambridge, UK, 2.Lancaster University, UK)

Hydrogen diffusion is modelled using a 2D multi-trap diffusion model. It takes into account trapping on crystal defects (dislocations, carbides and grain boundaries), as well as the presence of secondary phases with different hydrogen diffusivity and solubility. Secondary phases introduce local discontinuities in the hydrogen concentration field and this problem has not been modelled systematically in multiphase steels. The first studied case is a 2D simulation of thermal desorption in high-strength bainitic steels with varying fractions of retained austenite where the effects of austenite morphology are highlighted. The second case is a different thermal desorption problem in a high-temperature iron-nickel FCC alloy in which grain boundaries are known to be fast diffusion pathways. As the boundaries require a prohibitively fine discretisation in 2D, the microstructure is parameterised and reduced to 1D. The effects of grain boundary properties on hydrogen diffusion are studied. Lastly, we explore the application of the model to other interstitial elements and metallic systems, where the morphology and spatial arrangement of the microstructure strongly affects

elemental diffusion.

Symposium | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[SY-N7] Symposium N-7

Chair: Shotaro Hara(Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan)
Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room4

[SY-N7] Bridging Time Scales with Variationally Enhanced Sampling
○Omar Valsson （Max Planck Institute for Polymer Research, Germany）

[SY-N7] Simulations of Branched Polyelectrolytes
○Filip Uhlik （Charles University, Czech Republic）

[SY-N7] Adaptive resolution simulations coupling molecular dynamics to dissipative particle dynamic
○Matej Praprotnik （National Institute of Chemistry, Slovenia）

[SY-N7] Using Diffusive Molecular Dynamics Simulations to Investigate Grain Boundary Segregation and Grain Boundary Structural Transformations
Louis Hebrard, ○Chad W Sinclair （Dept. of Materials Engineering, University of British Columbia, Canada）

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room4)

[SY-N7] Bridging Time Scales with Variationally Enhanced Sampling

Invited

○Omar Valsson （Max Planck Institute for Polymer Research, Germany）

The usefulness of atomistic simulations is generally hampered by the presence of several metastable states separated by high barriers leading to kinetic bottlenecks. Transitions between metastable states thus occur on much longer time scales than one can simulate. Numerous enhanced sampling methods have been introduced to alleviate this time scale problem, including methods based on identifying a few crucial order parameters and enhancing their sampling through the introduction of an external biasing potential.

Here will we discuss Variationally Enhanced Sampling (Valsson and Parrinello, PRL 113 090601, 2014), a generally applicable enhanced sampling method where an external bias potential is constructed by minimizing a convex functional. We present numerous examples from physics and chemistry which show the flexibility and practicality of the method. We will furthermore show how the variational property of the method can be used to extend the method in various innovative ways, e.g.: to obtain kinetic information from atomistic simulation; to accelerate nucleation events by employing models from classial nucleation theory; and to incorporate experimental information into molecular simulations.

We will also introduce the VES code (http://www.ves-code.org), an open-source library for the PLUMED 2 plugin that implements methods based on Variationally Enhanced Sampling

---

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room4)

[SY-N7] Simulations of Branched Polyelectrolytes

○Filip Uhlik （Charles University, Czech Republic）

Polyelectrolytes (PEs) are polymers with ionizable groups. Under suitable conditions, PEs are soluble in aqueous media. This property makes them attractive for biological, medicinal and environment-friendly applications that require organization of matter at nanoscale. The applications of PEs range from drug carriers, water pollutants removal, oil recovery to sea water desalination. In some of them, *e.g.* as thickening agents or super-absorbents in diapers, they have already reached mass production.

In this contribution a general and efficient simulation technique based on hybrid Monte Carlo (HMC) method will be described. HMC uses dynamics for evolution, but dynamics of a long polymer with N beads is itself slow (Rouse time $\propto N^2$). For this reason we use a faster *unphysical* evolution with a modified Hamiltonian while still efficiently Monte Carlo sampling the Boltzmann distribution with the original one. The resulting simulation is much faster than molecular dynamics and other methods. It is
also well suited for simulations of coarse-grained models of PEs and allows for using reaction and other ensemble [F. Uhlik *et al.* Macromolecules 47 (2014) 4004].

Results for several types of branched PEs (*e.g.*, stars and combs) for different conditions of solvent quality, Bjerrum and Debye lengths will be given. While strong PEs remain fully ionized, the degree of ionization of weak PEs can be influenced by both changing pH and ionic strength. This results in a responsiveness to external stimuli needed in many applications. The conformations of weak PEs are coupled with charge redistribution and this can lead to unexpectedly complex behavior. For example, strong PE stars in marginally

poor solvents form bundles while weak PE stars redistribute charge and form core-shell structures with some arms uncharged and collapsed and others charged and extended. Behavior of other branching types as well as formation of inter-polyelectrolyte complexes will be also discussed.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room4)

[SY-N7] Adaptive resolution simulations coupling molecular dynamics to dissipative particle dynamic

○Matej Praprotnik （National Institute of Chemistry, Slovenia）

We present the hybrid coupling of the molecular dynamics (MD) and dissipative particle dynamics (DPD) methods, bridging the micro- and mesoscopic levels of detail. The coupling is achieved using the adaptive resolution scheme (AdResS), which is a linear momentum conserving multiscale method. Our methodology is thus suitable for simulations of liquids on the micro/mesoscopic scale, where hydrodynamics is crucial. The presented approach is showcased for water at ambient conditions. The supramolecular coupling is carried out by our clustering algorithm SWINGER that assembles, disassembles, and reassembles water clusters on demand during the course of the simulation. This allows for a seamless coupling between standard atomistic MD and DPD models.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room4)

[SY-N7] Using Diffusive Molecular Dynamics Simulations to Investigate Grain Boundary Segregation and Grain Boundary Structural Transformations

Louis Hebrard, ○Chad W Sinclair （Dept. of Materials Engineering, University of British Columbia, Canada）

We have investigated the time evolution of segregation on both grain boundary structural and chemical transitions in Al-Mg alloys by means of alloy diffusive molecular dynamics (a-DMD) calculations. The predictions with regard to segregation are compared with classic continuum approaches including the calculation of grain boundary free energy curves. The role that chemical segregation plays in grain boundary structural transitions (complexions) is studied and used to construct temperature-pressure-composition stability plots for one particular grain boundary.

Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D5] Symposium D-5

Chair: Jörg Neugebauer(MPIE, Germany)
Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room8

[SY-D5] Computational exploration of strong permanent magnet compounds
○Takashi Miyake[1,2,3] (1.CD-FMat, AIST, Japan, 2.ESICMM, NIMS, Japan, 3.CMI[2], NIMS, Japan)

[SY-D5] A machine-learning approach for finding new hard-magnetic phases
Johannes J. Möller, ○Daniel F. Urban, Christian Elsässer (Fraunhofer IWM, Freiburg, Germany)

[SY-D5] High-throughput optimization of finite temperature phase stabilities of Ce-based hard magnetic materials
○Tilmann Hickel, Halil Soezen, Fritz Koermann, Joerg Neugebauer (Max Planck Institut fur Eisenforschung, Germany)

[SY-D5] Understanding pairwise magnetic interactions in Fe-based materials with machine learning techniques
○Osamu Waseda, Omkar Hegde, Tilmann Hickel, Jörg Neugebauer (MPIE, Germany)

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room8)

[SY-D5] Computational exploration of strong permanent magnet compounds

Invited

○Takashi Miyake[1,2,3]　(1.CD-FMat, AIST, Japan, 2.ESICMM, NIMS, Japan, 3.CMI[2], NIMS, Japan)

Modern strong magnets are rare-earth magnets in which high saturation magnetization and high Curie temperature come from transition-metal 3d electrons, and strong magnetorcystalline anisotropy originates from rare-earth 4f electrons [1]. There are various types of crystal structures and chemical composition, and exploration of a new magnet compound is a hot topic. Among them, RFe$_{12}$-type compounds with the ThMn$_{12}$ structure are attracting renewed interest because of their high iron content. Recently synthesized NdFe$_{12}$N$_x$ film has higher saturation magnetization and anisotropy field than Nd$_2$Fe$_{14}$B, although its bulk phase is thermodynamically unstable. I will present a first-principles study on the effect of element substitution on magnetism and structural stability. I will also discuss how machine learning accelerates magnetic-materials discovery. Application to the Curie temperature of RFe$_{12}$-type compounds shows that Bayesian optimization offers an efficient way to optimize chemical composition of magnet compounds. Kernel ridge regression using orbital-field matrix as a descriptor reproduces the magnetic moment and formation energy of thousands of transition-metal compounds in reasonable accuracy [2], which can be utilized for virtual screening of new magnetic compounds. Bayesian optimization approach to crystal structure prediction is also presented [3].

