Wed. Oct 31, 2018

Room1

Plenary Talk | Plenary Talk

[PL4] Plenary Talk 4

Chair: Erik Bitzek(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)
8:30 AM - 9:20 AM Room1

[PL4] Plenary Talk 4

○Yuichi Ikuhara （The University of Tokyo/Japan Fine Ceramics Center, Japan）

Wed. Oct 31, 2018

Room1

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

[SY-C5] Symposium C-5

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

[SY-C5] **Plasticity and Fracture in Transition Metal Carbides**
○Giacomo Po[1], Suneel Kodambaka[2], Jeffrey M Wheeler[3], Davide Sangiovanni[4] （1.University of California Los Angeles, Mechanical Engineering Department, United States of America, 2.University of California Los Angeles, Materials Science and Engineering Department, United States of America, 3.Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Mechanics of Materials and Nanostructures, Swaziland, 4.Department of Physics, Chemistry and Biology, Linköping University, Sweden）

[SY-C5] Atomic Scale Investigation of Plasticity in Laves phases
○Julien Guenole[1], Fatim-Zahra Mouhib[1], Christoffer Zehnder[1], James Gibson[1], Blazej Grabowski[2], Sandra Korte-Kerzel[1] （1.Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Germany, 2.Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany）

[SY-C5] Nucleation of dislocation in ultra-hard ceramic nanoparticles modelled by molecular dynamics and nudged elastic band simulations
○Jonathan Amodeo[1], Emile Maras[2] （1.MATEIS, Univ. Lyon 1, France, 2.SRMP, DEN, CEA, Gif-sur-Yvette, France）

[SY-C5] Multiscale discrete dislocation dynamics modeling of nano-indentation near the grain boundary
○Xu Zhang, Songjiang Lu （School of Mechanics and Engineering, Southwest Jiaotong University, China）

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

[SY-C6] Symposium C-6

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

[SY-C6] Effect of interstitial solutes on the structure and mobility of screw dislocations in bcc metals
Berengere Lüthi[1], Lisa Ventelon[1], David Rodney[2], Emmanuel Clouet[1], Bernard Legrand[1], Fabienne Berthier[3], ○Francois Willaime[4] （1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, France, 2.Institut Lumière Matière, CNRS-Université Claude Bernard Lyon 1, France, 3.Synthèse, Propriétés et Modélisation des Matériaux /Institut de Chimie Moléculaire et des Matériaux d'Orsay, Université Paris-Saclay, France, 4.DEN-Département des Matériaux pour le Nucléaire, CEA, Université Paris-Saclay, France）

[SY-C6] Effect of solutes on dislocation motion in dilute hcp and bcc alloys
○Tomohito Tsuru[1,2], Mitsuhiro Itakura[1], Masatake Yamaguchi[1,2], Tomoaki Suzudo[1], Masato Wakeda[3], Shigenobu Ogata[2,4], Daryl C Chrzan[5] （1.Japan Atomic Energy Agency, Japan, 2.ESISM, Kyoto University, Japan, 3.National Institute for Materials Science, Japan, 4.Osaka University, Japan, 5.University of California, Berkeley, United States of America）

[SY-C6] Investigation of the energy pathway for generation of dislocations in silicon at $\Sigma 3$ grain boundaries with the kinetic Activation-Relaxation Technique
○Simen Nut Hansen Eliassen[1], Normand Mousseau[3], Mickaël Trochet[3], Yanjun Li[1], Jesper Friis[2], Inga Gudem Ringdalen[2] （1.Dept. of Materials Science and Engineering, Norwegian Univ. of Science and Technology, Norway, 2.SINTEF Materials and Chemistry, Norway, 3.Dept. of Physics, Univ. de Montréal, Canada）

[SY-C6] Prediction of mechanical twinning in post-perovskite structure
○Philippe Carrez, Alexandra Goryaeva, Patrick Cordier （Lille University, Lab. UMET UMR-CNRS 8207, France）

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

[SY-C7] Symposium C-7

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

[SY-C7] **Predictive simulations of crystal plasticity: multiscale or cross-scale?**
○Vasily V Bulatov[1], Alexander Stukowski[2], Luis A Zepeda-Ruiz[1], Tomas Oppelstrup[1] （1.Lawrence

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

[SY-C7] **Molecular dynamics simulations of dislocation avalanche emissions in FCC and BCC crystals**
○Javier Varillas[1,2], Jan Očenášek[2], Jorge Alcalá[1] (1.New Technologies Research Centre, University of West Bohemia in Pilsen, Czech Republic, 2.Department of Materials Science and Metallurgical Engineering, InSup, ETSEIB. Universitat Politècnica de Catalunya, Spain)

[SY-C7] Scrutinizing screw dislocation glide initiation at finite temperatures in BCC metals
○Tomoaki Suzudo[1], Takashi Onitsuka[2], Ken-ichi Fukumoto[2] (1.Japan Atomic Energy Agency, Japan, 2.Fukui Univ., Japan)

[SY-C7] Uranium plastic deformation: A multiscale approach
○Pavel A. Pokatashkin, Denis K. Ilnitsky, Alexei V. Yanilkin (Dukhov Research Institute of Automatics (VNIIA), Russia)

[SY-C7] Understanding the grain refinement mechanism in surface mechanical attrition treatment of Fe14Ni18Cr by molecular dynamics simulations
○Ali Rida[1], Matthieu Micoulaut[2], Emmanuelle Rouhaud[1], Ali Makke[1,3] (1.University of Technology of Troyes , France, 2.Sorbonne Université, France, 3.EPF, Engineering school, France)

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

[SY-C8] Symposium C-8

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

[SY-C8] Thermal fluctuations of dislocations reveal the interplay between their core energy and long-range elasticity.
○Pierre-Antoine Geslin[1,2,3], David Rodney[4] (1.Mateis lab, INSA Lyon/CNRS, France, 2.Institute for Materials Research, Tohoku University, Japan, 3.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan, 4.Institut Lumière Matière, Université Lyon 1, France)

[SY-C8] Tension of fluctuating dislocation lines
○Max Boleininger[1], Thomas D Swinburne[2], Laurent Dupuy[3], Sergei L Dudarev[1] (1.Culham Centre for Fusion Energy, UK, 2.Theoretical Division T-1, Los Alamos National Laboratory, United States of America, 3.DEN-Service de Recherches Métallurgiques Appliquées, CEA, France)

[SY-C8] Stress-Dependent Activation Parameters for Cross-Slip in FCC Metals
○Alon Malka-Markovitz, Dan Mordehai (Technion—Israel Institute of Technology, Israel)

[SY-C8] The influence of precipitate size and shape on the strengthening and hardening rate as observed within metallic alloys.
○Benjamin A Szajewski, Joshua Crone, Jaroslaw Knap (Army Research Laboratory, United States of America)

[SY-C8] Molecular dynamics simulations of dislocation dynamics
Eyal Oren, ○Guy Makov (Ben-Gurion University of the Negev, Israel)

Room2

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E5] Symposium E-5

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

[SY-E5] Use of FFT-based micromechanical modeling for analysis of synchrotron-based diffraction experiments
Vahid Tari[1], Ricardo A Lebensohn[2], Reeju Pokharel[2], Rachel E Lim[1], Darren C Pagan[3], Yufeng Shen[1], Joel V Bernier[4], Robert M Suter[1], ○Anthony D Rollett[1] (1.Carnegie Mellon University, United States of America, 2.Los Alamos National Laboratory, United States of America, 3.Cornell High Energy Synchrotron Source, United States of America, 4.Lawrence Livermore National Laboratory, United States of America)

[SY-E5] Computational Design of Hysteresis-Free and Linear Super-Elastic, and Ultralow Modulus Ferroelastic Materials
○Jiaming Zhu[1], Yipeng Gao[2], Dong Wang[3], Tong-Yi Zhang[4], Yunzhi Wang[2] (1.City University of Hong Kong, Hong Kong, 2.Ohio State University, United States of America, 3.Xi'an Jiaotong University, China, 4.Shanghai University, China)

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

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

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

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

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E6] Symposium E-6

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

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

○Ying-Jun Gao （Guangxi University, China）

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

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

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

○Michael Budnitzki （TU Bergakademie Freiberg, Germany）

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

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

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

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

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E7] Symposium E-7

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

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

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

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

○Tetsuya Ohashi （Kitami institute of technology, Japan）

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

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

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

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

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

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

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E8] Symposium E-8

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

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

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

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

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

Lu （Department of Physics, Beihang University, China）

[SY-E8] **Ab initio investigation on the stacking fault energy and the *c/a* ratio in hexagonal metals and alloys**
○Gang Zhou, Hao Wang, Dong sheng Xu, Rui Yang （Institute of Metal Research, Chinese Academy of Sciences, China）

[SY-E8] Role of vacancies and grain boundaries of 2D materials for the catalytic ammonia synthesis
○Qinye Li[1], Lizhong He[1], Chenghua Sun[2,3], Xiwang Zhang[1] （1.Monash University, Australia, 2.Swinburne University of Technology, Australia, 3.Dongguan University of Technology, China）

[SY-E8] First-principles Investigation on the Stability and Oxygen Adsorption Behavior of a Ti$_2$AlNb/TiAl Interface
○Yue Li, Jianhong Dai, Yan Song （School of Materials Science and Engineering, Harbin Institute of Technology at Weihai, China）

[SY-E8] **DFT predictions of hydrogen storage properties of Mg$_7$TiX$_2$ (X= F, O, S, P and Cl)**
○Yuying Chen, Jianhong Dai, Yan Song （School of Materials Science and Engineering, Harbin Institute of Technology at Weihai, China）

Room3

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

[SY-F5] Symposium F-5

Chair: Ingo Steinbach(Ruhr-University Bochum, Germany)
9:45 AM - 11:00 AM Room3

[SY-F5] Solidification microstructure formation by phase-field simulation with multi-GPU acceleration
○Tomohiro Takaki[1], Shinji Sakane[1], Munekazu Ohno[2], Yasushi Shibuta[3], Takayuki Aoki[4] （1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.The University of Tokyo, Japan, 4.Tokyo Institute of Technology, Japan）

[SY-F5] **Phase-field study of eutectic colony formation in NiAl-34Cr**
○Michael Kellner[1,2], Johannes Hötzer[1,2], Markus Linnenberg[1], Marco Seiz[1], Britta Nestler[1,2] （1.Institute of Applied Materials - Computational Materials Science (IAM-CMS), Karlsruhe Institute of Technology, Germany, 2.Institute of Digital Materials Science (IDM), Karlsruhe University of Applied Science, Germany）

[SY-F5] Solidification analysis by non-equilibrium phase field model using thermodynamics data estimated by machine learning
○Sukeharu Nomoto[1], Hiroshi Wakameda[1], Masahito Segawa[1], Toshiyuki Koyama[2], Akinori Yamanaka[3] （1.ITOCHU techno-Solutions Coorporation, Japan, 2.Materials Design Innovation Engineering, Nagoya Univ., Japan, 3.Department of Mechnical Systems Engneering, Tokyo University of Agriculture and Technology, Japan）

[SY-F5] Phase field modeling of deformation twinning in β-metastable titanium alloys
○Juba Hamma[1], Benoît Appolaire[2], Yann Le Bouar[1], Alphonse Finel[1] （1.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay F-92322 Châtillon, France, 2.IJL, UMR 7198 CNRS-Université de Lorraine, 54000 Nancy, France）

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

[SY-F6] Symposium F-6

Chair: Benoit Appolaire(Institut Jean Lamour, Univ. de Lorraine, France)
11:15 AM - 12:30 PM Room3

[SY-F6] Atomistically informed full-field simulation of tempered martensite:Quenching, tempering and mechanical characterization
○Ingo Steinbach （Ruhr-University Bochum, Germany）

[SY-F6] **Characterisation and modelling of drawn martensite**
○Marius Gintalas[1], Miguel A. Santajuana[2], Carlos Garcia-Mateo[2], David San-Martin[2], Jose A. Jiménez[2], Wim Van Haver[3], Pedro E. J. Rivera-Diaz-del-Castillo[4] （1.The University of Cambridge, Department of Materials Science &Metallurgy, 27 Charles Babbage Road, Cambridge CB3 0FS, UK, 2.Materalia research group, Department of Physical Metallurgy, Spanish National Centre for Metallurgical Research (CENIM-CSIC), Avda. Gregorio del Amo 8, Madrid E-28040, Spain, 3.NV Bekaert SA, Bekaertstraat 2, Zwevegem B-8550, Belgium, 4.The University of Lancaster, Department of Engineering, Engineering Building, Lancaster University, Gillow Ave, Bailrigg, Lancaster LA1 4YW, UK）

[SY-F6] 3D modeling of microstructure evolution in Ni-based superalloys under creep loading
○Maeva Cottura[1], Benoît Appolaire[1], Alphonse Finel[2], Yann Le Bouar[2] （1.Institut Jean Lamour , France, 2.LEM - CNRS/Onera, France）

[SY-F6] Phase field study of the effect of coherency strains and applied load in material couples

○Sourav Chatterjee, Nele Moelans （Department of Materials Engineering, KU Leuven, Belgium）

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

[SY-F7] Symposium F-7

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

[SY-F7] A Cosserat crystal plasticity and phase field theory for grain boundary migration

○Benoit Appolaire[1,2], Anna Ask[3], Samuel Forest[3], Kais Ammar[3] （1.Institut Jean Lamour, Univ. de Lorraine, France, 2.LEM, CNRS-Onera, France, 3.Centre des Materiaux, Mines ParisTech, France）

[SY-F7] Phase-field modeling of precipitation growth and ripening during heat-treatment conditions in Ni-base superalloys

○Michael Fleck, Felix Schleifer, Markus Holzinger, Yueh-Yu Lin, Uwe Glatzel （Metals and Alloys, University Bayreuth, Germany）

[SY-F7] Two-dimensional Simulation of Cyclic Phase Transformation in Fe-C-Mn-Si Alloy using Non-equilibrium Multi-Phase-Field Model

○Masahito Segawa[1], Nomoto Sukeharu[1], Akinori Yamanaka[2] （1.ITOCHU Techno-Solutions Corporation, Japan, 2.Division of Advanced Mechanical Systems Engineering, Institute of Engineering, Tokyo University of Agriculture and Technology, Japan）

[SY-F7] Prediction of the microstructure evolution in Electron Beam Melting Alloy 718 through phase field modelling

○Chamara Kumara[1], Dunyong Deng[2], Johan Moverare[2], Per Nylén[1] （1.Department of Engineering Science, University West, Sweden, 2.Department of Management and Engineering, Linköping University, Sweden）

[SY-F7] Phase-field simulation of solidification morphology in laser powder deposition of Fe-B alloys

○Xiaoxia Li, Xiangge Qin （School of Materials Science and Engineering, Jiamusi Univ., China）

