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-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_3Al: 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）

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.

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(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).

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)
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）

[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）

(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 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)

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:
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(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].

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[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.
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(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.

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

[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.

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(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

○Vera 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.

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[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

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[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.

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(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_3N_4/TiO_2(001) heterojunction

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

The formation of g-C_3N_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_3N_4/TiO_2

(001) interfaces were studied by first principles calculations. The stable g-C_3N_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_3N_4/TiO_2(001) interfacial zone. The electronic structures of g-C_3N_4/TiO_2(001) interface and boron doped systems were evaluated. Strong bonding interactions between the g-C_3N_4 and TiO_2(001) were found in the g-C_3N_4/TiO_2(001) interface, and the boron dopant can improve the charge transfers between g-C_3N_4 and TiO_2(001). Therefore, the boron may improve the photocatalytic properties of g-C_3N_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

○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].

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(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, how-ever, 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 mathemat-ical 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）

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room6)

[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.

(Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room6)

[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

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(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

U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

(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.

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)

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.

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)

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, ○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

○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 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）

Recently, hybrid MABX_3perovskites (MA= $CH_3NH_3^+$; 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**,

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(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

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(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].

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(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.

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[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.

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[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.

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(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.

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

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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.

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[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.

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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]
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(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

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

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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.

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[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.

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[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.

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[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)

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.

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[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.

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[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.

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[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.

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[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.

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[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.

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[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 $2\times10^{9}s^{-1}$ and $2\times10^{10}s^{-1}$ 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 1.6*nm* 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.

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[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.
This outcome has been achieved with the financial support of the Czech Science Foundation, project No. 16-00567S and the Ministry of Education, Youth and Sports of the Czech Republic under the “ National

Sustainability Programme I” (project No. LO1408 AdMaS UP).

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[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%.

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[PO-F1] Poster Session 1

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[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_3Al: 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）

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[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.

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[P1-34] Transition-metal alloying of γ'-Ni_3Al: 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 3*d* (Sc-Zn), 4*d* (Y-Cd) and 5*d* (Hf-Au) TM alloying elements on the ideal uniaxial compressive strength of γ'-Ni_3Al were investigated. The stress-strain relationships of pure Ni_3Al under [100], [110] and [111] compressive loads and the site occupancy behavior of TM elements in Ni_3Al 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_3Al under a deformation along the weakest compressive direction. Furthermore, the charge redistribution of Ni_3Al doped with 5*d* elements were also analyzed to understand the strengthening mechanisms of TM elements

in the γ'-Ni_3Al phase.

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[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.

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[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.

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[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.

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[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.

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[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.

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[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.

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[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.

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[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.

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[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.

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[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.

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[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）

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.

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[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）

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.

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

○Ian 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

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[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.

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[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.

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[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.

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[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.

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(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.

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[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.

This work was supported by the National Research Foundation of Korea (NRF) grants funded by the Korea

government (Ministry of Science and ICT) (NRF-2016R1C1B2011098, NRF-2017M3D1A1039422, and NRF-2014M3A6B3063711).

(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.

This work was supported by the National Research Foundation of Korea (NRF) grants funded by the Korea government (Ministry of Science and ICT) (NRF-2016R1C1B2011098, NRF-2017M3D1A1039422, and NRF-2014M3A6B3063711).

(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.

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[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.

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

[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.

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[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.

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[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）

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

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[P1-61] Interfacial charge transfer and enhanced photocatalytic mechanism for Bi_2WO_6/BiOCl heterostructure: A first-principles t heoretical study

○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.

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[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.

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(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.

Poster Session | J. Multiscale Modeling of Heterogeneous Layered Media

[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.

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

[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

○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

○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 (ϕ >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

○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

○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.

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(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

results were obtained within the implementation of the research project granted by the Czech Science Foundation - project No. GA17-14302S.

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.

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(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

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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.

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

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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.

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

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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.

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

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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.

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[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)