[1] Takashi Miyake and Hisazumi Akai, J. Phys. Soc. Jpn. **87**, 041009 (2018).
[2] T.L. Pham et al., Sci. Tech. Adv. Mater. **18**, 756 (2017).
[3] T. Yamashita et al., Phys. Rev. Mater. **2**, 013803 (2018).

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room8)

[SY-D5] A machine-learning approach for finding new hard-magnetic phases

Johannes J. Möller, ○Daniel F. Urban, Christian Elsässer　(Fraunhofer IWM, Freiburg, Germany)

Data-mining and machine-learning (ML) techniques play an increasingly important role in the discovery and development of new materials. In this contribution, we use kernel-based learning methods to predict optimal chemical compositions for new permanent magnets, which are key components in many green-energy technologies. The magnetic-property data used for training and testing the ML models were obtained by a combinatorial high-throughput screening (HTS) using density-functional theory calculations. For encoding the structural and chemical information of the HTS data in a machine-readable format, we use several existing and newly developed material descriptors and assess the predictive power of the ML models built with them. The accuracy of the ML models with an optimal choice of descriptor and model parameters enables the prediction of promising structurecomposition combinations for substitutes of state-of-the-art magnetic materials like Nd2Fe14B - with similar intrinsic hard-magnetic properties but no or less amounts of critical rare-earth elements.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room8)

[SY-D5] High-throughput optimization of finite temperature phase stabilities of Ce-based hard magnetic materials

○Tilmann Hickel, Halil Soezen, Fritz Koermann, Joerg Neugebauer （Max Planck Institut fur Eisenforschung, Germany）

While the present search for novel materials concepts to improve hard magnetic applications is concentrated on the magnetic properties of individual phases, their finite temperature phase stabilities are largely unknown. In the Ce-Fe-Ti ternary system, for example, the promising phase $CeFe_{11}Ti$ is competing with various Laves phases as demonstrated by energy-dispersive X-ray spectroscopy (EDS) measurements. We therefore use concepts of ab initio thermodynamics capturing vibrational, electronic and magnetic entropy contributions in order to determine the Helmholtz free energy of all relevant phases. Several additional elements have been considered within this formalism, to investigate their partitioning and impact on the relative phase stabilities. The insights obtained demonstrate how the screening of a complete set of transition metals in quarternary hard magnetic materials can be performed most efficiently and which alloying elements improve the stability of promising phases such as $CeFe_{11}Ti$ most substantially.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room8)

[SY-D5] Understanding pairwise magnetic interactions in Fe-based materials with machine learning techniques

○Osamu Waseda, Omkar Hegde, Tilmann Hickel, Jörg Neugebauer （MPIE, Germany）

Magnetic interactions are crucial to the stability of structural phases as well as for various thermophysical effects such as magnetocalorics. Despite their importance, there is no experimental procedure which allows for the understanding of magnetic interactions at the atomic level, and there is no exact theoretical model capable of describing them precisely except for expensive ab initio methods. It has been recently suggested that the Heisenberg Landau model has sufficient versatility to map the contribution of complex magnetic interactions of Fe-based materials to the free energy. Its original form, however, contains a high number of parameters which make it prone to overfitting. In this study, we mapped the magnetic interactions created from spin-polarised DFT calculations to extended Heisenberg-Landau models via various machine learning regression techniques. The free energy contribution of the magnetic interactions is then determined through Monte Carlo simulations for millions of atoms which would otherwise not be achievable with ab initio methods. The results enable us to understand the overall effects of impurities contained within microstructures on the magnetism in iron based materials.

Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D6] Symposium D-6
Chair: Daniel Urban(Fraunhofer IWM, Germany)
Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room8

[SY-D6] Novel two-dimensional materials: Materials discovery, data provenance, and workflow reproducibility.
○Nicola Marzari （EPFL, Switzerland）

[SY-D6] In silico screening of Metal-Organic Frameworks for adsorption driven heat pumps and chillers
○Mate Erdos[1], Martijn F. de Lange[1], Freek Kapteijn[2], Othonas A. Moultos[1], Thijs J. H. Vlugt[1]
 （1.Engineering Thermodynamics, Process &Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Netherlands, 2.Catalysis Engineering, Chemical Engineering Department, Delft University of Technology, Netherlands）

[SY-D6] Machine learning assisted by first-principles calculations for designing intermetallic-typed metallic glasses
○Tokuteru Uesugi, Manami Sakai, Yorinobu Takigawa, Kenji Higashi （Dep. of Materials Science, Osaka Prefecture Univ., Japan）

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room8)

[SY-D6] Novel two-dimensional materials: Materials discovery, data provenance, and workflow reproducibility.

Invited

○Nicola Marzari （EPFL, Switzerland）

Two-dimensional materials have seen in the past decade very dedicated experimental and theoretical efforts in the quest for novel physics and functionalities. Here, we systematically explore with first-principles calculations known inorganic materials, to identify those that could be exfoliated into two-dimensional layers. We start by curating experimental materials databases, collecting reliable data for 110,000 unique compounds. Then, we identify those that appear layered according to simple geometric and bonding criteria, and launch high-throughput calculations - based on van-der-Waals density-functional theory and 2D density-functional perturbation theory - to characterize binding energies, stability, and properties. Remarkably, we find close to 2000 inorganic compounds that could be exfoliated into novel two-dimensional materials, and recover in the process the known ones - from graphene to transition-metal dichalcogenides to boron nitride and black phosphorus. I'll provide a perspective on the promising properties we are uncovering - topological, electrical, magnetic, chemical - while highlighting the need for scalable approaches to data and calculations, able to persist and query the full provenance of the data and ensure reproducibility of the calculations' workflows.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room8)

[SY-D6] In silico screening of Metal-Organic Frameworks for adsorption driven heat pumps and chillers

○Mate Erdos[1], Martijn F. de Lange[1], Freek Kapteijn[2], Othonas A. Moultos[1], Thijs J. H. Vlugt[1] （1.Engineering Thermodynamics, Process &Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Netherlands, 2.Catalysis Engineering, Chemical Engineering Department, Delft University of Technology, Netherlands）

20% of the total energy demand is attributed to hot water production and space heating/cooling of buildings. Although, it is intended to produce more and more energy from clean low carbon sources for heating/cooling, 75% of it is still acquired by using fossil fuels. To ameliorate the dependence on fossil fuels and increase energy efficiency, several technologies have emerged recently, utilizing renewable energy sources for heating/cooling applications. Among these, adsorption driven heat pumps and coolers (AHP/ACs) are promising candidates because these devices can utilize thermal energy instead of electricity. However, a drawback of AHP/ACs systems is the lower performance compared to heat pumps based on absorption or chemical reactions. One possible way to improve the energy efficiency of AHP/ACs is by finding adsorbents with enhanced adsorption and thermophysical properties. Metal-Organic Frameworks in conjunction with alcohols (methanol, ethanol) are promising working pairs for this application.
A computational screening of MOFs is carried out to find the best performing structures for AC applications with methanol and ethanol as working fluids. Molecular simulations using Monte Carlo method are conducted to investigate 2930 structures. An efficient screening methodology is devised with 4 subsequent screening steps. The commensurate adsorption behavior of the adsorbates is exploited to reduce computational effort. In the last screening step, the 6 best performing MOFs with high deliverable working capacities (~0.6 ml working fluid in 1 ml structure) and diverse adsorption step locations are selected from

the original 2930 structures for each adsorbate. The finally selected structures show higher deliverable working capacities than the reported highest values (~0.45 ml working fluid in 1 ml structure).