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

[SY-F8] Symposium F-8

Chair: Martin Diehl(Max-Planck-Institut fuer Eisenforschung GmbH, Germany)
4:00 PM - 5:30 PM Room3

[SY-F8] From state parameter-based microstructure modeling to temperature and strain rate-dependent yield stress

○Ernst Kozeschnik （Institute of Materials Science and Technology, TU Wien, Austria）

[SY-F8] **Modelling of grain boundary segregation and precipitation in multi-component Al alloys subjected to heat treatment**

○Dongdong Zhao[1], Sylvain Gouttebroze[2], Jesper Friis[3], Yanjun Li[1] （1.Norwegian University of Science and Technology (NTNU), 7491, Trondheim , Norway, 2.SINTEF Materials and Chemistry, 0314 Oslo, Norway, 3.SINTEF Materials and Chemistry, 7491 Trondheim, Norway）

[SY-F8] Modeling the microstructure and electrical conductivity evolution during aging of Al-Mg-Si alloys

○Yijiang Xu, Yanjun Li （Norwegian University of Science and Technology , Norway）

[SY-F8] Thermo-kinetic modeling of long-term precipitate evolution in heat-resistant alloys

○Jae-Hyeok Shim[1], Magdalena Speicher[2], Mahesh Chandran[3], Woo-Sang Jung[1] （1.Korea Institute of Science and Technology, Korea, 2.Materials Testing Institute, Germany, 3.Indo-Korea Science and Technology Centre, India）

[SY-F8] **Simultaneous Transformation Kinetics Model for Additive Manufacturing**

○Narendran Raghavan, Srdjan Simunovic, John Turner （Oak Ridge National Laboratory , United States of America）

Room4

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

[SY-N1] Symposium N-1

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

[SY-N1] Increasing the power of accelerated molecular dynamics methods and plans to exploit the coming exascale

○Arthur F Voter （Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, United

States of America)

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

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

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

[SY-N2] Symposium N-2

Chair: Erik Bitzek(FAU Erlangen-Nuernberg, Germany)
11:15 AM - 12:15 PM Room4

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

○Nikolas Provatas (McGill University, Canada)

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

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

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

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

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

[SY-N3] Symposium N-3

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

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

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

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

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

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

○Ivan Novoselov[1,2], Alexey Yanilkin[1] (1.Dukhov Research Institute of Automatics, Russia, 2.Moscow Institute of Physics and Technology, Russia)

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

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

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

[SY-N4] Symposium N-4

Chair: Laurent Karim Beland(Queen's University, Canada)
4:00 PM - 5:30 PM Room4

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

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

[SY-N4] Accelerated Quantum Molecular Dynamics

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

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

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

Room5

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

[SY-O5] Symposium O-5

Chairs: Hitoshi Washizu(University of Hyogo, Japan), Sophie Loehle(TOTAL Marketing &Services, Solaize, France)
9:45 AM - 11:00 AM Room5

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

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

Freiburg, Germany）

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

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

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

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

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

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

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

[SY-O6] Symposium O-6

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

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

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

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

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

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

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

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

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

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

[SY-O7] Symposium O-7

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

[SY-O7] Toward Exascale Atomistic Simulations of Interfaces

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

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

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

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

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

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

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

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

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

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

[SY-O8] Symposium O-8

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

4:00 PM - 5:00 PM Room5

[SY-O8] Friction mechanism of nanostructured steel in lubricant: A coarse-grained molecular dynamics study

○Yoshitaka Umeno Umeno, Atsushi Kubo, Yuta Sudo （The University of Tokyo, Japan）

[SY-O8] Coarse-Grained Molecular Dynamic Simulation on the Wear Mechanism of Polymer Brush with Different Chain Topologies

○Zhongmin Liu, Shuichi Uehara, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Material Research,Tohoku Univ., Japan）

[SY-O8] Molecular Dynamics Simulation Study on Friction of Bottlebrush Polymer with a Cationic Anchor Block Adsorbed on Substrate

○Shuichi Uehara, Zhongmin Liu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Materials Research, Tohoku Univ., Japan）

[SY-O8] Temperature dependent dynamics simulation of traction fluid by molecular dynamics method

○Eiji Tomiyama[1,2], Takeshi Iwasaki[3], Hitoshi Washizu[2] （1.Research Organization for Information Science and Technology, Japan, 2.Graduate School of Simulation Studies, Univ. of Hyogo, Japan, 3.Lubricants Research Laboratory, Idemitsu Kosan Co., Ltd., Japan）

Room6

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A5] Symposium A-5

Chair: Sinisa Dj Mesarovic(Washington State University, United States of America)
9:45 AM - 11:00 AM Room6

[SY-A5] Parameters to consider in the modelling of dislocation boundary evolution

○Grethe Winther Winther （Technical University of Denmark, Denmark）

[SY-A5] Data Mining of Indentation Induced Dislocation Microstructures

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

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

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

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A6] Symposium A-6

Chair: Emma Griffiths(University of Cape Town, South Africa)
11:15 AM - 12:30 PM Room6

[SY-A6] Design of patchy nanoparticles via the self-assembly of triblock terpolymers in selective solvents

○Eliot Fried, Nicolás Moreno （Okinawa Institute of Science and Technology, Japan）

[SY-A6] Nanoporous Composites: Giving Polymers Strength and Helping Metals Move

○Emma Griffiths[1], Jana Wilmers[2], Swantje Bargmann[2], BD Reddy[1] （1.University of Cape Town, South Africa, 2.University of Wuppertal, Germany）

[SY-A6] Multiscale modeling of advanced materials for hybrid organic-inorganic solar cells

○Alexander E. Kobryn （Nanotechnology Research Center, National Research Council Canada, Canada）

[SY-A6] **From cellulose and lignin to kerogen: molecular simulations of a geological process**

○Roland PELLENQ[1], Pierre-Louis Valdenaire[1], Christophe Bichara[3], Franz Ulm[1], Jean-Marc Leyssale[2] （1.<MSE>2, MIT- CNRS - AMU, United States of America, 2.ISM, CNRS - Bordeaux U., France, 3.CINaM, CNRS - Aix-Marseille U., France）

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A7] Symposium A-7

Chair: Michael Zaiser(FAU University of Erlangen-Nuremberg, Germany)
2:00 PM - 3:30 PM Room6

[SY-A7] Mathematical challenges for a mesoscale theory of dislocations

○Thomas Hochrainer （TU Graz, Austria）

[SY-A7] **Dislocation multiplication in the discrete-continuum transition regime**

○Katrin Schulz[1], Markus Sudmanns[1], Kolja Zoller[1], Peter Gumbsch[1,2] （1.Karlsruhe Institute of Technology, Germany, 2.Fraunhofer Institute for Mechanics of Materials, Germany）

[SY-A7] The fundamental instability of dislocation transport equations

○Michael Zaiser, Ronghai Wu （FAU University of

Erlangen-Nuremberg, Germany)

[SY-A7] 2D continuum theory of dislocations
○Istvan Groma (Eotvos Lorand University, Hungary)

[SY-A7] Continuum dislocation dynamics for finite deformation mesoscale plasticity
○Anter El-Azab (Purdue University, United States of America)

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A8] Symposium A-8

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

[SY-A8] Pattern formation in doubly curved thin shells
○Eleni Katifori[1], Desislava Todorova[1], Octavio Albarran[2], Lucas Goehring[2] (1.University of Pennsylvania, United States of America, 2.Max Planck Institute, Germany)

[SY-A8] Phase-field model for microstructure change in $L1_0$ type ordering with lattice distortion
○Ryuichiro Oguma[1], Long-Qing Chen[2], Syo Matsumura[3] (1.Fukuoka Univ., Japan, 2.The Pennsylvania State Univ., United States of America, 3.Kyushu Univ., Japan)

[SY-A8] Coupling multi-component phase field models for oxide systems to thermodynamic databases - breaking the curse of dimensionality
○Inge Bellemans[1], Nico Vervliet[2], Lieven De Lathauwer[2,3], Nele Moelans[4], Kim Verbeken[1] (1.Department of Materials, Textiles and Chemical Engineering, Ghent University , Belgium, 2.Department of Electrical Engineering, KU Leuven, Belgium, 3.Group Science, Engineering and Technology, KU Leuven - Kulak, Belgium, 4.Department of Materials Engineering, KU Leuven, Belgium)

[SY-A8] A Sharp Phase Field Method
○Alphonse FINEL[1], Yasunori YAMADA[2], Yann LE BOUAR[1], Benoît DABAS[1], Benoît APPOLAIRE[1], Tetsuo MOHRI[2] (1.Laboratoire d'Etude des Microstructures, CNRS, ONERA, France, 2.Institute for Materials Research, Tohoku University, Japan)

Room7

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

[SY-I5] Symposium I-5

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

[SY-I5] **Heterogeneous disconnections nucleation mechanisms during grain boundary migration**
○Nicolas Combe[1,2], Frederic Mompiou[1], Marc Legros[1] (1.CEMES Toulouse, France, 2.Univ. Toulouse, UPS, France)

[SY-I5] Motion of Grain Boundaries Based on Disconnections
○Chaozhen Wei[1,2], Luchan Zhang[5], Yang Xiang[2], Jian Han[4], Spencer Thomas[4], kongtao Chen[4], David J. Srolovitz[3,1] (1.HKUST Jockey Club Institute for Advanced Study, Hong Kong University of Science and Technology, Hong Kong, 2.Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong, 3.Materials Science and Engineering, Mechanical Engineering and Applied Mechanics, Computer and Information Science, University of Pennsylvania, United States of America, 4.Materials Science and Engineering, University of Pennsylvania, United States of America, 5.Department of Mathematics, National University of Singapore, Singapore)

[SY-I5] Dislocation-mediated boundary motion, dislocation-boundary interaction, and their effect on the mechanical behavior in fcc materials
○Bob Svendsen[1,2], Jaber Rezaei Mianroodi[2], Juan Li[3], Christoph Kirchlechner[3], Gerhard Dehm[3] (1.Material Mechanics, RWTH Aachen University, Germany, 2.Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Germany, 3.Structure and Nano-/Micromechanics of Materials, Max-Planck-Institut für Eisenforschung GmbH , Germany)

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

[SY-I6] Symposium I-6

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

[SY-I6] Migration mechanisms of faceted vicinal grain boundaries
○Sherri Hadian[1], Blazej Grabowski[1], Mike W Finnis[2], Jörg Neugebauer[1] (1.Max-Planck-Institut fuer Eisenforschung, Germany, 2.Imperial College London, UK)

[SY-I6] Multiscale model for the structure and energy of low-angle general grain boundaries in Al, Cu and Ni
○Shuyang Dai[1], Yang Xiang[2], David Joseph Srolovitz[3]

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

[SY-I6] The influence of normal stress on the structural transformation and migration of grain boundaries

○Chuang Deng, Mohammad Aramfard （University of Manitoba, Canada）

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

[SY-I7] Symposium I-7

Chairs: Nicolas Combe(CEMES Toulouse, France), Brandon Runnels(University of Colorado Colorado Springs, United States of America)
2:00 PM - 3:30 PM Room7

[SY-I7] Insights into recrystallisation: atomistic simulations of the properties of grain boundaries in heavily deformed material

○Chris P Race （University of Manchester, UK）

[SY-I7] Continuum Dislocation Dynamic Based Grain Fragmentation Modeling for Severe Plastic Deformation in FCC Metals

○Ali Al-Hadi I. Kobaissy[1], Georges Ayoub[2], Mu'Tasem Shehadeh[1] （1.Department of Mechanical Engineering, American University of Beirut, Lebanon, 2.Department of Industrial and Manufacturing Systems Engineering, University of Michigan-Dearborn, United States of America）

[SY-I7] Atomistic Investigation on Interaction of Stress-Assisted Grain Boundary Motion with Crack

○Mohammad Aramfard, Chuang Deng （Univ. Manitoba, Canada）

[SY-I7] **Effect of grain boundary structure on its Dynamic Response using Molecular Dynamics**

○Saryu Fensin[1], Timothy Frolov[2] （1.Los Alamos National Lab, United States of America, 2.Lawrence Livermore National Laboratory, United States of America）

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

[SY-I8] Symposium I-8

Chair: Srikanth Patala(North Carolina State University, United States of America)
4:00 PM - 5:00 PM Room7

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

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

[SY-I8] **Grain Boundary Sliding: the best supporting role in ductile localization**

○Alexandre Dimanov[1], Jean Raphanel[1], Michel Bornert[2], Eva Héripré[3], Mathieu Bourcier[1], Ababacar Gaye[2], Alexandre El Sabbagh[1], Wolfgang Ludwig[4], Andrew King[5] （1.LMS, CNRS-UMR7649, Ecole Polytechnique, France, 2.Laboratoire Navier, CNRS-UMR8205, Ecole des Ponts, France, 3.MSSMAT, CNRS-UMR8579, Centrale-Supélec, France, 4.MATEIS, UMR5510, INSA-Lyon, France, 5.SOLEIL Synchrotron, Beam line Psiché, France）

[SY-I8] Polycrystal plasticity with anisotropic grain boundary energy described on the five-dimensional grain boundary space

○Nikhil Chandra Admal[1], Javier Segurado[2,1], Jaime Marian[1] （1.University of California Los Angeles, United States of America, 2.IMDEA, Spain）

Room8

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

[SY-G1] Symposium G-1

Chairs: Byeongchan Lee(KyungHee Univ., Korea), Keonwook Kang(Yonsei University, Korea)
9:45 AM - 11:00 AM Room8

[SY-G1] A systematic method to develop a potential model for harsh environments

○Takuji Oda, Sehyeok Park, Woonghee Cho （Dept. of Nuclear Engineering, Seoul National Univ., Korea）

[SY-G1] Molecular dynamics study of the bulk cascades in W-Re alloy

○Hyunggyu Lee[1], Byeongchan Lee[2], Keonwook Kang[1] （1.yonsei university, Korea, 2.kyung hee university, Korea）

[SY-G1] Defect Energetics in W-Based Transition-Metal Ternary Systems

○Younggak Shin, Byeongchan Lee （KyungHee Univ., Korea）

[SY-G1] A numerical study of channel deformation and fracture in irradiated stainless steel single crystals

○Jean-Michel Scherer[1,2], Samuel Forest[2], Jacques Besson[2], Benoit Tanguy[1], Jérémy Hure[1] （1.DEN-Service d'Etudes des Matériaux Irradiés, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette cedex, France, France, 2.MINES ParisTech, PSL-Research University, Centre des matériaux, CNRS UMR 7633, 63-65 rue Henri Auguste DesbruèresBP 87 91003 Evry Cedex, France, France)

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

[SY-G2] Symposium G-2

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

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

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

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

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

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

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

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

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

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

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

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

[SY-G3] Symposium G-3

Chairs: Seunghwa Ryu(Korea Advanced Institute of Science and Technology, Korea), Keonwook Kang(Yonsei University, Korea)
2:00 PM - 3:30 PM Room8