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room8)

[SY-D6] Machine learning assisted by first-principles calculations for designing intermetallic-typed metallic glasses

○Tokuteru Uesugi, Manami Sakai, Yorinobu Takigawa, Kenji Higashi （Dep. of Materials Science, Osaka Prefecture Univ., Japan）

Metallic glasses have interesting properties such as low Young's moduli, high corrosion resistance and high wear resistance and are considered new materials in many fields. The factors that contribute to the glass-forming ability (GFA) are an important consideration in the design of new metallic glasses. Ternary metallic glasses are classified into three types on the basis of their atomic size distribution. The factors that affect the GFAs of the metallic glasses are presumed to vary among the three types. However, metallic glasses with two alloying elements exhibit irregular composition ratios or atomic radii; thus, in these cases, the contributing factor is unclear. The binary metallic glasses usually crystallize only intermetallic crystalline phase after heating. For example, Ti-Cu and Ti-Ni binary metallic glasses crystallized as only TiCu and Ti_2Ni intermetallic compounds. Therefore, these metallic glasses such as Ti-Cu and Ti-Ni are able to be called as intermetallic-typed metallic glasses (IMG). In this work, we aimed to elucidate the design criteria of IMG and design new metallic glasses based on the machine learning assisted by the first-principles calculations. First, the first-principles calculations were performed on intermetallic compounds and then, explanatory variables were calculated. Second, a regression systems of GFA was constructed using artificial neural networks (ANN) and logistic regression analysis (LRA). The results of ANN validation showed very high accuracy than the results of LRA validation. The partial regression coefficients of LRA indicated the design criteria of intermetallic-typed metallic glasses. The obtained regression systems were applied to intermetallic compounds whose GFA are unknown, and the alloy systems of a novel metallic glass were predicted.

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H11] Symposium H-11

Chair: Erik Van der Giessen(University of Groningen, Netherlands)
Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room9

[SY-H11] A Hierarchical Multiscale Simulations Approach for Modeling Failure in Polymer Matrix Composites

Xiawa Wu[1], Amin Aramoon[1], Christopher Woodward[2], ○Jaafar A. El-Awady[1] （1.Johns Hopkins University, United States of America, 2.Air Force Research Laboratory, United States of America）

[SY-H11] Some Positive Aspect of Structural Defects in Graphene/Polymer Nanocomposites Studied by Abinitio,Molecular Dynamics, and Continuum Approaches

○Seunghwa Yang[1], Janghyuk Moon[1], Maenghyo Cho[2] （1.School of Energy Systems Engineering, Chung-Ang University, Korea, 2.School of Mechanical and Aerospace Engineering, Seoul National University, Korea）

[SY-H11] Linear and non-linear viscoelastic properties of model fractal-like aggregates polymer nanocomposites

○Samy MERABIA[1], Yang WANG[1], François DETCHEVERRY[1], Marc COUTY[2], Gaëtan MAUREL[2] （1.CNRS and Universite Lyon 1, France, 2.MFP Michelin, Clermont-Ferrand , France）

[SY-H11] **Topological defect structure in the self-assembly of semiflexible polymers under spherical confinement**

○Mihir Khadilkar, Arash Nikoubashman （Johannes GutenBerg University Mainz, Germany, Germany）

[SY-H11] Molecular dynamics simulation of the detachment force between graphene and epoxy resin

○Kazuki Mori[1], Makoto Yabe[2], Yuji Kohno[2], Jun Koyanagi[3] （1.ITOCHU Techno-Solutions Corporation, Japan, 2.Yokohama National University, Japan, 3.Tokyo University of Science, Japan）

[SY-H11] Relation between deformation and electrical conductivity for electroconductive polymer nanocomposites with highly segregated structure

○Oleg V. Lebedev[1], Sergey Abaimov[1], Alexander Ozerin[2], Anton Trofimov[1], Iskander Akhatov[1] （1.Center for Design, Manufacturing and Materials, Skolkovo Institute of Science and Technology, Russia, 2.Laboratory of the Structure of Polymer Materials, N.S. Enikolopov Institute of Synthetic Polymer Materials of RAS, Russia）

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room9)

[SY-H11] A Hierarchical Multiscale Simulations Approach for Modeling Failure in Polymer Matrix Composites

Xiawa Wu[1], Amin Aramoon[1], Christopher Woodward[2], ○Jaafar A. El-Awady[1] (1.Johns Hopkins University, United States of America, 2.Air Force Research Laboratory, United States of America)

Polymer matrix composites (PMCs) are widely used in many automotive, marine, and aerospace applications. Predicting the damage and failure of such systems is of crucial interest for their reliable performance. In this work, a coarse-grained MD model has been developed to characterize the evolution of free volume density (voids) in DGEBA polymers under loading and its subsequently plastic deformation (e.g. hardening and failure). A detailed atomic monomer is coarsened to create the tailored plastic behavior. Cross-linked polymer networks are created under different curing conditions, including temperature, and cross-linker functionality using a dynamic cross-linking algorithm. The effect of chain size, and degree of cross-linking are also investigated. The free volumes are measured as a function of strain by fitting the largest ellipsoids between neighboring chains in the network. From these simulations we develop a direct correlation between the evolution of plastic deformation and the free volume density. The results of these simulations are then upscaled into a finite element simulations to model the damage and failure of PMCs.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room9)

[SY-H11] Some Positive Aspect of Structural Defects in Graphene/Polymer Nanocomposites Studied by Abinitio,Molecular Dynamics, and Continuum Approaches

○Seunghwa Yang[1], Janghyuk Moon[1], Maenghyo Cho[2] (1.School of Energy Systems Engineering, Chung-Ang University, Korea, 2.School of Mechanical and Aerospace Engineering, Seoul National University, Korea)

In this study, we reveal some positive aspect of the intrinsic defect commonly observed in two dimensional nanocarbon structure of graphene as a multifunctional reinforcement. Among the intrinsic defects commonly observed in graphene, we focus on the crystallographic defect of the Thrower-Tone-Wales (TSW) defect. Since the formation of the TSW defects in graphene involves 90 degree of rotation of the two covalently bonded neighboring carbon atoms and the resultant change in electron density, we firstly adopt the density functional theory to investigate the adhesion characteristics of the carbon atoms in TSW defect to the to the polypropylene (PP) monomers. In order to observe the effect of the arbitrarily generated TSW defect on representative volume element level mechanical properties, we modeled transversely isotropic molecular unit cell model of single layer graphene reinforced PP nanocomposites. The stress-strain curves in tension and shear are predicted from a constant strain rate ensemble simulation at below the glass transition temperature of the PP matrix and at the atmospheric pressure. At the same time, the mechanical properties of single layer graphene embedding the TSW defect is studied using the same ensemble simulations. To correlate the locally rippled configuration of the TSW defected sites to the macroscopic stress-strain relation, we analyzed the surface roughness of the graphene according to the density of TSW defects. Finally, a multiphase micromechanics model incorporating the weakened interface between graphene and PP matrix is applied to study the stress-strain relation of poly-dispersed nanocomposites with random graphene orientation. The two rivalling effects of the degradation of the graphene and improvement of the interfacial shear load transfer are evaluated from parametric studies on the effect of the aspect ratio and the volume

fraction of the defected graphene on overall stress-strain relation of poly-dispersed nanocomposites.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room9)

[SY-H11] Linear and non-linear viscoelastic properties of model fractal-like aggregates polymer nanocomposites

○Samy MERABIA[1], Yang WANG[1], François DETCHEVERRY[1], Marc COUTY[2], Gaëtan MAUREL[2] （1.CNRS and Universite Lyon 1, France, 2.MFP Michelin, Clermont-Ferrand , France）

Dispersing solid fillers into a polymer matrix is a common strategy to enhance and tailor its properties. Polymer nanocomposites (PNCs) so obtained with fractal-like aggregates have exceptional rheological behavior that have long been exploited in the tire industry. However, due to disparity of time and length scales, our understanding of the relation between nanocomposites structure and rheology remains far from complete.