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

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

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

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

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

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

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

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

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

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

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

[SY-G4] Symposium G-4

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

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

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

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

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

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

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

Room9

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

[SY-H3] Symposium H-3

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

[SY-H3] Polydomain liquid crystal elastomers1

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

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

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

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

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

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

[SY-H4] Symposium H-4

Chair: Meredith Silberstein(Cornell University, United States of America)
11:15 AM - 12:30 PM Room9

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

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

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

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

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

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

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

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

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

[SY-H5] Symposium H-5

Chair: Alexey Lyulin(Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands)
2:00 PM - 3:30 PM Room9

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

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

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

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

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

○Sumit Basu （Indian Institute of Technology Kanpur,

India）

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

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

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

[SY-H6] Symposium H-6

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

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

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

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

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

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

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

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

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

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

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

Room10

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

[SY-B1] Symposium B-1

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

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

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

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

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

[SY-B1] **Properties of interstitials in concentrated Fe-Cr alloys from first principles**

○Marcin Roland Zemla[1], Jan Stanislaw Wrobel[1], Marek Muzyk[1], Tomasz Wejrzanowski[1], Duc Nguyen-Manh[2], Sergei L. Dudarev[2], Luca Messina[3], Par Olsson[3], Christophe Domain[4] （1.Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland, 2.CCFE, Culham Centre for Fusion Energy, Abingdon, Oxon OX14 3DB, UK, 3.KTH Royal Institute of Technology, Nuclear Engineering, 106 91 Stockholm, Sweden, 4.Dép artement Matériaux et Mécanique des Composants, EDF-R&D, Les Renardières, F-77250 Moret sur Loing, France）

[SY-B1] **Defect production in cascade overlap with defect clusters in iron and tungsten**

○Jesper Byggmastar[1], Fredric Granberg[1], Andrea E Sand[1], Kai Nordlund[1] （1. Department of Physics, University of Helsinki, Finland）

[SY-B1] Multiscale modelling of radiation damage evolution in Fe and Fe-based alloys

○Fredric Granberg[1], Haixuan Xu[2], Kai Nordlund[1] （1.Department of Physics, University of Helsinki, Finland, 2.Department of Materials Science and Engineering, University of Tennessee, United States of America）

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

[SY-B2] Symposium B-2

Chair: Davide Pizzocri(Politecnico di Milano, Italy)
11:15 AM - 12:30 PM Room10

[SY-B2] Atomic scale calculations of nuclear fuel properties to sustain multiscale modeling of fuel behavior

○Emeric Bourasseau, Marjorie Bertolus, Michel Freyss, Gérald Jomard, Ibrahim Cheik Njifon, Martin-Stéphane Talla Noutack, Cyrille Takoukam Takoundjou

（CEA/DEN/DEC, Centre CEA de Cadarache, France）

[SY-B2] Influence of vibrational entropy on the concentrations of uranium vacancies in UO_2
○Jean-Paul Crocombette[1], Fabien Bruneval[1], Aurélien Soulié[1], Mihai-Cosmin Marinica[1], Samuel Murphy[2]
（1.CEA Saclay, France, 2.Lancaster University, UK）

[SY-B2] **Modelling of defect and rare gas transport properties in UO_2 from the atomic to the grain scale**
○Marjorie Bertolus, Michel Freyss, Emerson Vathonne, Emeric Bourasseau, Serge Maillard, Gérald Jomard
（CEA, DEN, Département d'Etude des Combustibles, Centre de Cadarache, 13108 Saint-Paul-lez-Durance, France）

[SY-B2] **Intragranular bubble impact on nuclear fuel thermomechanical properties**
Fabienne Ribeiro[1], Mehdi Colbert[1], ○Jack Arayro[1], Guy Tréglia[2] （1.Institut de Radioprotection et de Sûreté Nucléaire/PSN-RES/SEMIA/LPTM, France, France, 2.Centre Interdisciplinaire de Nanoscience de Marseille, CNRS, France, France）

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

[SY-B3] Symposium B-3

Chair: Kazuto Arakawa(Shimane University, Japan)
2:00 PM - 3:15 PM Room10

[SY-B3] **Formation of radiation-induced Re and Os precipitation in W and its effects on mechanical properties**
○Guang-Hong Lu, Yu-Hao Li, Hong-Bo Zhou （Beihang University, China）

[SY-B3] **Elastic fields and interaction between self-interstitial atom defects in bcc metals.**
○Sergei L Dudarev, Pui-Wai Ma （UK Atomic Energy Authority, UK）

[SY-B3] Molecular dynamics simulation study of the interaction of Re with interstitial defects in tungsten bulk
Yangchun Chen[1], Jingzhong Fang[1], Ning Gao[2], Hong-Bo Zhou[3], Wangyu Hu[4], Fei Gao[4,5], ○Huiqiu Deng[1,4]
（1.School of Physics and Electronics, Hunan University, China, 2.Institute of Modern Physics, Chinese Academy of Sciences, China, 3.Department of Physics, Beihang University, China, 4.College of Materials Science and Engineering, Hunan University, China, 5.Department of Nuclear Engineering and Radiological Science, University of Michigan, United States of America）

[SY-B3] **Hydrogen super-saturated layers in plasma loaded tungsten: a global model combining Density Functional Theory data, Thermodynamic and Kinetic models**
○Yves Ferro, Etienne Hodille （Aix-Marseille University, France）

[SY-B3] Mobility of small vacancy and interstitial prismatic dislocation loops in BCC tungsten
○Jan Fikar[1], Roman Gröger[1], Robin Schäublin[2]
（1.Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic, Switzerland, 2.Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, Switzerland）

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

[SY-B4] Symposium B-4

Chair: Gary S Was(University of Michigan, United States of America)
4:00 PM - 5:15 PM Room10

[SY-B4] **Kinetics of Precipitation in Fe-Cr and Fe-Cr-C alloys under Irradiation**
○Frederic Soisson （CEA Saclay, France）

[SY-B4] **The complex problem of the experimental validation of atomistic and microstructural evolution models**
○Lorenzo Malerba （ CIEMAT, Energy, Environment and Technology Research Centre, Spain）

[SY-B4] Physically based prediction of radiation hardening: application to steels and model alloys
○Ghiath Monnet （EDF - R&D, MMC, France）

[SY-B4] **Oxygen diffusion in bcc Fe under the influence of foreign atoms and vacancies**
○Xiaoshuang Wang, Matthias Posselt, Jürgen Faßbender
（Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany）

Wed. Oct 31, 2018

Poster Hall

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

[PO-A2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-01] Multiscale model of solid state amorphization during processing of pharmaceutical materials
Chunyu Li[1], Yifei Zeng[1], Lorena Alzate-Vargas[1], Pilsun Yoo[1], Rachel Frocino[2], Jeff Brum[2], Peilin Liao[1], Marisol Koslowski[1], ○Alejandro Strachan[1] （1.Purdue University, United States of America, 2.GlaxoSmithKline, Analytical Sciences and Development, United States of America）

[P2-02] FTMP-based Modeling and Simulations of HCP Mg Single Crystal
○Takahiro Kitano, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P2-03] Nonlinear elasticity on Riemannian manifold and its application to general surface development
○Yuto Horikawa[1], Ryuichi Tarumi[2], Yoji Shibutani[1] （1.Dept. of Mechanical Engineering, Osaka Univ., Japan, 2.Grad. Sch. of Engineering Science, Osaka Univ., Japan）

[P2-04] The challenge of achieving quantitative phase field models for microstructure evolution in irradiated solids - the case of voids
○Anter El-Azab （Purdue University, United States of America）

[P2-05] A Molecular-Dynamics Study of Surface Tension: From Alloy Droplets to Bubbles in Molten Alloy
○Xiangming Ma, Hongtao Liang, Yang Yang （East China Normal Univercity, China）

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

[PO-B2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-06] Effects of rhenium on the mechanical behavior of irradiated tungsten: a molecular dynamics study using neural-network potential
○Ryo KOBAYASHI （Nagoya Institute of Technology (NITech), Japan）

[P2-07] Diffusion behavior and temperature dependence of hydrogen in tungsten and molybdenum under isotropic strain state
○QuanFu Han[1], Yue-Lin Liu[2], Ying Zhang[1], Guang-Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

[P2-08] **Diffusion of Point Defects on Tungsten Surface**
Jiannan Hao[1], ○Shuo Jin[1], Haixuan Xu[2], Xiaolin Shu[1], Guanghong Lu[1] （1.School of Physics and Nuclear Energy Engineering, Beihang University, China, 2.Department of Material Science and Engineering, The University of Tennessee, Knoxville, United States of America）

[P2-09] Influence of anisotropic strain and temperature on hydrogen dissolution in tungsten
○Ying zhang[1], Quan Fu Han[1], Yue lin Liu[2], Guang Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

[P2-10] Screw dislocation-interstitial solute coevolution in W-O alloys using atomistically-informed kinetic Monte Carlo simulations
○Yue Zhao[1], Lucile Dezerald[3], Jaime Marian[1,2] （1.Dept. of Materials Science and Engineering, University of California, Los Angeles, United States of America, 2.Dept. of Mechanical Engineering, University of California, Los Angeles, United States of America, 3.Institut Jean Lamour, University of Lorraine, France）

[P2-11] Kinetic Monte-Carlo Simulations of Radiation Damage in W(Re,Os) Alloys
○Matthew James Lloyd[1,2], David Armstrong[1], Enrique Martinez Saez[3], Duc Nguyen-Manh[2] （1.Department of Materials, University of Oxford, UK, 2.Culham Centre for Fusion Energy, UK, 3.Los Alamos National Laboratory, United States of America）

[P2-13] **Dynamics of Magnetism in Neutron Irradiated Iron-Chromium Steels**
○Jacob B. J. Chapman, Pui-Wai Ma, Sergei L. Dudarev （Culham Centre for Fusion Energy (CCFE), UK）

[P2-14] **Atomistic insights into the grain boundaries interaction with radiation-induced point defects in bcc Fe-Cr alloys**
○Marcin Roland Zemla, Jan Stanislaw Wrobel, Tomasz Wejrzanowski （Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland）

[P2-15] Production and Process of Cascade Development in Irradiated Pure α-Zr from Molecular Dynamics Simulations
○Rongjian Pan[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Bang Wen[1], Wen He[1], Y.R. Ovcharenko[3], D.O.

Kharchenko[3] （1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine）

[P2-16] Microstructure evolution of cascade annealing in irradiated pure α-Zr from molecular dynamics simulations

○Bang Wen[1], Rongjian Pan[1], Wei Zhang[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3] （1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine）

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

[PO-C2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-18] **Prediction of Biaxial Tensile Deformation Behavior of Aluminum Alloy Sheets using Crystal Plasticity Finite Element Method and Machine Learning**

○Kota Koenuma[1], Akinori Yamanaka[1], Ikumu Watanabe[2], Toshihiko Kuwabara[1] （1.Tokyo University of Agriculture and Technology, Japan, 2.National Institute of Materials Science, Japan）

[P2-19] MobiDiC: A 3-D Dislocation Dynamics Simulation

○Ronan MADEC[1], Laurent COLOMBET[1], Ladislas KUBIN[2] （1.CEA, DAM, DIF, France, 2.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay, France）

[P2-20] Temperature dependence of fatigue crack growth in Ti-6Al-4V

○Bhargavi Rani Anne, Masaki Tanka, Tatsuya Morikawa （Dept. of Materials Science and Engineering, Kyushu University, Japan）

[P2-21] Parametric model of discrete dislocation dynamics based on mathematical theory of moving curves

○Miroslav Kolar, Jan Kratochvíl, Petr Pauš, Michal Beneš （Czech Technical University in Prague, Czech Republic）

[P2-22] On Visualization of Multiscale Information Transfer/Exchange Processes via FTMP-based Duality Diagram Representation Scheme

○Takuya Takagi, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P2-23] **Rotational Field Evolutions based on Field Theory of Multiscale Plasticity (FTMP)**

○Tadashi Hasebe[1], Yasutaka Matsubara[2] （1.Kobe Univ., Japan, 2.Graduate School of Kobe Univ., Japan）

[P2-24] **A 2D MESOSCALE STUDY OF DISLOCATIONS, CRACKS AND MARTENSITIC PHASE TRANSFORMATIONS**

○Rachel Derby, Michael Budnitzki, Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

[P2-25] Effects of Stress Distribution on the Plastic Deformation of Metallic Glasses under Different Geometries

○Chih-Jen Yeh[1], Hsuan-Teh Hu[1], Chang-Wei Huang[2], Yu-Chieh Lo[3] （1.National Cheng Kung University, Taiwan, 2.Chung Yuan Christian University, Taiwan, 3.National Chiao Tung University, Taiwan）

Poster Session | D. Data-Driven and Physics-Informed Materials Discovery and Design

[PO-D2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-26] Generalized nano-thermodynamic model for predicting size-dependent surface segregation in multi-metal alloy nanoparticles from smaller particles

○Abhijit Chatterjee （Dept. of Chemical Engg., Indian Institute of Technology Bombay, India）

[P2-27] Development of thermodynamic database of Nd-Fe-B-based permanent magnet alloys

○Jiang Wang, Lei Xu, Kaicheng Yang, Qingrong Yao, Guanghui Rao, Huaiying Zhou （School of Material Science and Engineering, Guilin University of Electronic Technology, China）

[P2-28] Design of proteins and biopolymers: role of directional interactions and of water.