In this contribution, we propose a mesoscopic model to describe the dynamics and the rheology of aggregate PNCs. While aggregates are described explicitly as groups of interacting particles, we use for the polymer matrix an implicit description based on generalized Langevin equation, that captures the average effect of a viscoelastic medium. These two-level description allows us to simulate large PNCs systems containing dozens of aggregates.

We focus on the linear and non-linear viscoelastic properties of PNCs. We characterize the influence of aggregate size, rigidity and volume fraction. We show that compared to nanoparticles, aggregates may display levels of reinforcement considerably larger. We also demonsrate that the stress relaxation of aggregates display long relaxation times, which originates in the slow rotation of the aggregates. As concerns non linear properties, we concentrate on the Payne effect characterized by a drop of the storage modulus for small deformation amplitudes. We relate the Payne effect to the deformation and alignment of the aggregates under the imposed deformation direction. We also discuss memory effects, and in particular the slow recover kinetics subsequent to a first deformation. All these considerations may help in building connections between the macroscopic mechanical response of the PNCs and the mesoscopic morphology of the nanofillers.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room9)

[SY-H11] Topological defect structure in the self-assembly of semiflexible polymers under spherical confinement

○Mihir Khadilkar, Arash Nikoubashman   (Johannes GutenBerg University Mainz, Germany, Germany)

Static and dynamic properties of macromolecules are often strongly affected in confinement, due to the enforced constraints on polymer motion and conformation. Moreover, for semiflexible polymers like DNA and actin, the confinement effects also compete with the enthalpic costs of bending. Using coarse-grained molecular dynamics simulations, we explore the phase behavior of semiflexible polymers confined to spheres and thin spherical shells. We observe a disordered-to-nematic ordering transition as a function of chain stiffness accompanied by the emergence of topological defects on the surface. Each of the configuration

variables including chain length, packing density, chain stiffness and shell thickness uniquely affects the phase behavior, including the nature and relative orientation of the defects. Systemic trends observed could pave the way for a better understanding of the links between topological defects and elastic properties of the macromolecules. Further, controlling the nature and locations of these defects could also be crucial in understanding other multiscale biological processes involving these biomolecules like chromosomal packing of DNA and gene regulation.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room9)

[SY-H11] Molecular dynamics simulation of the detachment force between graphene and epoxy resin

○Kazuki Mori[1], Makoto Yabe[2], Yuji Kohno[2], Jun Koyanagi[3] （1.ITOCHU Techno-Solutions Corporation, Japan, 2.Yokohama National University, Japan, 3.Tokyo University of Science, Japan）

We introduced a computational method to investigate the shear detachment strength at a carbon fiber/epoxy resin interface using molecular dynamics simulations. In the computational model, the graphene molecular structure was assumed to be that of a simple carbon fiber. The interaction energies calculated for the epoxy bulk phase were in good agreement with the experimental data in our previous work [1], however, the estimates of surface energy between carbon fiber and epoxy resin were missing. In this work, we calculated the surface energy and estimated the correlation between surface energy and shear detachment strength of the carbon fiber/epoxy resin interface. All calculations were performed using Exabyte.io platform [2]. The calculated surface energy was confirmed to be related to the experimental shear strength: the surface energy increased with increase in the resin density near graphene. In addition, molecular structures of bulk resin and the resin near graphene surface regions were found to be different. Our results suggest that the carbon fiber and epoxy resin have strong interaction at the interface. In the vicinity of graphene, the resin molecular structure deformed into a flattened state. We propose this to happen due to the influence of CH/π orbitals. The CH/π interaction is a weak interaction (0.1 kcal/mol), however, the compound effect of the numerous weak interaction forces leads to the rise of a strong interaction at the surface between graphene and resin. Because of this, the carbon composite becomes a high-strength material. We further simulated the stress-strain curve of the graphene/epoxy composite model because the above interaction might be related to tensile stress. We found that the crack formation started from the epoxy interface layer and progressed to the bulk epoxy layer.

[1] K. Mori, N. Matsumoto, S. Nomoto, K. Tsuruta, OJCM (2017) 7, 179-184
[2] https://exabyte.io/

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room9)

[SY-H11] Relation between deformation and electrical conductivity for electroconductive polymer nanocomposites with highly segregated structure

○Oleg V. Lebedev[1], Sergey Abaimov[1], Alexander Ozerin[2], Anton Trofimov[1], Iskander Akhatov[1] （1.Center for Design, Manufacturing and Materials, Skolkovo Institute of Science and Technology, Russia, 2.Laboratory of the Structure of Polymer Materials, N.S. Enikolopov Institute of Synthetic Polymer Materials of RAS, Russia）

Polymer composites with highly non-uniform distribution of nanoscale filler in a matrix (filler forming a so-called segregated structure) possess many interesting properties, such as very low percolation threshold and distinct non-linear piezoresistance effect. To study the dependence of the loss in electrical conductivity on the uniaxial deformation and 3D expansion degree, multiscale finite-element analysis was conducted for polymer matrix containing carbon nanotubes. At the first stage of this work, a uniform distribution of dense-packed and entangled nanotubes was created within a thin planar RVE with polyethylene properties. The response of RVE's electrical conductivity to a variety of loading conditions was studied to simulate the response of different parts of a segregated structure on the nano-level to the external loading applied at macro-level. In particular, the planar RVE was oriented at different angles relatively to the axis of macroscopic uniaxial loading and progressively deformed to observe non-linear effects. For each pair angle/deformation, a value of effective electrical conductivity was calculated by an external procedure (Python script), accounting for the Kirchhoff's circuit laws. In the result, an analytical functional dependence of the electrical conductivity on RVE's angle and degree of deformation was developed and compared with the experimental results obtained for uniaxially-deformed electroconductive nanocomposite. At the second stage, a finite-element micro-level model of the segregated structure, recreated from the experimentally observed filler distribution in a composite, was created. The elements of the volume corresponding to the segregated highly filled areas were modeled as having effective electroconductive properties that obey the previously developed conductivity and angle/deformation analytic relation. The micro-level model was uniaxially deformed and thermally treated to introduce expansion of the matrix, and for each degree of deformation or expansion the effective electrical conductivity of the material was calculated. For the obtained dependencies, an analytical expression was developed and was compared with the experimental results for a composite with highly segregated structure.

[SY-H12] Symposium H-12

Fri. Nov 2, 2018 11:15 AM - 12:00 PM Room9

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B9] Symposium B-9

Chair: Michael Tonks(University of Florida, United States of America)

Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room10

[SY-B9] Ab Initio Modeling of Self-Interstitial and Vacancy Migration in Zirconium

○Emmanuel Clouet[1], Céline Varvenne[2]　(1.CEA Saclay, France, 2.CNRS - Aix-Marseille University, France）

[SY-B9] Atomistic modelling of point defect clusters in zirconium and impact on the microstructure evolution and crystal growth under irradiation

Benjamin CHRISTIAEN[3], Christophe DOMAIN[3,2], ○Ludovic THUINET[1,2], Antoine AMBARD[3,2], Alexandre LEGRIS[1,2]　(1.UMET, UMR CNRS 8207, Lille university, F-59655 Villeneuve d'Ascq, France, 2.EM2VM, EDF-CNRS, France, 3.EDF R&D, MMC, Les Renardieres, F-77810 Moret-sur-Loing, France）

[SY-B9] Modeling of dislocation climb assisted glide in crystal plasticity models

○Alankar Alankar, Vikram Phalke, Ritesh Dadhich, Ashish Mishra　(IIT Bombay, India）

[SY-B9] The role of oxide grain boundaries in the oxidation of zirconium alloy fuel cladding

○Maria S Yankova[1], Felicity Baxter[1,2], Alistair Garner[1], Philipp Frankel[1], Christopher P Race[1]　(1.Materials Performance Centre, School of Materials, University of Manchester, UK, 2.Corrosion and Materials Science, Wood. PLC, UK）

[SY-B9] Advances in X-ray Diffraction Line Profile Analysis of Dislocation Loops in Zr - Insights from Atomistic Modelling.