○Valentino Bianco[1], Ivan Coluzza[2] （1.University of Vienna, Austria, 2.CIC biomaGUNE, center for cooperative research in biomaterials, Spain）

[P2-29] Aquatic pollutant removal by adsorption in zeolite structures: An experimental and molecular simulation study

○Mate Erdos[1], Nan Jiang[2], Sebastian G. J. Heijman[2], Othonas A. Moultos[1] （1.Process &Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Netherlands, 2.Department of Water Management, Faculty of Civil Engineering and Geosciences, Delft University of Technology, Netherlands）

[P2-30] Optimizing elastic moduli of the silicate glasses through high-throughput atomistic modeling and machine learning techniques

Yong-Jie Hu[1], Ge Zhao[2], Tyler Del Rose[1], ○Liang Qi[1] （1.Dept. of Materials Science and Engineering, University of Michigan, United States of America, 2.Department of Statistics, Pennsylvania State University, United States of America）

[P2-31] High pressure phase transition and structural stability of transition metal compounds

○Fanyan Meng[1], Wandong Xing[1,2], Rong Yu[2] （1.Dept. of Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-32] Development of artificial neural network model for prediction of electronic density of states in atomistic systems

○Atsushi Kubo, Yoshitaka Umeno （Institute of Industrial Science, the University of Tokyo, Japan）

[P2-33] Development of First-principles Platform Technology for Energy Research

○Kanghoon Yim[1], Chan-Woo Lee[1], Jehyun Lee[1], Incheol Jeong[2], Yong Youn[3], Seungwu Han[3] （1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Dept. of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science &Technology, Korea, 3.Seoul National University, Korea）

Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-34] Dynamics of a solidification front made by invasion of fluid with a different temperature

○So Kitsunezaki, Chika Yamanaka （Nara Women's Univ., Japan）

[P2-35] Strengthening through solid solution in $W_{1-x}Ta_xB$ system

○lijuan liu[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-36] Desiccation crack patterns based on phase-field modeling and their statistical properties

○Shin-ichi Ito[1], Satoshi Yukawa[2] （1.The Univ. of Tokyo, Japan, 2.Osaka Univ., Japan）

[P2-37] Ce-terminated (111) surface of CeO_2

○YaNan Zhao[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-39] **Numerical analysis of elasto-plastic behavior of metallic architectured materials**

○Filip Siska[1], Ivo Dlouhy[1], Jan Cizek[2], Hanus Seiner[3] （1.Institute of Physics of Materials, Czech Academy of Sciences, Czech Republic, 2.Institute of Materials Science and Engineering, Brno University of Technology, Czech Republic, 3.Institute of Thermomechanics, Czech Academy of Sciences, Czech Republic）

[P2-40] Automatic analysis and numerical prediction of flow stress curves for aluminium alloys

○Evgeniya Kabliman, Johannes Kronsteiner, Ana-Helena Kolody （Light Metals Technologies Ranshofen, Center fo Low-Emission Transport, Austrian Institute of Technology, Austria）

[P2-41] Comparison of different alkali activated mortars with hemp fibres response during fracture test by acoustic emission method

Libor Topolar[1], ○Hana Simonova[1], Barbara Kucharczykova[1], Zbynek Kersner[1], Jelena Dragas[2], Ivan Ignjatovic[2], Miroslav Komljenovic[3], Violeta Nikolic[3] （1.Brno University of Technology, Faculty of Civil Engineering, Czech Republic, 2.University of Belgrade, Faculty of Civil Engineering, Serbia, 3.University of Belgrade, Institute for Multidisciplinary Research, Serbia）

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

[PO-F2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-43] Design of spontaneous formation-based 3D plasmonic optical structure, using multyphysics modeling

○Jihwan Song[1], Inhee Choi[2], Yonghee Shin[3], SoonGweon Hong[5], Younggeun Park[5], Dongchoul Kim[4], Taewook Kang[3], Luke Lee[5] （1.Dept. of Mechanical Engineering, Hanbat National University, Korea, 2.Dept. of Life Science, University of Seoul, Korea, 3.Dept. of Chemical and Biomolecular Engineering, Sogang

University, Korea, 4.Dept. of Mechanical Engineering, Sogang University, Korea, 5.Dept. of Bioengineering and Berkeley Sensor and Actuator Center, University of California, Berkeley, United States of America)

[P2-44] **Characterization of $K_xNa_{1-x}NbO_3$ powders and ceramics prepared by hydrothermal synthesis**

○Jing Yang, Aifen Tian, Xuan Xi, Huiling Du (Dept. of Materials Science and Engineering, Xi An Univ. of Science and Technology, China)

[P2-45] Numerical and experimental investigation of liquid metal dealloying of Cu-Ni alloy in liquid silver.

○Pierre-Antoine Geslin[1,2,3], Takumi Suga[2], Takeshi Wada[2], Hidemi Kato[2] (1.INSA Lyon/CNRS, France, 2.Institute for Materials Research, Tohoku University, Japan, 3.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan)

[P2-46] **Application of DLVO theory to predict dispersion stability of ZrO_2 submicron particles in electrolyte solutions**

○Ming-Hong Chiueh, Tien-Jung Huang (Industrial Technology Research Institute, Taiwan)

[P2-47] Multi-GPU large-scale phase-field lattice Boltzmann simulation of dendrite growth with thermal-solutal convection

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

[P2-48] Stress analysis of 4H-SiC power devices via FEM and Raman spectroscopy

○Hiroki Sakakima[1], Asuka Hatano[1], Akihiro Goryu[2], Kenji Hirohata[2], Satoshi Izumi[1] (1.The Univ. of Tokyo, Japan, 2.Toshiba, Japan)

[P2-49] A Functionally Graded Multi-Phase Micromechanical Model for Carbon Nanotube - Polymer Composites

○Vahidullah Tac[1,2], Ercan Gurses[1] (1.Middle East Technical University, Turkey, 2.Turkish Aerospace Industries, Turkey)

[P2-50] **Atomic surface treatment of copper nanowires by electron beam irradiation simulated by first principle calculation**

○Shih Kuang Lee (National Chiao Tung University, Taiwan)

[P2-51] Molecular-Dynamic Simulation of Rapid Solidification of Dipolar Molecular Crystal from Its Melt

○Xianqi Xu, Yang Yang (East China Normal University, China)

[P2-52] Intrinsic Analysis of Structural Order Parameter at Equilibrium Crystal-Melt Interfaces

○Wenliang Lu, Hongtao Liang, Yang Yang (EAST CHINA NORMAL UNIVERSITY, China)

[P2-53] Multiscale Modelling of Indirect-to-Direct Band Gap Transition in Silicon Nanosheets

○Byung-Hyun Kim[1], Chan-Woo Lee[1], Mina Park[2], Gyubong Kim[2], Kersti Hermansson[3], Peter Broqvist[3], Heon-Jin Choi[4], Kwang-Ryeol Lee[2] (1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Computational Science Research Center, Korea Institute of Science and Technology, Korea, 3.Dept. of Chemistry-Ångström Laboratory, Uppsala University, Sweden, 4.Dept. of Materials Science and Engineering, Yonsei University, Korea)

Poster Session | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[PO-G2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-54] **Component-wise Effect of Incompatibility Tensor on Misorientation Development in Lath Block Structure Model based on FTMP**

○Yuta Amano, Tadashi Hasebe, Yasutaka Matsubara (Dept. of Mechanical Engineering, Kobe Univ., Japan)

[P2-55] Construction of virtual ITZ specimens using extended stochastic optimization and evaluation of their permeability

○Se-Yun Kim, Tong-Seok Han (Dept. of Civil and Environmental Engineering, Yonsei Univ., Korea)

[P2-56] Estimation for probabilistic distribution of material response according to microstructural characteristics

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

[P2-57] **Hypervelocity impact and shock behavior of pillared graphene foams**

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

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

[PO-H2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-58] Studying the kinetics of a self-propelled cruiser in 2D granular media under gravity

○Guo-jie Jason Gao (Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan)

[P2-59] A Discrete Tetris model showing two flow regimes for hard particles exiting a hopper with an adjustable obstacle

○Tomoya Yasuno[1,2], Guo-jie Jason Gao[1] (1.Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan, 2.Dept. of Complex Systems Science, Nagoya Univ., Japan)

[P2-60] Effect of water molecules on polymer chain motion in dense chain ensembles of nafion membrane

○Isamu Riku, Ryoma Oka, Koji Mimura (Osaka Prefecture Univ., Japan)

[P2-61] A Coarse-Grained Model for Competitive Adsorption on the Surface of Inorganic Nanomaterials

○Stefano Poggio[1], Hender Lopez[2], David Power[1], Vladimir Lobaskin[1] (1.School of Physics, University College Dublin, Ireland, 2.Institute Laue-Langevin, Grenoble, France)

[P2-62] Molecular Dynamics of Inorganic and Organic Interfaces with Force-Field Parameters Based on DFT Simulations

○Kosuke Ohata, Hiroya Nitta, Kenta Chaki, Taku Ozawa (JSOL Corporation, Japan)

[P2-63] **Molecular dynamics screening for developing compounds of electrolytes with high performance in lithium ion batteries**

○Yoshihiro Takai[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] (1.Graduate school of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan)

[P2-64] Molecular dynamics study on transmission mechanism of torsional deformation in cellulose nanofibers with hierarchical structure

○Kentaro Takada[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] (1.Graduate School of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan)

[P2-65] Bubble dynamics of foam flow around an obstacle

○Antti Puisto, Juha Koivisto, Leevi Viitanen, Mikko J Alava (Aalto University, Department of Applied Physics, Finland)

[P2-66] Shape Deformation and Mechanical Relationship of Ionic Droplet Under An Electric Field

Bo-Yu Shih[1], ○Wei-Chun Lin[1], Alice Hu[2], Hsuan-Teh Hu[1], Yu-Chieh Lo[3] (1.Department of Civil Engineering,National Cheng Kung University, Taiwan, 2.Department of Mechanical and Biomedical Engineering, City University of Hong Kong, Hong Kong, 3.Department of Materials Science and Engineering, National Chiao Tung University, Taiwan)

[P2-67] Multiscale modeling of surface functionalized graphene/polymer nanocomposites: insight into the effect of covalent grafting

○Jeong-ha Lee[1], Seunghwa Yang[2] (1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea)

[P2-68] Durability analysis on the environmental aging of epoxybased nanocomposite

○Sunyong Kwon[1], Man Young Lee[2], Seunghwa Yang[3] (1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Agency for Defense Development, Korea, 3.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea)

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

[PO-I2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-69] **Topological evolution of the microstructures of thin films during grain growth**

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

[P2-70] Molecular dynamics simulations of phase transformations in nanocrystalline NiTi shape-memory alloys

○Won-Seok Ko (University of Ulsan, 93 Daehak-ro, Nam-gu, Ulsan, 44610, Korea)

[P2-71] An attempt to connect migration of grain boundaries to their atomic
structures with help of Molecular Dynamics

Zakaria El Omari, ○Sylvain Queyreau, Charlie Kahloun, Brigitte Bacroix （Universite Paris XIII, Sorbonne Paris Cite, Laboratoire des Sciences des Procedes et des Materiaux, LSPM UPR 3407, France）

[P2-72] Disconnection interaction in Cu grain boundaries

○Christian Brandl （Karlsruhe Institute of Technology, Germany）

[P2-73] Phase-field Approach to Thermo-mechanical Behavior of Through-silicon Vias

Wooju Lee, ○jaekeun yoon, Dongchoul Kim （Sogang Univ., Korea）

[P2-74] **Grain-Growth in Nanocrystalline Metals under Ion Irradiation: A Thermal Spike Model**

○Djamel Kaoumi[1], Robert Birtcher[2], Arthur Motta[3] （1.North Carolina State University, United States of America, 2.Argonne National Laboratory, United States of America, 3.Penn State University, United States of America）

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

[PO-N2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-75] **Why the structure-property relationship in metallic glasses should be established beyond short-range order: Insight from potential energy landscape**

○Dan Wei[1,2], Yunjiang Wang[1,2], Lanhong Dai[1,2] （1.University of Chinese Academy of Sciences, China, 2.Institute of Mechanics, Chinese Academy of Sciences, China）

[P2-76] Vacancy segregation analysis near grain boundaries in metallic systems by long-time atomistic simulations

○Shotaro Hara （Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan）

[P2-77] **EXPERIMENTAL AND DENSITY FUNCTIONAL THEORY STUDIES OF PRECIPITATE INTERFACES IN ALUMINIUM ALLOYS, WITH FOCUS ON β" & β**

○Haris Rudianto, Deni Hariadi, Andriansyah Andriansyah （Gunadarma University, Indonesia）

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

[PO-O2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-78] Adsorption of Volatile Organic Compounds (VOCs) on Silicene by Density Functional Theory Calculations

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

[P2-79] Atomistic insights into defect formation mechanism in single crystal SiC based on molecular dynamics simulation

○Kenji Nishimura[1], Koji Miyake[1], Ken-ichi Saitoh[2] （1.AIST, Japan, 2.Kansai Univ., Japan）

[P2-80] **Potential cathode material Na_xVOPO_4 for rechargeable Sodium - ion batteries: DFT investigation**

○Duc Huu Luong[1], An Van Dinh[1,2], Yoshitada Morikawa[3], Yoji Shibutani[2,1] （1.Nano Technology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan, 3.Department of Precision Science and Technology, Graduate School of Engineering, Osaka University, Japan）

[P2-81] **Two-dimensional Na_xSiS as a promising anode material for rechargeable Sodium-based batteries: Ab initio material design.**

Thi Dung Pham[1], ○Van An Dinh[1,2], Kazunori Sato[3], Yoji Shibutani[1,2] （1.Nanotechnology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan, 3.Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, Japan）

[P2-82] Modelling and analysis of SiO2 interfaces of non-firing solids

○Tomohiro Sato[1], Ken-ichi Saitoh[1], Masayoshi Fuji[2], Chika Yamashita Takai[2], Hadi Razavi[2], Masanori Takuma[1], Yoshimasa Takahashi[1] （1.Dept. of Mechanical Engineering, Kansai Univ., Japan, 2.Advanced Ceramics Reserch Center, Nagoya Institute of Technology, Japan）

Plenary Talk | Plenary Talk

[PL4] Plenary Talk 4

Grain boundary sliding, fracture and dislocation motion in ceramics
Chair: Erik Bitzek(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)
Wed. Oct 31, 2018 8:30 AM - 9:20 AM Room1
Yuichi Ikuhara

[PL4] Plenary Talk 4

○Yuichi Ikuhara （The University of Tokyo/Japan Fine Ceramics Center, Japan）

(Wed. Oct 31, 2018 8:30 AM - 9:20 AM Room1)

[PL4] Plenary Talk 4

Grain boundary sliding, fracture and dislocation motion in ceramics

○Yuichi Ikuhara （The University of Tokyo/Japan Fine Ceramics Center, Japan）

Ceramics have been widely used for structural applications because of their superior mechanical properties at high temperatures. It has been known that the behavior of GB sliding is strongly dependent on the GB characters such as misorientation angle between two adjacent crystals and GB plane, however, such effect has not been clarified yet. In addition, this effect in much influenced by dopant segregation at GBs. In this study, in order to clarify the atomistic mechanisms of GB sliding and its dopant effect, bicrystal studies have been performed to find the relationship between the atomic structures, chemistry and GB sliding behavior of Al2O3 ceramics. Several kinds of bicrystals including GBs with specific geometrical configuration were fabricated, and some of them were doped by rare-earth elements to enhance the GB segregation.
It has been reported that several oxides can be plastically deformed even at R.T. by dislocation slip like metals. So far, many experimental investigations have been tried for understanding the dislocation-grain boundary interaction, but these experiments were mostly carried out statically, and the fundamental processes are still not well understood yet. In this study, the nanoindentation experiments were conducted for SrTiO3 crystals their bicrystals inside TEM. Several kinds of TEM specimens for in situ nanoindentation experiments were prepared, that are single crystals and bicrystals including various types of GBs. The SrTiO3 single crystals were indented with the sharp diamond tip and successfully observed the dislocation dynamics. In the case of the GBs, the interaction between the introduced lattice dislocations and the GBs were directly observed. The dislocation-GB interaction and its dependence on the GB characters will be discussed in detail.