○Chris P Race, Rory Hulse, Tamas Ungar　(University of Manchester, UK）

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room10)

[SY-B9] Ab Initio Modeling of Self-Interstitial and Vacancy Migration in Zirconium

◯Emmanuel Clouet[1], Céline Varvenne[2] (1.CEA Saclay, France, 2.CNRS - Aix-Marseille University, France)

Irradiation in hexagonal close-packed zirconium leads to the creation of point-defects, both vacancies and self-interstitials. Migration and clustering of these point-defects control the microstructure evolution under irradiation. In particular, the faster diffusion of self-interstitial in the basal planes than along the c axis is often assumed to explain the self-organization of the microstructure observed in irradiated Zr as well as the breakaway growth visible for high irradiation dose. As no direct experimental measurement characterizing a possible diffusion anisotropy is possible, at least for the self-interstitial, ab-initio calculations appear as a suitable alternative.
We model with ab initio calculations all possible configurations of the self interstitial and calculat with NEB the different migration barriers between these configurations [1]. The attempt frequencies corresponding to the different migration events are deduced from phonon calculations thanks to the harmonic approximation and the transition state theory. We thus fully characterize the migration of both the self-interstitial and the vacancy. The obtained ab initio data is validated by modeling internal friction in irradiated zirconium and comparing the low temperature peaks with the ones observed in experiments [2]. Once this validation step performed, diffusion coefficients are calculated and diffusion anisotropy is characterized.

[1] C. Varvenne, F. Bruneval, M.-C. Marinica and E. Clouet, Phys. Rev. B 88, 134102 (2013).
[2] R. Pichon, E. Bisogni and P. Moser, Radiation Effects 20, p. 159 (1973).

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room10)

[SY-B9] Atomistic modelling of point defect clusters in zirconium and impact on the microstructure evolution and crystal growth under irradiation

Benjamin CHRISTIAEN[3], Christophe DOMAIN[3,2], ◯Ludovic THUINET[1,2], Antoine AMBARD[3,2], Alexandre LEGRIS[1,2] (1.UMET, UMR CNRS 8207, Lille university, F-59655 Villeneuve d'Ascq, France, 2.EM2VM, EDF-CNRS, France, 3.EDF R&D, MMC, Les Renardieres, F-77810 Moret-sur-Loing, France)

Zirconium alloys are used to manufacture fuel cladding as well as fuel assemblies of pressurized water nuclear reactors. Under irradiation, they show a dimensional change commonly called growth. Experimental observations have shown that above a threshold dose, these alloys are subject to accelerated growth called "breakaway". It has been well established that the irradiation formation of and <c> dislocation loops is directly responsible for the growth of irradiated zirconium alloys and that the appearance of <c> loops is correlated with this growth acceleration. However, the nucleation mechanisms of the <c> loops are still poorly understood. In order to improve our understanding, atomic-scale calculations based on the density functional theory (DFT) and empirical potentials are used to determine the properties of clusters of point defects (vacancies as well as self-interstitials) in terms of formation energy, binding energy and eigenstrain, of prime importance to assess their influence on the deformation of the material. In particular, DFT simulations of dislocation loops in large supercells allow to revisit their energies used as input parameters of mesoscale models (Object KMC), resulting in prediction of growth and its acceleration. Moreover, pyramids of stacking

faults are studied in more detail and their characterization sheds light on their plausible role in the nucleation sequence of <c> loop, which allows to propose an original scenario for their appearance.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room10)

[SY-B9] Modeling of dislocation climb assisted glide in crystal plasticity models

○Alankar Alankar, Vikram Phalke, Ritesh Dadhich, Ashish Mishra　(IIT Bombay, India)

We present crystal plasticity modeling of climb assisted glide in fcc, bcc and hcp metals. Dislocation density is divided into edge and screw characters. Dislocation density evolution takes care of non-schmid effect and the effect of screw dislocation core assymetry in hcp metals. A chemical stress component due to non-equilibrium vacancy concentration acts on edge dislcoations and is called drag-stress. This chemical stress component depends strongly on crystallographic orientation as well if the vacancy concentration is low. Evolution of chemical stress and thus dislocation climb rate is discussed as a function of dislocation density, strain, crystallographic orientation and temperature. Model is calibrated against data from literature. The model is able to predict mechanical behavior under conditions of creep. Also, depending on whether creep occurs or not, the model is able predict crystallographic texture during deformation. Such model has been used for modeling of irradiation in Zr and zircaloys.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room10)

[SY-B9] The role of oxide grain boundaries in the oxidation of zirconium alloy fuel cladding

○Maria S Yankova[1], Felicity Baxter[1,2], Alistair Garner[1], Philipp Frankel[1], Christopher P Race[1]　(1.Materials Performance Centre, School of Materials, University of Manchester, UK, 2.Corrosion and Materials Science, Wood. PLC, UK)

Oxidation of the Zr alloy fuel cladding in light water reactors is one of the key degradation mechanisms, limiting the amount of fuel burned. The structural and electronic properties of monoclinic and tetragonal zirconia grain boundaries strongly affect the transport of species through the oxide layer. Improving the understanding of oxygen transport through the oxide grain boundaries, and its interaction with dopant point defects, is an important factor in achieving a more mechanistic knowledge and better control of the corrosion process. We are exploiting a combination of density functional theory (DFT) simulation, scanning precession electron diffraction in the transmission electron microscope (SPED-TEM) and novel Python-based texture analysis to obtain an improved mechanistic understanding of the oxide microstructure. We have investigated the effect of oxygen defects and key alloying elements such as Sn and Nb on the structural and electronic properties of representative oxide grain boundaries using DFT. We have investigated dopant-oxygen vacancy binding which can have a significant effect on oxygen conductivty. We have characterised the grain boundary misorientation distribution in non-irradiated and irradiated oxides with estimates on the relative boundary energetics. We have further used the results of our DFT calculations to test a range of empirical potentials for the Zr-O system to establish their suitability for computational modelling of zirconia at microstructural length-scales.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room10)

[SY-B9] Advances in X-ray Diffraction Line Profile Analysis of Dislocation Loops in Zr - Insights from Atomistic Modelling.

○Chris P Race, Rory Hulse, Tamas Ungar （University of Manchester, UK）

Irradiation-induced growth (IIG) of Zr-alloy nuclear fuel cladding can limit the service life of nuclear fuel. It involves a macroscopic shape change driven by the formation and growth of populations of dislocation loops.

Efforts to create Zr-alloys that are resistant to IIG thus rely on accurate determination of the size distribution and number density of dislocation loops in irradiated candidate alloys. X-ray diffraction (XRD) can, in principle, provide this information via an analysis of changes to the diffraction peak shapes. Such methods are well developed in the study of plastic deformation, but the different character of the defects formed under irradiation complicates the analysis. An improved understanding of the effect of dislocation loops on the diffraction peak shapes is therefore required.

We have constructed atomistic models of controlled defect populations in Zr and generated theoretical XRD profiles. We have compared these with experimental profiles and analysed changes in lineshape in terms of contributions from the strain fields of individual defects. In particular, we are able to explain the appearance of features in the experimental profiles that are peculiar to irradiated material. We show that these new features contain information about the character of the dislocation loops in irradiated material.