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

[SY-C5] Symposium C-5

Chair: Christopher Woodward(Air Force Research Laboratory, United States of America)
Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room1

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

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

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

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

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

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

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

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

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room1)

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

Invited

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

Current and future applications in hypersonic flight, re-entry vehicles, propulsion, and power production create an insatiable demand for materials capable to perform in severe environments. Materials for these applications must possess a rare combination of properties, which include high specific strength, elevated melting temperature, high thermal conductivity, and low thermal expansion coefficient. Ultra-High Temperature Ceramics are being considered for applications in extreme environments, especially when oxidation is a major concern. Currently, the factor limiting the use of UHTCs as structural materials is their low-temperature brittleness. This talk focuses on the plasticity and fracture mechanisms of the transition metal carbide TaC, one of the highest melting temperature materials known to mankind. *In-situ* micro-pillar compression experiments carried out at different temperatures and orientations reveal unexpected intrinsic ductility of TaC, which contrasts its well-known bulk brittleness. These findings unveil new properties of the material, such as a pronounced non-Schmid behavior and a remarkable temperature/orientation dependence of the yield strength. A variety of multiscale modeling techniques ranging from *ab-initio* to discrete dislocation dynamics simulations are employed to understand the small-scale behavior of TaC. Computer simulations shed light on the room-temperature brittleness of TaC by explaining the link between plastic deformation and fracture.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room1)

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

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

The strengthening mechanisms in magnesium alloys are strongly related to the complex intermetallic precipitates that spread all over the microstructure. In particular, the hard and brittle Laves phases [1] commonly observed in such alloys exhibit a complex atoms stacking with largely unknown plasticity mechanisms [2].

We propose here a numerical atomistic approach at the cross-road of experiments and *ab initio* simulations, to shed light on the responsible mechanisms for the plasticity in hexagonal Mg_2Ca (C14) Laves phases. Elastic and plastic properties of bulk Laves phase are investigated by both first principle and classical atomistic simulations. Molecular dynamics/statics simulations with a robust MEAM interatomic potential are performed to study the propagation of dislocations, by a combination of nudge-elastic-band (NEB) methods and nano-mechanical tests. In particular, the cross-slip to pyramidal slip planes, the propagation of dislocations in the basal plane by the so called synchroshear mechanism [3,4] and the influence of temperature on slip systems activation, are investigated at the atomic scale. All these results are finally correlated and discussed by considering experimental findings, especially from micro-pillar compression

tests. Our goal is to improve the understanding of the largely unknown plasticity of Laves phases.

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(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room1)

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

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

Micro- and nano-sized structures have attracted substantial interest due to their special mechanical behavior: they generally show an increased yield strength compared with the bulk material as well as an improved ductility. Among them, nanoparticles (NPs) which are generally used for their shape-dependent functional properties also appear as perfect candidates for submicronic plasticity investigations due to their broad range of sizes and their variety of shapes. While metallic and silicon NPs have been widely investigated since almost two decades, less is known about the strength of ceramic NPs maybe due to the brittleness of their bulk counterparts.
In the light of recent but preliminary in situ TEM observations, we investigate here the mechanical behavior of <100>-oriented MgO nanocubes. First, incipient plasticity mechanisms are investigated using molecular dynamics simulations (MD) of virtual nanocompression tests at constant strain rate. Results show that the plastic deformation of MgO nanocubes starts with the nucleation from the surface of perfect ½<110>{110} dislocations under ultra-high stresses, one order of magnitude larger than what is generally observed in fcc metals. However, as MD simulations can only be carried out at strain rates several orders of magnitude larger than experimental ones,we used the nudged-elastic-band method to calculate the activation energy for the nucleation of the dislocation as a function of stress, particle size and dislocation nucleation site. With the help of the transition state theory, the nucleation stress can then be estimated as a function of temperature and experimental strain rate. We find that due to the large stiffness of the activation energy *vs.*stress curve, the strain rate has a much smaller influence on the nucleation stress than what is found for metallic nanocrystals and therefore, that the nucleation stress estimated using MD is close to that corresponding to experimental strain rate.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room1)

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

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

Nano-indentaiton is a convenient method to investigate the mechanical properties of material by utilizing the low-loads and small-scale displacements. However, grain boundary (GB) effect on nano-indentation response needs detailed microstructure and mechanism analysis, which has been a long technique challenge. We developed a three-dimensional multiscale modeling framework, which couples the three-dimensional discrete dislocation dynamics with finite element method, and use it to investigate the GB effects on nano-indentation of aluminum bicrystal. The interaction between dislocations and GB is physically considered by introducing a penetrable GB, where dislocation pile-ups can penetrate through GB and dislocation debris at GB can be re-emitted into grain interior. In the simulation, we confirmed two experimentally observed phenomena, i.e., pop-in events and the dependence of indentation hardness on distance to GB. The pop-in events are correlated with the activation and multiplication of dislocations, especially, the GB pop-in event results from the dislocations penetration through GB. By changing the distances from indenter to GB, the simulation shows that the indentation hardness increases with the decrease of GB-indenter distance. The size effect of nano-indentation results from the geometrically necessary dislocation density distributed within the constraint volume between GB and the indenter.

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

[SY-C6] Symposium C-6

Chair: Jaime Marian(Dept. of Materials Science and Engineering, University of California Los Angeles, United States of America)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room1

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

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

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

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

[SY-C6] Investigation of the energy pathway for generation of dislocations in silicon at Σ3 grain boundaries with the kinetic Activation-Relaxation Technique

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

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

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

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room1)

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

Invited

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

There is ample experimental evidence of the effects of solute interactions with dislocations, such as Cottrell atmospheres and dynamical strain ageing (DSA). In this work we investigated, using Density Functional Theory (DFT) electronic structure calculations, the interaction between interstitial solute atoms, in particular carbon, and screw dislocation cores in body centered cubic (bcc) metals, in particular iron.
First considering carbon in bcc Fe, our calculations evidence a strong attractive interaction of carbon with screw dislocation cores inducing an unexpected reconstruction towards a hard-core configuration, which is unstable in pure metals. The carbon atoms are at the center of regular trigonal prisms formed by the Fe atoms. Around this decorated core, the 4th nearest neighbor octahedral sites are found to be also highly attractive for carbon. The complex thermodynamic behavior of carbon segregation on these dislocation sites, as function of temperature and bulk carbon concentration, is modelled using mean field and Monte Carlo methods. The parameters of the Hamiltonian, fitted to DFT calculations, account for the C-C repulsions between neighboring sites. It is concluded that in the temperature range corresponding to the occurrence of DSA, the carbon atoms occupy every other prismatic sites, while the other sites are essentially empty. This configuration is then used to study the kink-pair mechanism suggested by in situ straining experiments. The results obtained for the kink-pair formation energy and single kink migration energies are consistent with the activation energy of the end of DSA regime.
The solute segregation on dislocation-core prismatic sites was investigated for other solutes in Fe and for C in other bcc metals. A behavior similar to Fe-C is exhibited for B, N and O in Fe and for C in group 6 metals, Mo and W, but with solute-solute interactions between prismatic sites which can be either attractive or repulsive. By way of contrast, the configuration of lowest energy in group 5 consists of the dislocation in its easy core and the carbon atom in a fifth nearest neighbor octahedral site. We show that this group dependence is consistent with the carbon local environment in the stable stoichiometric carbide structures, namely cubic NaCl-type for group 5 and hexagonal WC-type for group 6.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room1)

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

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

Unlike fcc metals, where dislocation motion associated with solutes is reproduced by the effect of solute on the stacking fault energy and conventional hardening law, solutes in bcc and hcp metals induce more unique

effects such as softening and dramatic change in plastic deformation. Recently, modeling of dislocations based on first-principles calculations was developed, and the modeling for various crystallographic structure were systemized. Especially for BCC metals, solid-solution model was established based on the thermally-activated process of double-kink nucleation and kink migration related to Orowan’ s relation. Furthermore, DFT calculations found to have a great role in providing fundamental properties of these kink-related process and reproduced solution softening behavior. While the Burgers vector of the primary slip system in HCP metals is generally dislocation, the slip plane differs depending on the material, which mainly belongs to basal and prismatic plane according to the its stacking fault energy. Solute atoms have a large variety of the influence on dislocation motion resulting in dramatic change in plastic deformation.
In the present study, we implemented first-principles calculations to obtain corresponding data to the fundamental properties of dislocation motion. We will discuss the effect of transmutation product on solid solution softening in BCC tungsten and the change in slip system caused by a specific solute in HCP titanium.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room1)

[SY-C6] Investigation of the energy pathway for generation of dislocations in silicon at Σ3 grain boundaries with the kinetic Activation-Relaxation Technique

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

Multicrystalline silicon (mc-Si) is widely used for solar cell applications due to the low production costs and high efficiency. However, the crystallization processes of mc-Si induces different kinds of defects in the structure which reduces the overall conversion efficiency. Regions containing a high density of defects such as dislocations are especially detrimental. The origin of dislocations is an ongoing debate. Previous studies indicates that generation of dislocations in mc-Si can occur at Σ3 grain boundaries; however, a detailed atomistic description of the mechanisms governing the generation of dislocations is lacking. To cast light on the mechanisms behind generation of dislocations, we have deployed the kinetic Activation-Relaxation Technique (k-ART), an off-lattice Kinetic Monte Carlo code with an on-the fly cataloging of events. K-ART allows us to construct an extensive description of the energy landscape around defects and obtain the energy barriers of diffusion pathways. Furthermore, this is achievable at a time scale and in a temperature regime relevant to experimental observations. In this work, we have constructed a model structure containing an asymmetric and a symmetric Σ3 grain boundary which are joined together to form a kink. We present here an energy pathway for generation of dislocations from the kink with the associated energy barriers, and how the energy barriers is affected when the system is subjected to a shear force.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room1)

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

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

The plastic properties of $MgSiO_3$ post-perovskite are believed to be one of the key issues for the understanding of the recorded seismic anisotropy at the bottom of the Earth in a thin layer at the boundary between Earth mantle and Earth core. Indeed, the seismic waves velocities are sensitive to the development of crystallographic preferred orientations directly related to the plastic properties of the phases. Experimental results from high pressure deformation experiments, have unfortunately led to several conflicting interpretations regarding slip systems and dislocation activities in the various investigated post-perovskite material. Whereas, plastic slip in post-pervoskite has attracted much more attention, twinning mechanism has not been addressed despite some experimental evidence on low-pressure analogues such as $CaIrO_3$ compounds.

In this work, we present a twin nucleation model in $MgSiO_3$ and $CaIrO_3$ post-perovskite based on a hierarchical mechanical model of the emission of 1/6<110> partial dislocations. Relying on first-principles calculations, we show that {110} twin wall formation resulting from the interaction of multiple twin dislocations occurs at rather low stresses, suggesting that twinning is a strain producing mechanism as competitive as dislocation activities in our understanding of the development of preferred orientations in post-perovskite materials.

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

[SY-C7] Symposium C-7

Chair: David Rodney(Institut Lumiere Matiere, Universite Lyon 1, France)
Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room1

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

○Vasily V Bulatov[1], Alexander Stukowski[2], Luis A Zepeda-Ruiz[1], Tomas Oppelstrup[1] （1.Lawrence Livermore National Laboratory, United States of America, 2.Darmstadt University, Germany）

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

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

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

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

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

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

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

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

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room1)

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

Invited

○Vasily V Bulatov[1], Alexander Stukowski[2], Luis A Zepeda-Ruiz[1], Tomas Oppelstrup[1] （1.Lawrence Livermore National Laboratory, United States of America, 2.Darmstadt University, Germany）

Prediction of crystal plasticity from atomic motion has been regarded over the years as a poster child context for multiscale modeling, given that the relevant scales were inaccessible to direct MD simulations and, at the same time, dislocation lines offer a natural, concise and accurate way to coarse-grain crystal microstructure. The method of Discrete Dislocation Dynamics (DDD) is regarded as a key and most challenging element in the multiscale modeling hierarchy developed to enable such predictions. We will discuss results of a recently completed direct Molecular Dynamic (MD) simulation of dislocation dynamics in which a single crystal of tantalum was compressed at rate 10^5/s. Termed Livermore BigBig (LBB) simulation, LBB is by far the largest MD simulation ever performed. LBB generated a fully dynamic trajectory of over 2.1 billion atoms simulated over 5 microseconds of compressive straining. The simulation generated nearly 80 exabytes of recordable trajectory data a fraction of which was saved on disk in a highly compressed/post-processed form available for further analysis. As opposed to multiscale, LBB simulation can be regarded *cross-scale* being sufficiently large to be statistically representative of collective action of dislocations resulting in the macroscopic flow stress and yet fully resolved to every atomic “jiggle and wiggle”. Importantly, LBB is sufficiently large to be used as a critical test of the DDD-based multi-scale approach. To enable an “apples to apples” comparison, we carefully calibrated our DDD model (in ParaDiS) to match our LBB model at the level of single dislocation mobilities, shape and dimensions of the simulation volume, straining rate, temperature, straining axis, positioning and shape of initial dislocation sources, etc. Our first comparisons of the so-calibrated DDD simulations with LBB - which in this case serves as an exact benchmark for comparison - are far from satisfactory suggesting, in particular, that in our DDD model the dislocations do not know how to multiply. The exact origin of the uncovered discrepancies still unclear, we intend to make available to the community all the relevant atomistic simulation data (including the LBB results) thus challenging the DDD practitioners to match our LBB predictions.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room1)

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

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

Plastic deformation in crystalline materials is characterized by intermittent collective dislocation glide processes, or dislocation avalanches [1, 2, 3]. Here we perform a comprehensive set of molecular dynamics (MD) simulations to investigate the influence of strain-rate effects upon the emission of dislocation avalanches in body-centered cubic (BCC) and face-centered cubic (FCC) microcrystals. The MD simulations comprise periodic (representative) cells containing dense dislocation arrangements injected prior to the application of uniaxial displacement. Our results enable assessment of the transition from a continuous deformation mode, developed under a large strain-rate, to the characteristic serrated discontinuous mode

(indicating dislocation-mediated crystal plasticity) under a lower strain rate. In the latter, the stress-strain curves can be essentially probed under strict displacement control, enabling direct comparison with the avalanche-size distributions from quasi-static micropillar compression experiments [3]. Moreover, our findings shed new light on the role of strain hardening and dislocation cross-slip in FCCs as well as on the thermally-activated glide of screw dislocations in BCCs upon the avalanche distributions, including avalanche truncation at large plastic slip events [3].

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(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room1)

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

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

Plasticity of body-centered-cubic (BCC) metals at low temperatures is determined by screw dislocation kinetics. Because the core of screw dislocation in BCC metals has non-planar structure, its motion is complex and unpredictable. For example, although density functional theory (DFT) predicts slip on a {110} plane, the actual slip plane departs from the prediction at elevated temperatures, its mechanism having been a mystery for decades. In the current study, we conducted molecular dynamics simulations at finite temperatures using a recently-developed empirical potential that has the single-hump Peierls barrier for 1/2<111> the screw dislocation jump and examined the dislocation jump process.

In our molecular dynamics, the dislocation glides on the {110} plane with the highest Schmidt's factor, as predicted by DFT at low temperatures, while the dislocation approximately glides on a {112} plane at higher temperatures. Thus, our molecular dynamics simulations successfully reproduced the transition of the slip plane observed in experiments. To examine how the glide-plane transition takes place, we particularly developed a post-analysis tool to scrutinize the initiation of screw dislocation jumps from one Peierls valley to the next with high spatiotemporal resolution. The results indicated that heaved motion of screw dislocation line inside a Peierls valley sometimes causes a double-kink nucleation on a {110} plane with lower Schmidt's factor. Because of the twinning/anti-twinning asymmetry of the core structure, the average slip plane over the long kinetics departed from the original {110} plane and approximately becomes {112}. This suggests that thermal fluctuation of screw dislocation line are responsible for the transition of the slip plane.

We also observed a jerky dislocation motion at low temperatures similar to experiments. Close investigation of this motion using the new post-analysis tool indicates that inertial effect causes the jerky motion, i.e., a previous jump beyond the Peierls barrier can directly cause the double-kink nucleation for the next jump.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room1)

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

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

Uranium is a key element in nuclear technology. We focus on studying plastic deformation of the high-temperature BCC phase. On the one hand, classical molecular dynamics is used for obtaining material parameters, necessary for dislocation dynamics. Dislocation motion involves various mechanisms. The significance of their contribution to plastic response is studied on the other hand.

We show dislocation climb can be observed at nanosecond timescale. Imposing external shear results in gliding of the dislocation, making dislocation climb even more significant. Studying of those mechanisms is performed and quantitative parameters e.g. phonon drag coefficient, activation energy, activation volume are obtained. We emphasize that qualitative results remain the same for all three interatomic potentials considered in our study. Both discrete and continuum dislocation dynamics simulations are performed based on the results obtained from atomistic simulations. Synergy between two approaches of multiscale modeling results in better understanding of uranium plastic deformation.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room1)

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

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

In surface mechanical attrition treatment the surface of a treated material is submitted to a severe local plastic deformation. This deformation results from the random impacts of spherical shots with high velocity on the surface of the specimen. Therefore, a nanocrystalline layer is generated on the surface. The thickness of this layer can reach a depth of 50 micrometers. The grain refinement mechanisms that lead to the formation of the nanocrystalline layer are still not well understood. In this work, molecular dynamics simulation has been employed to simulate the compression of a single crystal Fe14Ni18Cr at strain rate of $5.10^9\ s^{-1}$ in order to analyze its main plastic deformation mechanisms. Therefore, the relationship between the impacts of the shots and the refinement mechanisms in a grain has been investigated. A combination of dislocation slips and mechanical twinning have been found to be the main refinement mechanisms. High density of dislocations and twins nucleation are observed on the surface. Moreover, the large density of generated twin boundaries modify the monocrystal into lamellar twin-matrix blocks with a nanometer sized thickness. Finally, twin-twin and twin-dislocation interactions lead to the transformation of the twin-matrix blocks to small grains.

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

[SY-C8] Symposium C-8

Chair: Yinan Cui(Mechanical and Aerospace Engineering Department, University of California, Los Angeles, United States of America)

Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room1

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

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

[SY-C8] Tension of fluctuating dislocation lines

○Max Boleininger[1], Thomas D Swinburne[2], Laurent Dupuy[3], Sergei L Dudarev[1] （1.Culham Centre for Fusion Energy, UK, 2.Theoretical Division T-1, Los Alamos National Laboratory, United States of America, 3.DEN-Service de Recherches Métallurgiques Appliquées, CEA, France）

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

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

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

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

[SY-C8] Molecular dynamics simulations of dislocation dynamics

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

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room1)

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

Invited

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

Thermal fluctuations of dislocations control their mobility and set the time-scale of thermally activated events such as cross-slip or obstacles by-pass. While dislocation vibrations have been previously investigated using simplified line tension descriptions and numerical dislocation dynamics models, we analyze them by the means of an analytical approach combined with atomistic simulations. Within the framework of the non-singular dislocation theory, we derived an analytical expression for the elastic energy of a weakly perturbed dislocation, which controls the amplitude of the equilibrium thermal fluctuations through the equi-partition theorem. Comparing this analytical prediction with molecular dynamics calculations performed in aluminum shows that a core energy (proportional to the dislocation length) has to be incorporated in addition to long-range elasticity. Adding this contribution allows to reproduce very accurately the fluctuation spectra obtained from molecular dynamics simulations and yields quantitative estimates for the core parameter of the non-singular theory and for the magnitude of the core energy. We also discuss the transferability of these parameters to the bowing-out of a dislocation between obstacles. Finally, a deeper analysis of the time-dependence of the fluctuations yields valuable insights on the dynamical behavior of dislocations, namely their mass and phonon damping.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room1)

[SY-C8] Tension of fluctuating dislocation lines

○Max Boleininger[1], Thomas D Swinburne[2], Laurent Dupuy[3], Sergei L Dudarev[1] (1.Culham Centre for Fusion Energy, UK, 2.Theoretical Division T-1, Los Alamos National Laboratory, United States of America, 3.DEN-Service de Recherches Métallurgiques Appliquées, CEA, France)

Fusion materials will be subjected to high lifetime doses of irradiation at high temperatures. To accurately predict changes in mechanical properties of materials under fusion conditions, we need to simulate complex stochastically-driven evolution of radiation damage defect networks over a broad range of temperature and timescales.

Recent analysis shows that fundamental concepts underpinning defect dynamics require re-examination. In stark disagreement with atomistic simulations, linear elasticity theory predicts that straight dislocations have negative line tension with respect to small fluctuations, suggesting that dislocations are unstable to bow-out. Consequently, a dislocation dynamics model based solely on linear elasticity is unable to cope with stochastic thermal fluctuations.

A consistent treatment of dislocation cores is a prerequisite for correctly describing dislocation line tension in a continuum model. We present a new solution of the discrete Multi-String Frenkel-Kontorova (MSFK) model, which in the continuum limit unifies linear elasticity and the Peierls-Nabarro model for an edge dislocation. The core (misfit) energy and core width are controlled by a single parameter. We find the

continuum displacement fields in agreement with atomistic displacements derived from molecular dynamics simulations of edge dislocations in bcc iron and tungsten. We investigate line tension of the continuum MSFK model with respect to bow-out and find that the misfit energy plays a crucial role in controlling the stochastic line instabilities.

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 633053. Also, it has been part-funded by the RCUK Energy Programme (Grant Number EP/P012450/1). The views and opinions expressed herein do not necessarily reflect those of the European Commission.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room1)

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

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

Cross-slip is a thermally activated process by which screw dislocations can change their glide plane. Quantifying the activation parameters for cross-slip in a general stress field is imperative to model cross-slip in dislocation-based simulations. In most discrete dislocation dynamics (DDD) simulations, only the contribution of the resolved shear stress is considered. Recently, the contributions of Escaig stresses on the primary and cross-slip planes were accounted for. In this work, we propose a model for cross-slip of screw dislocations in Face-Centered Cubic (FCC) metals by employing the line-tension model to calculate the free-energy barrier under a general stress field.

When only Escaig stresses are applied, we show that cross-slip is favorable only when Escaig stress in the primary plane is larger than in the cross-slip plane. The free-energy barrier decreases nonlinearly with Escaig stresses, whereas it decreases stronger with Eacsig stress in the primary plane. Using our model, we show that there is typical length for cross-slip, which is a means to quantify the region that bows-in towards constriction. The typical length scale varies when applying different Escaig stresses on both the primary and the cross-slip planes.

Schmid stresses in the cross-slip plane break the symmetry of the solution, and the partial dislocations bow-out in the cross-slip plane after constricting. The application of Schmid stresses is shown to remove the divergence in the free-energy barrier and cross-slip is possible for all combination of Escaig stress. We propose an Escaig and Schmid stress-dependent closed-form expression for the free-energy barrier for a cross slip in a large range of stresses without any fitting parameters. The proposed expression captures qualitatively the essentials found in atomistic simulations and is in good agreement with previous models. This closed-form activation energy function can be easily implemented in DDD simulations, owing to its simplicity and universality.

Malka-Markovitz A. and Mordehai D., Philos. Mag. 98 (2018) 347-370.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room1)

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

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

The interaction between glissile dislocations and precipitates within a continuum is responsible for marked increases in material strength. Due to their desirable engineering features, dislocation-obstacle interactions have been the subject of theoretical study for many decades. Despite ongoing efforts, these studies have often been limited to crude approximations whose validity is difficult to assess. Towards enhancing our understanding of these complex interactions, we employ a three dimensional coupled dislocation dynamics and finite element method computational scheme to directly compute the strength (i.e. bypass stress) of a variety of dislocation-precipitate interactions. The coupled framework accounts for elastic mismatch between the host matrix and precipitates via the inclusion of elastic image stresses and stress concentrations computed through the finite elements. Our simulations span a range of elastic mismatch, linear obstacle densities, degrees of ellipticity and size. Through our simulations, we demonstrate the influence of these four parameters on both the dislocation-precipitate strength, and hardening rate. We devise a simple mechanical model which yields insight into the results of both our numerical simulations as well as others found within the literature.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room1)

[SY-C8] Molecular dynamics simulations of dislocation dynamics

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

Dislocations are of fundamental importance in plasticity and mechanical deformation of solids and their properties are required for understanding of numerous phenomena related to mechanical response. Molecular dynamics simulations allow the study of dislocation motion at the short time and length scales which are difficult to access by experimental means, but require careful convergence for physical meaning. Highly converged simulations were performed on long dislocations in large FCC copper crystal supercells with full periodic boundary conditions, incorporating a dislocation dipole with zero net Burgers vector. Kinematics were studied by accelerating dislocations at constant stress and temperature. The relation between stress and terminal velocity at cryogenic and room temperatures for both screw and edge dislocations was obtained. A transition from viscous behaviour to near sonic asymptotic behaviour was identified and the velocity dependence of the drag force was characterised. At higher stresses a shift into the transonic regimes occurs and the mechanism and stability of this transition is examined. The thermally activated process of cross-slip was simulated multiple times creating statistical data from which the kinetics and activation parameters were calculated. The effects of stresses in the cross slip and in the glide planes on the activation volumes were determined. Finally, the rate controlling step of the cross-slip process was identified producing insight into the cross-slip mechanism.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E5] Symposium E-5

Chairs: Anthony D Rollett(Carnegie Mellon University, United States of America), Evgeniya Kabliman(Austrian Institute of Technology, Austria)

Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room2

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

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

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

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

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

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

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

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

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room2)

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

Invited

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

This presentation describes use of image-based modeling to analyze synchrotron-based High Energy Diffraction Microscopy (HEDM) stress-strain experiments. HEDM is both in-situ and non-destructive and was used to measure micromechanical fields such as strain and orientation at the grain scale developed under macroscopic tensile loading of Ti-7Al. Taking the 3D image of the experimentally measured initial microstructure as input, elasto-viscoplastic modeling based on the Micromechanical Analysis of Stress-Strain Inhomogeneities with Fourier transforms (MASSIF) was used to compute the micromechanical fields that develop during loading. To validate the MASSIF calculations, we compared the calculated fields with the ones measured by HEDM. The initial comparisons showed that MASSIF can reproduce the macroscopic stress/strain curve but poor agreement was found between calculated and measured fields at the grain scale. The differences at the grain scale were hypothesized to be caused by the initial residual stress state that was induced during prior material processing, and which was not incorporated in the MASSIF calculation. We used eigenstrain concept to incorporate residual stress in the MASSIF calculation by converting it to an initial eigenstrain field. The results reveal that incorporation of residual stress results in good agreement between calculated and measured fields at the grain scale, thereby validating the computational approach. MASSIF was further used to model an experiment in which a polycrystalline sample of Ti-7Al was cyclically deformed and mapped using boxbeam near field(nf)-HEDM and far field(ff)-HEDM. The ff-HEDM results show a decrease in residual elastic strain over the first cycle followed by a steady increase in (elastic) strain. The initial residual strain in each grain was anti-correlated with the change in that same strain component over the first cycle. The distribution in the von Mises stress, which is a scalar measure of deviatoric stress, broadens as cycles accumulates and develops a long upper tail. Initially, a graph of hydrostatic stress against stress coaxiality angle shows a positive correlation but after about 65 cycles, the trend-line has rotated to a negative correlation. Simulations with MASSIF are used to analyze and understand these results.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room2)

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

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

A unique characteristics of ferroelastic materials is their highly non-linear stress-strain curves with plateaus and large hysteresis. We show by computer simulations how to render ferroelastic materials nearly hysteresis-free and linear super-elastic (with an elastic strain limit of 2.7%), and ultralow modulus (<20 GPa) by creating appropriate concentration modulations (CMs) in the parent phase via spinodal decomposition and by pre-straining. The CM causes phase stability modulations, suppresses autocatalysis in nucleation, imposes nano-

confinement on growth and hinders long-range order of transformation strain during martensitic transformation (MT) and, thus, turns the otherwise sharp first-order transition into a broadly smeared, macroscopically continuous transition over a large stress range. The pre-straining yields retained martensitic particles that are stable at the test temperature without applied load and act as operational nuclei in subsequent load cycles, eliminating the stress-strain hysteresis and offering an ultralow apparent Young’s modulus. This study demonstrates a novel and universal approach to design new ferroelastic materials with unprecedented properties.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room2)

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

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

Composite materials are widely used in high value manufacturing industries like aerospace and auto- motive. However, they are often compromised by high costs, long development time, and poor quality due to manufacturing defects. Therefore, numerical simulation for composite manufacturing processes has attracted much attention in academic and industrial communities, with the twin objectives of improving product quality and decreasing production time.

Typically, carbon fibre composite components are made by layering a series of thin carbon fibre layers, pre-impregnated with resin, onto a tool surface. During this lay-up process the stack of plies is consolidated at moderate temperatures and pressures to remove air trapped between layers. The consolidation of composite laminates prior to curing strongly influences the formation of defects which ultimately hinder the components structural integrity.

The deformation of uncured composite laminates is complex. It depends on the individual constitutive behaviour of the plies and interface, as well as the geometric constraints that arise from the layers fitting and moving together. Theoretically, uncured composites can be modelled using detailed finite element calculations in which each layer and interface is defined explicitly. Experimental characterization have led to much better understanding of the shearing, bending, flow and consolidation mechanics of uncured laminate composites. This data has been parameterized largely via simplified heuristic models and have yet to be translated into rigorous 3D continuum models.