[SY-B10] Symposium B-10
Chair: Frederic Soisson(CEA Saclay, France)
Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room10

[SY-B10] Sink strengths of point defects near tilt grain boundaries: A phase field model

○Pengchuang Liu[1], Songlin Zheng[2], Pengcheng Zhang[1], Sanqiang Shi[3], Kaiguo Chen[2]
（1.Institute of Materials, China academy of engineering physics, China, 2.Institute of Fluid Physics, China academy of engineering physics, China, 3.Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hong Kong）

[SY-B10] Modelling swelling and growth under irradiation using the phase field method

○Daniel Schwen, Andea M. Jokisaari （Dept. of Fuels Modeling and Simulation, Idaho National Laboratory, United States of America）

[SY-B10] Phase-field modelling of dislocation loop evolution under irradiation : application to radiation induced segregation prediction near the dislocation cores

○Gabriel Franck BOUOBDA MOLADJE[1], Ludovic THUINET[1], Alexandre LEGRIS[1], Charlotte BECQUART[1], Maylise NASTAR[2], Frédéric SOISSON[2] （1.CNRS, université de Lille, France, 2.CEA, Université Paris-Saclay, France）

[SY-B10] Theoretical derivation of the ABVI model from cluster expansion Hamiltonian

○Antonio Fernandez Caballero[1,2], Jan Wrobel[3], Paul Mummery[1], Duc Nguyen-Manh[2] （1.School of Mechanical, Aerospace and Civil Engineering, University of Manchester, UK, 2.Department of Materials Science and Scientific Computing, CCFE, United Kingdom Atomic Energy Authority, Abingdon OX14 3DB, UK, UK, 3.Faculty of Materials Science and Engineering, Warsaw University of Technology, Ul. Wołoska 141, 02-507 Warsaw, Poland, Poland）

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room10)

[SY-B10] Sink strengths of point defects near tilt grain boundaries: A phase field model

○Pengchuang Liu[1], Songlin Zheng[2], Pengcheng Zhang[1], Sanqiang Shi[3], Kaiguo Chen[2]　（1.Institute of Materials, China academy of engineering physics, China, 2.Institute of Fluid Physics, China academy of engineering physics, China, 3.Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hong Kong）

Dislocations and grain boundaries are perfect sinks for point defects (PDs), the ability of sinks to absorb point defects is a critical factor for the irradiation damage behaviors of materials. Phase field (PF) method was used to describe low angle tilt grain boundaries which composed of edge dislocations. Evolution processes of tilt grain boundaries and PDs were coupled in a same PF model. We considered the climbing mechanism rather than fixed dislocations. Sink strengths of grain boundaries were computed based on the obtained steady-state average PDs concentrations. We studied the saturation properties of tilt grain boundaries and obtained the relations between sink strengths and dislocation densities. PDs generation rate represents the irradiation intensity, it is also undemanding to take into account in this PF model. Elastic interactions of point defects and dislocations have great impacts on the sink properties of tilt grain boundaries. We compared the effects of different eigenstrains and applied stresses and got the connections between sink strengths and climbing speeds of dislocations. A physical phase-field model was built, which covered material processes to study sink properties of tilt grain boundaries without additional assumptions. We compared the calculated results with the theoretical and existing ones, clarified the inherent differences between them, results are favorable for designing extremely radiation tolerant materials.

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room10)

[SY-B10] Modelling swelling and growth under irradiation using the phase field method

○Daniel Schwen, Andea M. Jokisaari　（Dept. of Fuels Modeling and Simulation, Idaho National Laboratory, United States of America）

In extreme environments with high point defect production rates, some materials can experience macroscopic dimensional changes due to the mechanisms of swelling and growth. Both processes are related to preferential absorption of different point defect species at different sinks. In the case of swelling this entails the creation of voids which act as vacancy sinks, while interstitials are absorbed at dislocations or grain boundaries where new lattice sites are created, leading to a total volume increase of the sample. Growth occurs if anisotropic interstitial and vacancy fluxes with differing spatial orientations lead to lattice site creation and removal along non-parallel lattice planes, leading to a volume conserving shape change. Prediction of swelling and growth behavior requires an understanding of the defect transport and reaction processes at the mesoscale. The phase field method has been established as a standard modeling technique on these length scales.

In this work we develop a modified set of phase field equations that allow for the local and anisotropic creation and destruction of lattice sites at sinks using a tensor field describing the local lattice site changes. We apply this method to study the effects of microstructure on swelling and growth behavior in polycrystalline materials, in the presence of applied mechanical loading, and microstructural features such as

precipitates.

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room10)

[SY-B10] Phase-field modelling of dislocation loop evolution under irradiation : application to radiation induced segregation prediction near the dislocation cores

○Gabriel Franck BOUOBDA MOLADJE[1], Ludovic THUINET[1], Alexandre LEGRIS[1], Charlotte BECQUART[1], Maylise NASTAR[2], Frédéric SOISSON[2] （1.CNRS, université de Lille, France, 2.CEA, Université Paris-Saclay, France）

Understanding and predicting the microstructural evolution of metallic alloys constituting the reactor vessels are crucial issues for safety in the nuclear industry. Under irradiation, point defects (PD) are created and diffuse towards microstructural defects such as dislocations. These microstructural defects will evolve according to their ability to absorb PD, also known as sink strength. Dislocation climb is one consequence of PD absorption and leads to growth or shrinkage of dislocation loops. Phase field (PF) models have already been proposed to describe dislocation climb when only vacancies are considered, which couple non-conservative dislocation motion and vacancy diffusion through an absorption term. To simulate growth/shrinkage of dislocation loops under irradiation in metallic alloys where vacancies but also self-interstitials are created, a new formulation of these models is required, and this will constitute the first part of the presented work. In particular, it will be shown that such a formulation is not a straigthforward generalization of the existing models. Thanks to this new PF model, well-known phenomena observed under irradiation, such as radiation induced segregation, will be studied near the dislocation cores. The particular influence of climb and elastic interactions between PDs and dislocations, generally ignored in RIS calculations, will be discussed in detail.

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room10)

[SY-B10] Theoretical derivation of the ABVI model from cluster expansion Hamiltonian

○Antonio Fernandez Caballero[1,2], Jan Wrobel[3], Paul Mummery[1], Duc Nguyen-Manh[2] （1.School of Mechanical, Aerospace and Civil Engineering, University of Manchester, UK, 2.Department of Materials Science and Scientific Computing, CCFE, United Kingdom Atomic Energy Authority, Abingdon OX14 3DB, UK, UK, 3.Faculty of Materials Science and Engineering, Warsaw University of Technology, Ul. Wołoska 141, 02-507 Warsaw, Poland, Poland）

In nuclear fusion research, degradation of material microstructure and nanostructure by radiation damage is of interest both from experimentally and modelling perspectives. Modelling from first principles can be used to rationalize mechanisms behind degradation phenomena caused by the simplest type of damage produced by radiation: vacancies and interstitials and their clusters. Recent studies found that density functional theory and kinetic monte carlo can be used to investigate radiation induced segregation and precipitation[1] incorporating both vacancy and interstitial into Ising-like ABVI model Hamiltonian[2]. The kinetic processes of solute transport both by vacancies and interstitials can be captured by a Hamiltonian parametrised by

bond energies and derived from DFT.

In this work, we treat multi-body defect-solute or solute-solute interactions as cluster entities from the cluster expanded Hamiltonian of the alloy system containing point defects. Binding energies for elements within defect cluster are expressed in terms of effective interactions parameters found from the cluster expansion of the Hamiltonian of the system containing vacancies and interstitials. Local effects from defect surroundings are incorporated by offseting the binding enery by the cluster expanded reference energy depending on chemical compositions of the surroundings[3,4]. This model can be used to investigate the kinetic simulations of segregation and precipitation of binary alloys under irradiation.

[1] *G. Martin, 1980, Phys. Rev. B 21, 2122*

[2] *C. Huang and J. Marian, 2016, J. Phys.: Condens. Matter 28 425201*

[3] *J.S. Wrobel, D. Nguyen-Manh, K.J. Kurzydlowski, S.L. Dudarev, 2017, Journal of Physics: Condensed Matter, 29 145403.*

[3] *A. Fernandez-Caballero, J.S. Wrobel, P.M. Mummery, D. Nguyen-Manh, 2017, J. Phase Equilibrium and Diffusion, 38 391-403.*

[SY-K4] Symposium K-4

Chairs: Tetsuo Mohri(IMR, Tohoku University, Japan), Akihiro Nakatani(Dept. of Adaptive Machine Systems, Osaka Univ., Japan)
Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room11

[SY-K4] Disclination dipole model of kink deformation in layered solid
○Akihiro Nakatani[1], Xiao-Wen Lei[2]　(1.Dept. of Adaptive Machine Systems, Osaka Univ., Japan, 2.Dept. of Mechanical Engineering, Univ. of Fukui, Japan）

[SY-K4] Large-scale coarse-grained molecular dynamics simulations on fracture processes of lamellar structure in crystalline polymers
○Yuji Higuchi　(The University of Tokyo , Japan）

[SY-K4] Grain boundary sliding within the entropy production rate theory
○Tetsuo Mohri　(IMR, Tohoku University, Japan）

[SY-K4] Molecular Dynamics Simulation on Intergranular Cracking Mechanism of Iron Material in High Temperature Pressurized Water Environment
○Qian Chen, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo　(Institute for Materials Research, Tohoku University, Japan）

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room11)

[SY-K4] Disclination dipole model of kink deformation in layered solid

Invited

○Akihiro Nakatani[1], Xiao-Wen Lei[2] (1.Dept. of Adaptive Machine Systems, Osaka Univ., Japan, 2.Dept. of Mechanical Engineering, Univ. of Fukui, Japan)

Kink deformation is commonly observed in layered solid for a wide variety of scales from atomistic layers to geological structures, and their structural similarity means possibility of universal application of deformable body mechanics. In our previous works, the deformation mechanism of kink deformation in a layered solid with a single-slip system has been studied and it is shown that the fundamental process of kink deformation is represented by disclination dipole model.

In this study, first, we review the relationship between generalized continuum theories and the disclination dipole dynamics from a multiscale point of view.

Secondly, nucleation of kink deformation under a compressive force in the direction parallel to the layers is studied using configulational force of disclination dipole based on instability theory, in which the deformation mechanism is discussed from the viewpoint of the instability theory with the Maxwell's equal area rule.

Third, we use cellular automaton as a discretized model of disclination dipole theory, in which each layer is divided into segments and the amount of Frank vector of each segment is encoded using integers. In this study, total strain energy is calculated as sum of the local bending strain energy of each layer and inter-layer energy, in which the local strain energy density is evaluated as a linear function of square of curvature and inter-layer energy is assumed to be expressed by a form of Lennard-Jones 12-6 potential. The Metropolis Monte Carlo Method is adopted to evolve the state of the material system. The result of this scheme is verified on the classical problem of buckling of Euler's column with comparing analytical solution. After that, simulation of kinking deformation is examined for various values of the inter-layer strength parameter.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room11)

[SY-K4] Large-scale coarse-grained molecular dynamics simulations on fracture processes of lamellar structure in crystalline polymers

○Yuji Higuchi (The University of Tokyo , Japan)

Understanding the fracture processes of crystalline polymers such as polyethylene by molecular theory is one of the big challenges, which contributes to the increase in the toughness of polymeric materials in industry. To reveal the fracture process, coarse-grained molecular dynamics simulation is effective; however the fracture processes of the most fundamental crystal structure, lamellar structure consisting of amorphous and crystalline layers, in polyethylene has not been revealed. The reason is the difficulty of the construction of the lamellar structure due to the small simulation size in the order of 10^4 beads. Thus, we propose a crystallization method for the large-scale lamellar structure in the order of 10^6 beads and perform the fracture simulation.

In the fracture process of the lamellar structure by coarse-grained molecular dynamics simulation, mechanical properties are consistent with the experiment, confirming the validity of the simulation results. We also reveal that the movement of chain ends from amorphous layers to crystalline layers causes the deformation and void generation in the amorphous region, indicating that the chain ends act as defect [1, 2].

In the large scale simulations, the buckling of crystalline layer and its fragmentations are observed, which can be compared directly with the experimental observation by electronic microscope. Our large-scale coarse-grained molecular dynamics simulations are useful to reveal the fracture process of polymers at molecular level. We develop the above molecular technology which can reveal the fracture processes of polymeric materials at the molecular level and successfully apply it to the fracture process of double network gels [3].

[1] Y. Higuchi et al., Macromolecules 50, 3690-3702 (2017).
[2] Y. Higuchi, Polym. J. in press (2018).
[3] Y. Higuchi et al., Macromolecules in press (2018).

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room11)

[SY-K4] Grain boundary sliding within the entropy production rate theory

○Tetsuo Mohri （IMR, Tohoku University, Japan）

It is a challenging task to clarify the underlying principle of deformation behavior of an alloy. In high temperatures, an alloy undergoes various deformation modes driven by dislocations movement, grain boundary sliding etc. Under a given strain rate (tensile test) or a given stress (creep test), how does an alloy adjust internal structures to accommodate externally imposed deformation conditions such as deformation rate and applied stress? This is the question the author addresses in the present paper. By taking a grain boundary sliding as an example, we formulated deformation behavior in terms of average rotation rate of a grain and density of rotating grains based on entropy production rate theory within the linear regime. The physical implications of grain boundary sliding at an extremum of entropy production rate are main focus of the discussion, and thermodynamic similarity between grain boundary sliding and dislocations driven deformation is addressed. Furthermore, it will be briefly touched upon how to extend the formulation of grain boundary sliding for an alloy to larger scale deformation phenomena.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room11)

[SY-K4] Molecular Dynamics Simulation on Intergranular Cracking Mechanism of Iron Material in High Temperature Pressurized Water Environment

○Qian Chen, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Materials Research, Tohoku University, Japan）

Iron-based materials are widely used in power plants, and usually serve in high temperature pressurized water environment. The severe water environment causes stress corrosion cracking (SCC), resulting in potentinally catastrophic accidents. It is therefore important to understand the chemical reaction dynamics at the iron-water interface and the SCC mechanism during failure process in order to improve corrosion resistance. However, it is difficult to achieve that by experimental observation, particularly in high temperature pressurized water. Thus, the SCC mechanism for iron-based materials in such an environment is still unclear. In this study, we employed molecular dynamics simulation to study the failure process in high temperature pressurized water environment. To investigate chemical reactions, a reactive force field was used in this study. Since intergranular cracking is more common than transgranular cracking during the

fracture processes of iron materials, a $\Sigma 5(310)$ grain boundary was modeled. To investigate the crack growth process under stress conditions, we applied external tension along the perpendicular direction of the pre-crack model with water arranged on the surface. The simulation results showed structural change due to plastic deformation around the pre-crack, and the structural change was found to be attributable to twinning by partial dislocations. In addition, small cracks were observed in the lateral direction of the pre-crack tip. To investigate the effect of high temperature pressurized water, we also simulated the model without water for comparison. It was revealed that crack propagation was promoted by suppressing structural relaxation due to the chemical reactions in the high temperature pressurized water condition.