At In this study, we have developed a new continuum model for uncured carbon fibres plies to capture the non-linear visco-elastic behaviour of uncured laminates considering shear, bending, flow, and consolidation mechanisms based on the recent experimental characterization results. The model is developed from a biphasic continuum theory allowing for coupling between the solid and fluid responses. It includes the deformation mechanisms of the fibres as an anisotropic hyper-elastic material as well as resin flow through the fibre network. This work is the first part of a larger research effort to develop an efficient multi-scale numerical framework for composite manufacturing process of full scale components.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room2)

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

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

When material deformation occurs at elevated temperatures, one has to take into account the simultaneous evolution of grain, sub-grain structure and microchemistry (dissolution and precipitation of phase particles). In the present work, we present current results on the implementation of a computational strong coupling scheme between material deformation and microchemistry/microstructure evolution. For this purpose, we introduce a Dyna2Micro Material Model, which is implemented into a Finite Element Code (LS-DYNA of LSTC) and allows a simultaneous calculation of the (sub)-grain structure and phase kinetics at every integration point and time step. Dynamic processes, such as, work hardening and recovery are calculated by using a dislocation based model (MD^2 Model) implemented into a user defined subroutine, while the phase dissolution and precipitation is calculated by the thermo-kinetic software package MatCalc. Computational efficiency is realized by a new remote control feature implemented in MatCalc specially developed for this project as command interface between the user subroutine and a running MatCalc session. The simulations are checked by simulation of multi-step hot compression tests using a 3D axisymmetric cylindrical model of samples according to the experimental set up. For the material, we choose an Al-Cu-Mg alloy, where precipitation and dissolution of Al_2Cu and Al_2CuMg is considered. The whole simulation process from solidification, pre-heat treatment, deformation and post heat treatment is then controlled by the SProC (Smart Process Control) Toolkit.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E6] Symposium E-6

Chairs: Ying-Jun Gao(Guangxi University, China), Masaki Tanaka(Kyushu Univ., Japan)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room2

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

○Ying-Jun Gao （Guangxi University, China）

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

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

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

○Michael Budnitzki （TU Bergakademie Freiberg, Germany）

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

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

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

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

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room2)

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

○Ying-Jun Gao （Guangxi University, China）

Phase field crystal (PFC) method is used to simulate cracks propagation as a function of grain orientation. The results show that when the direction of tensile stress is perpendicular to the grain orientation, the crack exhibits cleaving extension characteristics with straight and smooth edges. As the angle between the grain orientation and the direction of the applied stress changes, the extension of the cracks begins to present a structure with saw teeth on the edge. Then, with the change of the angle increasing, a dislocation is emitted in front of the crack tip. Along with the dislocation slipping, it generates a series of micro holes. These holes further develop and grow to connect each other, and form a crack, which presents a ductile crack growth process. It can be seen that the change of the angle between the direction of the applied stress and the orientation of the grains can lead to a transformation of the ductile-brittle behavior of the fracture.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room2)

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

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

Spatial correlations of plastic strain fluctuations in a shear-driven amorphous solid are investigated in the vicinity of a hard wall with a molecular-scale corrugation [1]. Within thin slabs parallel to the wall plane, normalized correlations are enhanced when the slab center is closer to the wall. The amplitude of these correlations, however, is found to be suppressed by the wall. It is shown in this work that the enhancement of the normalized correlations quantitatively matches with the wall-induced enhancement of the elastic propagator within continuum elasticity [1,2]. The decrease of strain amplitude, on the other hand, is shown to originate from molecular scale wall effects on the size of the nearest neighbor cage, explored by particles on intermediate times scales [1]. These results highlight the fundamental role of elasticity for the correlation of plastic activity in glassy systems [3].

[1] M. Hassani, P. Engels and F. Varnik, Wall effects on spatial correlations of non-affine strain in a 3D model glsss (Europhysics Leters 2018, in press).
[2] A. Nicolas and J.-L. Barrat, A mesoscopic model for the rheology of soft amorphous solids, with application to microchannel flows, Faraday Discuss. 167, 567 (2013).
[3] F. Varnik, S. Mandal, V. Chikkadi, D. Denisov, P. Olsson, D. Vagberg, D. Raabe, and P. Schall, Correlations of plasticity in sheared glasses, Phys. Rev. E 89, 040301 (2014).

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room2)

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

○Michael Budnitzki （TU Bergakademie Freiberg, Germany）

Partially stabilized zirconia (PSZ) based ceramics are known for their excellent mechanical properties and bio-compatibility. The material's ability to undergo stress-induced phase transitions results in a very high fracture toughness, making it ideal for applications such as dental implants. In MgO-stabilized zirconia (MgO-PSZ) the martensitic phase transformation is restricted to lenticular inclusions of retained tetragonal phase embedded in a cubic matrix.

We use semi-analytical models as well as phase-field methods based on Ginzburg-Landau theory to account for various aspects of microstructure formation. Using phase-field it is possible to directly simulate the phase morphology and investigate the influence of geometric and crystallographic aspects. The semi-analytical model allows to study the effects of material parameters, such as surface energies, on the transformation stress as well as the inelastic strain in the inclusions and allows for the application of homogenization techniques in order to assess the effective constitutive response. Both approaches complement each other in order to achieve a more quantitative understanding of the micromechanics of zirconia.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room2)

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

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

Wire-drawn fully pearlitic steel was twisted at room temperature. As a result, a delamination crack propagated along the longitudinal direction of the wire. The fracture surface of the delamination crack was compared with the fracture surface obtained by an impact test at 120K, demonstrating that the delamination crack is neither a simple cleavage nor ductile shear one. Backscattered electron and transmission electron microscopy images indicated that the cementite lamellae immediately beneath the delamination crack had vanished. In addition to that, a fine-grained structure was observed. This indicated that the delamination fracture was not a brittle one but a shear one associated with local severe plastic deformation.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room2)

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

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

Against highly complex hierarchical material systems as in high Cr heat-resistant ferritic steels exhibiting inhomogeneous recovery-triggered accelerated creep rupture, the present study tackles a series of problems about their practically-feasible multiscale modeling and simulations based on FTMP. The targeted system here is composed of martensite laths with high-dense dislocations (Scale A), lath blocks/packets (Scale B) embedded within a prior austenitic grain (Scale C). The objectives are (a)reproduction of the experimentally-observed accelerated degradation of the creep strength due to inhomogeneous recovery of the microstructures under relatively low stress conditions, and (b)identification of the minimal conditions for (a) to occur, focusing on the interactions between Scales A and B. Creep analyses, considering the interior high-dense dislocations evaluated by the spontaneously-evolved incompatibility tensor field in Scale B, are conducted for single lath block models first. They exhibit pronounced local instability due to local recovery brought about by the interaction incompatibility field. Thus-developed models are further combined to construct single packets and embedded packet models, respectively, and the same series of analyses are performed on them. The fluctuating incompatibility field in Scale A, concurrently enhanced by the interaction term, is demonstrated to promote the local recovery. We further clarify the contributions of the projection directions of the incompatibility tensor in evaluating the Scale A dislocation density. The projection to the slip plane normal direction is turned out to play exclusively-dominant roles, implying the critical contribution of the climb-related elementary processes to the enhanced localized recovery. An attempt is also made to replace the above recovery model to improve the consistency of the current approach.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E7] Symposium E-7

Chairs: Daisuke Matsunaka(Shinshu Univ., Japan), Shiyu Du(Chinese Academy of Sciences, China)
Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room2

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

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

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

○Tetsuya Ohashi （Kitami institute of technology, Japan）

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

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

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

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

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

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

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room2)

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

Invited

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

Metallic faceted nanoparticles exhibit ultra-high strength, since their deformation involves the nucleation of dislocations on their surfaces. In this work, we employ molecular dynamics (MD) simulations to study the strength of molybdenum faceted nanoparticles and its relation to the activation parameters for dislocation nucleation [1]. We show that under compression, the nanoparticles yield by nucleating dislocations at the vertices, which are points of stress concentration. For each temperature, the simulation is repeated 30 times with different atomic velocities. Since dislocation nucleation is a thermally-activated process, the calculated strength varies between the different simulations. The strength distribution can be exploited to calculate the activation parameters. We show that the distribution can be approximated by a normal distribution, with a standard-deviation that corresponds directly to the activation volume at the given temperature and stress. Accordingly, the activation volumes are calculated from the MD simulation results at different temperatures and stresses. In addition, the dependence of the most-probable nucleation stress on the temperature is calculated. With the help of classical nucleation theory, the activation free-energy and the activation entropy are calculated. We find that the dependence of the activation free-energy on the stress obeys a power-law near the conditions for spontaneous nucleation, with a critical exponent that is equal ˜1.5. This critical exponent is typical for simple bifurcation problems. In addition, the activation entropies are found to be in the range of 0-15k_B, with some deviations form the Meyer-Neldel compensation rule. Based on the calculated activation parameters, the probabilistic nature of the strength at this scale is discussed.

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(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room2)

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

○Tetsuya Ohashi （Kitami institute of technology, Japan）

Density evolution of atomic vacancies during plastic slip deformation is evaluated by crystal plasticity analyses where evolution of dislocation density is calculated by the model of Kocks and Mecking[1] and the dislocation mean free path is given by an effective average distance of forest dislocations and a microstructure length scale[2, 3]. We slightly modified the model by Essmann and Mughrabi[4] for the evolution of atomic vacancy density and implemented to the crystal plasticity software code.
Analysis results[5] show that the vacancy density sometimes reaches at the order of 10^{24} /m^3, which is at the order of 10^{-4} in terms of concentration. Increase rate of the atomic vacancy is shown to depend largely on the microstructure length scale and slip multiplication on different systems.

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(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room2)

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

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

Magnesium (Mg) alloys with long-period stacking ordered (LPSO) structures show excellent mechanical performances such as high yield strength and ductility. The LPSO structures consist of periodic arrangement of basal stacking faults (SFs) and enrichment of solute atoms in the vicinity of the SFs. HAADF-STEM measurements observed that the $L1_2$-type clusters of solute atoms are formed and aligned at each SF. The $L1_2$ clusters at each SF have a solute-enriched region of four close-packed planes. As SFs are periodically introduced, each type of the LPSO structures has the specifc close-packed layers between the quadrople solute-enriched layers. While a previous first-principles study showed that the binding energy of solute atoms to SF and the solute-solute pair interaction can describe the formation of the $L1_2$ clusters, the physical origin of the periodic arrangement of the quadrople solute-enriched layers with the $L1_2$ clusters remains controversial.

In order to elucidate the periodic arrangement of the quadrople solute-enriched layers, we investigate interactions mediated by electrons or phonons between the neiboring quadrople solute-enriched layers. The formation energy of the $L1_2$ cluster evaluted by first-principles calculations shows that the electron-mediated interaction is short-range repulsive with respect to the distance of the quadrople solute-enriched layers. On the other hand, we investigate effects of phonon on the inter-planer ordering of the solute-enriched layers using the 1-dimensional chain model with mass change. For heavy mass change, the ordering of the mass changes is stabilized by phonons and the energy gain increases with the concentration of the mass changes, i.e., the short LPSO period is favorable. Thus, a promising mechanism of the inter-planer ordering of the LPSO structures is the phonon-mediated interaction of the quadrople layers where heavy solute atoms are enriched as the $L1_2$ clusters at SFs.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room2)

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

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

High entropy alloys (HEAs) are random solid solution alloys with 5 or more components, usually of near equi-composition. HEAs exhibit excellent mechanical properties, including high strength, high ductility, and high fracture toughness [1]. Guiding the design of new HEAs across the vast composition space requires an ability to compute necessary underlying material parameters via first-principle calculations. Here, a methodology is proposed to compute, via density functional theory (DFT), the elemental misfit volumes, as well as alloy lattice constant, elastic constants and stable stacking fault energy, in the fcc noble metal HEA RhIrNiPdPtCu

[2]. These properties are then used in a recently developed solute strengthening model [3, 4] for temperature and strain-rate dependent yield strength, with the prediction of 563 MPa is in excellent agreement with the experimentally measured value of 527 MPa [5]. This methodology links the alloy composition with the yield strength prediction, indicating a general methodological path for exploring new potential high-strength HEAs in this and other alloy classes.

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[2] B. Yin and W. A. Curtin, in preparation.

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(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room2)

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

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

Carbon nanotubes (CNT) possess excellent mechanical properties in terms of axial elastic stiffness and rupture strength. It is therefore an obvious question whether these properties can be harnessed for structural applications by using such nanoparticles as fillers in low-melting lightweight metals such as Al or Mg nanocomposite. To this end, homogeneous dispersion of CNT in the metal matrix and strong interfacial bonding are essential factors since agglomerated nanoparticles with weak bonding into the surrounding metal matrix might act as flaws which actually deteriorate, rather than improve, the mechanical properties of composites. However, good dispersion and strong interfacial bonding are hindered by the low affinity of CNT to Al or Mg. To overcome this problem, interface engineering approaches such as coating CNT with an appropriate metal such as Nitweight , or by decorating them with metal nanoparticiles, may offer a promising approach towards the efficient fabrication of lightweight metal-CNT nanocomposites.
In this work we study how metal coated or metal decorated carbon nanotubes affect the mechanical properties of aluminium/CNT composites. In particular we look at the pullout behaviour of pristine as well as Ni coated or Ni decorated CNT from an aluminium matrix. Our result shows that Ni coating produces an extended interface (“intephase”) where a significant amount of energy is dissipated during CNT pull-out, leading to a high pull-out force. We then investigate the interaction of embedded CNT with and without coating/decoration with cracks and with dislocations during simulated tensile tests. We discuss the results in view of promising approaches for engineering CNT-metal interfaces such as to achieve high strength and high toughness of the metal-CNT composites.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E8] Symposium E-8

Chairs: Hao Wang(Institute of Metal Research, CAS, China), Jun-Ping Du(Kyoto University, Japan)
Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room2

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

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

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

○Zhong Zhu Li, Yu Hao Li, Hong Bo Zhou, Guang Hong Lu （Department of Physics, Beihang University, China）

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

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

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

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

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

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

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

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

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room2)

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

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

Hydrogen can be either an intentional constituent or unwelcome impurity in metals. The fact that excess hydrogen can enhance greatly the self-diffusion of atoms in metals has been explained by the appearance of superabundant vacancies, because the vacancy formation energy decreases substantially with increasing H concentration, while individual vacancy diffusion is supposed to be slowed down due to the increased jumping energy barrier of H-vacancy complexes based on the previous first-principles studies. Here, performing first-principles calculations of appearance probability of possible H-vacancy configurations and activation energy of possible vacancy jumping pathways in combination with molecular dynamics (MD) simulations, we found at certain H concentrations and temperatures, the diffusivity of vacancy in face-centered cubic Cu can be accelerated by H, which is caused by H-enhanced diffusion attempt frequency and environmental H-assisted vacancy diffusion pathway. The MD simulations demonstrated that the promoting effect of H can also be found in dynamical processes. The uncovered H-vacancy diffusion processes in metals can advance our understanding of the H behavior in metals.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room2)

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

○Zhong Zhu Li, Yu Hao Li, Hong Bo Zhou, Guang Hong Lu （Department of Physics, Beihang University, China）

Tungsten (W) is one of the most promising candidates for the plasma facing materials (PFMs) in future fusion devices. Vacancy is the typical defect in W, and plays key role in the microstructure and mechanical properties of W. Vacancies can aggregate to form voids by migrating, and further lead to swelling, hardening and embrittlement of W. Therefore, the behaviors of vacancy in W have attracted many attentions. Generally, the presence of vacancy is accompanied with the disappearance of normal W atom, and induces local lattice distortion and forms stress field. Thus, one can expect that the external strain/stress field should have effect on vacancy behaviors in W, while little work focuses on this aspect so far.