[SY-K5] Symposium K-5

Chairs: Masanori Kohyama(AIST, Japan), Masatake Yamaguchi(Japan Atomic Energy Agency, Japan)
Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room11

[SY-K5] **Effects of a bulk-region size in the first-principles tensile test of a grain boundary**

○Masanori Kohyama[1], Hao Wang[2], Shingo Tanaka[1] （1.AIST, Japan, 2.Shanghai Univ., China）

[SY-K5] **Combined analysis of first-principles calculations and fracture mechanics experiments on intergranular embrittlement of an alloy steel**

○Masatake Yamaguchi （Center for Computational Science and e-Systems, Japan Atomic Energy Agency, Japan）

[SY-K5] **First-principles local energy analysis of grain boundary segregation of sp-elements on bcc Fe**

○Kazuma Ito[1,2], Somesh Kr. Bhattacharya[3], Shingo Tanaka[3], Masanori Kohyama[3], Hideaki Sawada[2], Shigenobu Ogata[1] （1.Osaka University, Japan, 2.Nippon Steel &Sumitomo Metal Corporation, Japan, 3.National Institute of Advanced Industrial Science and Technology, Japan）

[SY-K5] **Fast and scalable prediction of local energy at grain boundaries: Machine-learning based modeling of first-principles calculations**

○Tomoyuki Tamura[1,2], Masayuki Karasuyama[1,2,3], Ryo Kobayashi[1,2], Ryuichi Arakawa[1], Yoshinori Shiihara[4], Ichiro Takeuchi[1,2,5] （1.Nagoya Institute of Technology, Japan, 2.Center for Materials Research by Information Integration (CMI2), Research and Services Division of Materials Data and Integrated System (MaDIS), National Institute for Materials Science (NIMS), Japan, 3.PRESTO, JST, Japan, 4.Toyota Technological Institute, Japan, 5.RIKEN Center for Advanced Intelligence Project, Japan）

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room11)

[SY-K5] Effects of a bulk-region size in the first-principles tensile test of a grain boundary

◯Masanori Kohyama[1], Hao Wang[2], Shingo Tanaka[1]　（1.AIST, Japan, 2.Shanghai Univ., China）

The first-principles tensile test (FPTT) of a grain boundary (GB) is a powerful tool to clarify intrinsic tensile strength and failure process of a GB, according to natural behaviors of electrons and atoms, corresponding to a slow tensile test at zero temperature [1]. This is quite effective to clarify the effects of segregated impurities [2]. This can provide intrinsic energy-strain and stress-strain curves of a GB, which should be useful to construct separation-energy curves for "cohesive zone model" in a continuum model as a multi-scale simulation technique. However, there are several unsolved issues in interpreting FPTT results compared to real mechanical properties of GBs. In the present study, we investigate the effects of the bulk-region size in the GB supercell, where usually two symmetric interfaces of a coincidence-site lattice (CSL) GB are alternately stacked between bulk slabs with some thickness. We show that the bulk-region thickness seriously affect the features of energy-strain and stress-strain curves around the failure point by comparing the FPTTs of the same Al GB with different bulk-region thicknesses, which are also analyzed by local-energy and local-stress techniques [3]. The difference is dominated by the relation between the Griffith and stress conditions for failure, depending on the bulk-region thickness. From this viewpoint, we re-interpret our previous FPTT results of Al GBs with various segregated impurities [2].

[1] M. Kohyama, Phil. Mag. Lett. 79, 659 (1999); Phys. Rev. B, 65, 184107 (2002)

[2] G. H. Lu et al., Phys. Rev. B, 73, 224115 (2006)

[3] H. Wang et al., Modell. Simul. Mater. Sci. Eng. 25, 015005 (2017)

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room11)

[SY-K5] Combined analysis of first-principles calculations and fracture mechanics experiments on intergranular embrittlement of an alloy steel

◯Masatake Yamaguchi　（Center for Computational Science and e-Systems, Japan Atomic Energy Agency, Japan）

A significant loss of fracture toughness (K_{Ic}) is induced by intergranular (grain boundary; GB) segregation of metalloid solute (Sb, Sn, and P) in a Ni-Cr steel. However, the atomistic mechanism has not been clarified from a multiscale point of view. From first-principles calculations, it is shown that segregated solute with higher energetic stability on fracture surfaces causes a larger linear reduction in the ideal work to intergranular fracture ($2\gamma_{int}$); i.e. the energy difference between a GB and its two fracture surfaces. The combined analysis with first-principles calculations and fracture mechanics experiments found several orders of magnitude more energy loss in K_{Ic} for a specific range in the $2\gamma_{int}$ within only a few tenths of J/m^2. These results illustrate that the GB of steel has the threshold energy of atomic cohesion under which catastrophic failure occurs [1]. [1] M. Yamaguchi and J. Kameda: Phil. Mag. 94, 2131-2149 (2014).

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room11)

[SY-K5] First-principles local energy analysis of grain boundary segregation of sp-elements on bcc Fe

○Kazuma Ito[1,2], Somesh Kr. Bhattacharya[3], Shingo Tanaka[3], Masanori Kohyama[3], Hideaki Sawada[2], Shigenobu Ogata[1]　(1.Osaka University, Japan, 2.Nippon Steel &Sumitomo Metal Corporation, Japan, 3.National Institute of Advanced Industrial Science and Technology, Japan)

In polycrystalline materials, grain boundary segregation of impurity elements and alloying elements may have a great influence on the material properties. Particularly in steel materials, it is known that the sp-elements such as P and S segregate at the grain boundary, thereby remarkably lowering hot ductility and low temperature toughness. However, the microscopic mechanism of grain boundary segregation of these elements has not been fully clarified.

In this study, grain boundary segregation energies for sp-elements (Al,Si,P and S) in bcc Fe are calculated by first-principles calculations. Furthermore, to investigate the microscopic mechanism, the contribution of each physical origin to the grain boundary segregation energies is evaluated numerically by using first-principles local energy analysis. We will also discuss the relationship between the contribution of each physical origin and the geometric structure or the electronic state of the grain boundary.

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room11)

[SY-K5] Fast and scalable prediction of local energy at grain boundaries: Machine-learning based modeling of first-principles calculations

○Tomoyuki Tamura[1,2], Masayuki Karasuyama[1,2,3], Ryo Kobayashi[1,2], Ryuichi Arakawa[1], Yoshinori Shiihara[4], Ichiro Takeuchi[1,2,5]　(1.Nagoya Institute of Technology, Japan, 2.Center for Materials Research by Information Integration (CMI2), Research and Services Division of Materials Data and Integrated System (MaDIS), National Institute for Materials Science (NIMS), Japan, 3.PRESTO, JST, Japan, 4.Toyota Technological Institute, Japan, 5.RIKEN Center for Advanced Intelligence Project, Japan)

A GB is the interface between two grains or crystallites in a polycrystalline material, and the atomic configurations and chemical bonds near GB are distinct from those of the bulk crystal. Thus, the properties of materials with GBs can greatly differ from those of a single crystal. Since it is possible to improve various properties of materials significantly by GB engineering, it is of great importance to investigate physical and chemical properties of each atoms or local regions near GBs. By virtue of the development of efficient computational techniques of large-scale density functional theory (DFT) calculations and the rapid progress of parallel computers including supercomputers, we can deal with relatively large supercells for GB models. But, it needs much computational costs to perform DFT calculations with larger supercells, and it is impossible to cover all GB models.

We proposed a new scheme based on machine learning for the efficient screening in GB engineering. A set of results obtained from DFT calculations for a small number of GB systems is used as a training data set. In our scheme, by partitioning the total energy into atomic energies using a local-energy analysis scheme, we can increase the training data set significantly. We use atomic radial distribution functions and additional

structural features as atom descriptors to predict atomic energies and GB energies simultaneously using the least absolute shrinkage and selection operator (LASSO). In the test study with fcc-Al [110] symmetric tilt GBs, we could achieve enough predictive accuracy to understand energy changes at and near GBs at a glance, even if we collected training data from only ten GB systems. The present scheme can emulate time-consuming DFT calculations for large GB systems with negligible computational costs, and thus enable the fast screening of possible alternative GB systems.