Here, we have investigated the migration of vacancy in W under strain using a first-principles method in combination with the activation volume tensor and thermodynamic models. In general, vacancy inevitably induces local tensile stress field, tending to contract the lattice. Thus, it is considered that the mobility of vacancy responds to strain “monotonically”, i.e., the migration energy of vacancy will decrease (increase) with the increasing tensile (compressive) strain. The mobility of vacancy in W under triaxial strain follows this rule. Surprisingly, we have discovered that the vacancy mobility can always be promoted by anisotropic (biaxial) strain in W, independent of the sign of strain. In a wide range of strain values, the vacancy mobility is enhanced in the strained W. This anomalous behavior is found to be caused by an unusual variation of the vacancy activation volume tensor induced by anisotropic strain, which is originated from the Poisson effect. Further, it is found that the diffusivity of the vacancy in W with 5% tensile (compressive) biaxial strain will be increased by 3 (2) orders at 600K based on the Arrhenius equation. Meanwhile, the onset temperature for vacancy diffusion will also be markedly reduced by biaxial strain. Consequently, our finding suggests that anisotropic strain will significantly enhance vacancy mobility in W and promote the formation and growth of hydrogen/helium bubbles.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room2)

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

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

For structural materials with hexagonal close-packed structures, the stacking fault energy and the ratio of *c/a* are key factors which have strong correlation with many properties, such as the critical shear stress of dislocations and deformation twinning. We thus employed high-throughput *ab initio* calculations to investigate the stacking fault energy and the *c/a* ratio in hexagonal metals, Mg, Ti, Zr, Be and Zn, as well as in alloyed Mg and Ti. The result indicates that the ratio of the unstable stacking fault energy on the prism plane over that on the basal plane, γ^p/γ^b, is primarily relevant to the *c/a* ratio. In Be, Mg and Zn, γ^p/γ^b increases with *c/a* leading to increasing preference of basal slip, whereas in Ti and Zr, γ^p/γ^b changes unperceivably with *c/a* leading to the preference of prism slip. In alloyed Mg and Ti, alloying varies both the stacking fault energy and the *c/a* ratio and certain alloying elements significantly affect -slip preference in Mg, while alloying exhibits negligible influence on -slip preference in hexagonal Ti.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room2)

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

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

Ammonia has been extensively synthesized by human beings, dominatedly by Haber-Bosch process at high temperature and high pressure. It results in large amount of carbon emisson and energy consumption. This work aims to investigate the role of vacancies and grain boundaries for catalysts design used in ammonia synthesis. They are employed as active sites for the design of single-atom catalyst design. As revealed by DFT calculations, single Fe/Co/Mo atoms can actively adsorb on these defects and offer high performance for N2 activation. Fe-doped MoN2 has been identified as an excellent catalyst for nitrogen reduction.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room2)

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

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

The stability of a interface between O-phase Ti_2AlNb (1 -1 0) surface and B2-phase TiAl (2 1 -1) surface was studied by first principles calculations to investigate the atomic matching behavior. A coherent twin boundary with extremely small misfit degree was found, The calculated formation energy and the electronic structure illustrate that the interaction is strong. The adsorption of a single oxygen atom at the interface was estimated thermally stable by adsorption energy. The present research indicates the existence of O/B2 interface may lead to influences on both the mechanical strength and the oxidation resistance of Ti_2AlNb alloys.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room2)

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

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

Stability and reversibly de/hydrogenation properties of presumed Mg_7TiX_2 (X= F, O, S, P and Cl) were predicted using Density Functional Theory. Hypothetical Mg_7TiX_2 and its hydride are energetically stable with respect to the individual elements involved and they may be synthesized experimentally. The stability of alloy highly relate to the formation energy of Mg-X compound because that distance of Ti-X is large than that of Mg-X. The considered systems possess preferable hydrogen adsorbing capacity, and their hydrogen adsorption energies lie in the range from -0.5 eV to -0.05 eV. The dehydrogenation of the $Mg_7TiX_2H_{14}$ were calculated and found that H-Mg bond and Ti-Mg bond have significant effect on dehydrogenation process. The study of desorption energy of X atoms found that P atoms are less stable than H atoms and will escape from system before H atoms that lead system collapse, thus Mg_7TiP_2 is not available to hydrogen storage. Our studies indicated that Mg_7TiX_2 (X= F, O, S and Cl) can realize reversible hydrogen storage properties.

Keywords: Density Functional Theory; Hydrogen Storage; Stability; Reversibility; Mg_7TiX_2.

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

[SY-F5] Symposium F-5

Chair: Ingo Steinbach(Ruhr-University Bochum, Germany)
Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room3

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

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

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

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

[SY-F5] Solidification analysis by non-equilibrium phase field model using thermodynamics data estimated by machine learning

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

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

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

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room3)

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

Invited

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

Accurate prediction of material microstructures is crucial for the production and design of high performance material. Phase-field method has emerged as a powerful numerical model for predicting the formation process of complicated material microstructure. Now, it is well accepted as the most accurate and promising model for microstructure formation in the mesoscale. On the other hand, a large computational cost due to the diffuse interface is a major drawback, and usually the phase-field simulation is limited to the small domain. To overcome this drawback, we need a high-performance computing for the phase-field simulation.

In this talk, we introduce our recent progresses in the high-performance phase-field simulation using multi-GPU acceleration. Here, we focus on the dendritic solidification where the microstructure is formed through the competitive growth among multiple dendrites. We introduce the phase-field simulations of dendrite competitive growth during directional solidification of a binary alloy in single crystal [1], bicrystal [2], and polycrystal [3]. In addition, the liquid flow drastically changes the solidification microstructure. We also introduce the large-scale phase-field simulations of dendrite growth with liquid flow [4-6]. The above all simulations have been performed by the GPU supercomputer TSUBAME at the Tokyo Institute of Technology.

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(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room3)

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

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

The properties of a material are mainly defined by their chemical composition and by their underlying microstructure. Therefore, the development of tailored microstructures is crucial for the applicability in high-performance materials with specified properties. Depending on the material properties and process conditions, multi-scale microstructures evolve during the directional solidification of eutectics. Beside the microscopic eutectic lamellar and/or fibrous structures, macroscopic structures like eutectic colonies occur at certain process conditions. Eutectic colonies are mainly observed in ternary systems when the

composition of the alloy is in the vicinity of a binary eutectic reaction. The formation of colonies is driven by microscopic instabilities in a macroscopic planar solidification front, due to the impurities by the third component that diffuse from the two solidifying phases into the liquid.

To simultaneously investigate the formation processes of micro- and macroscopic structures in their complex spatial arrangement, two- and three-dimensional large-scale phase-field simulations based on a Grand potential formalism are conducted for the high-performance material NiAl-34Cr. By systematic variations of the solidification velocity beyond the stability range the underlying mechanisms leading to the formation of eutectic colonies are studied. Further the interactions and the coherences between the eutectic rod-like structure of NiAl-34Cr and the arrangement of the eutectic colony are investigated. Especially the contact zones between the colonies are of interest, as these are indicated to be the weak points for the applicability. In additional studies the stability of the colonies for different temperature gradients and off-eutectic melt compositions is observed.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room3)

[SY-F5] Solidification analysis by non-equilibrium phase field model using thermodynamics data estimated by machine learning

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

A multi-phase field (MPF) model coupled with finite interface dissipation proposed by Steinbach et al. is applied to simulate the dendritic solidification in Fe-Cr-Ni-Mo-C steel. Thermodynamic calculation using CALPHAD database is replaced by machine learning prediction procedure in this MPF program. Solidification calculations are performed in a case of quinary system: Fe-16Cr-2Mo-10Ni-0.08C. We confirm that the microstructure evaluated by using machine learning parameter is good agreement with one directly coupled with CALPHAD database. Furthermore, this calculation is also confirmed to be approximately five times faster than the direct CALPHAD calculation method.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room3)

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

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

Recently, new β-metastable titanium alloys, so-called "TRIP/TWIP titanium alloys" (TRIP for TRansformation Induced Plasticity and TWIP for TWinning Induced Plasticity), have been developed to exhibit improved mechanical properties at ambient temperature. These properties are attributed to very complex microstructures engendered by the mechanical destabilization of the initial bcc phase (β) in the course of the deformation. Indeed, the microstructure features numerous twins following the peculiar {332}<113>

twinning mode of the β phase, specific to β-titanium alloys, as well as the orthorhombic (α") phase ensued from concomitant displacive transformations. Moreover, experimental observations revealed the possible activation of secondary deformation mechanisms, i.e. the formation of secondary twins and/or α" inside primary twins of the β phase.

To get a better understanding of the formation of the complex microstructures described above, we propose a numerical model using the phase field method. This method provides a thermodynamically consistent framework to couple the mechanisms at the origin of the microstructure evolution. As a first step of modeling the evolution of the β-metastable titanium alloys microstructure upon deformation, we focus on the {332}<113> twinning mode of the bcc phase β. In this work, we propose a phase-field model relying on (i) a finite strain formalism; and (ii) the possibility of taking into account the activation of secondary twinning inside primary twins. We will show with simple calculations the capabilities of the model to describe the {332}<113> twin growth. A comparison with a model formulated in a small strain formalism will also be presented to show the influence of the geometrical non-linearities introduced in the finite strain framework.

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

[SY-F6] Symposium F-6

Chair: Benoit Appolaire(Institut Jean Lamour, Univ. de Lorraine, France)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room3

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

○Ingo Steinbach （Ruhr-University Bochum, Germany）

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

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

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

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

[SY-F6] Phase field study of the effect of coherency strains and applied load in material couples

○Sourav Chatterjee, Nele Moelans （Department of Materials Engineering, KU Leuven, Belgium）

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room3)

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

Invited

○Ingo Steinbach （Ruhr-University Bochum, Germany）

A scale bridging modelling and simulation strategy of virtual production and virtual testing is presented which starts with parametrization of continuum constitutive relations by quantum mechanical calculations at the atomistic scale. These models are integrated into a full-field framework at the scale of microstructures in technical materials. The phase-field method is employed to simulate the microstructure evolution during processing: virtual production. Finally micromechanical simulations of deformation and damage evolution till catastrophic failure are performed utilizing the full information about the microstructure, composition and residual stresses resulting from the production route: virtual testing. The approach is applied to tempered martensite, describing the evolution of the microstructure under quenching, tempering and testing.

The quenching simulation reproduces the martensite transformation under consideration of the Kurdjumov-Sachs relationship. Based on these results, tempering is simulated. Diffusion is enabled at elevated temperatures and cementite carbides are nucleated, which decreases carbon composition in the martensite, which also decreases the tetragonal distortion. A virtual tension test provides then information about strain hardening, damage as well as the macroscopic response of the material to the loading. Different microstructures, as resulting from different alloy composition and different tempering conditions are compared regarding their mechanical performance.

[1] Atomistically Informed Extended Gibbs Energy Description for Phase-Field Simulation of Tempering of Martensitic Steel, Oleg Shchyglo, Thomas Hammerschmidt, Miroslav Čak, Ralf Drautz, Ingo Steinbach, Materials 9 (8), 669

[2] Microstructure Design of Tempered Martensite by Atomistically Informed Full-Field Simulation: From Quenching to Fracture, Efim Borukhovich, Guanxing Du, Matthias Stratmann, Martin Boeff, Oleg Shchyglo, Alexander Hartmaier, Ingo Steinbach, Materials 9 (8), 673

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room3)

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

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

There has been an extensive work on microstructural refinement via severe plastic deformation, which leads to improved strength in metallic materials. However, due to the complexity of the microstructural changes involved, the mechanisms responsible for the strength enhancement of the cold deformed marteniste have not been completely revealed. This work summarises advanced experimental and modelling activities carried out on heavily drawn martensite. These include slow heating high resolution dilatometry, high resolution transmission electron microscopy and high resolution X-ray diffraction conducted with both synchrotron and lab x-ray sources. The purpose of employing various characterisation techniques is to collect data to gain a comprehensive understanding on the microstructural evolution with respect to applied strain. The modelling work aims to propose a novel martensite strength model to describe the relationship between microstructure and mechanical properties, including the effects of applied strain upon severe plastic deformation. The strengthening model is validated using stress-strain data of martensite drawn at various strain levels.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room3)

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

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

Many materials used in everyday life have a complex internal structure organized at different scales with a texture of grains, and a complex pattern of thermodynamic phases at lower scale. This microstructure strongly impacts the movement of crystalline defects in the materials and therefore controls the mechanical behaviour. The phase field method has emerged as a well-suited method for tackling microstructure evolutions during phase transformations when elastic coherency stresses are generated. In addition, in many materials and especially at high temperature, the microstructure evolution is coupled with plasticity, and there is currently a great research effort to extend the phase field method to take this coupling into account. In this context, we will show how to couple a classical phase field model (for the description of the phase transformation) with a crystal plasticity model based on dislocation densities. The latter model uses a storage-recovery law for the dislocation density of each glide system and a hardening matrix to account for the short-range interactions between dislocations. The proposed model will be applied to study rafting of ordered precipitates observed in Ni-based superalloys. We will present 3D calculations of microstructure evolution under [100], [110] and [111] creep loading as well as different shear creep tests.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room3)

[SY-F6] Phase field study of the effect of coherency strains and applied load in material couples

○Sourav Chatterjee, Nele Moelans （Department of Materials Engineering, KU Leuven, Belgium）

We investigate the role of coherency strains and applied load on phase growth and morphological evolution in binary diffusion couples using the phase field method. We employ the Kim-Kim-Suzuki model for the chemical contribution in the free energy. The elastic energy contribution to the free energy is evaluated using a suitable interpolation scheme considering the elastic heterogeneity between the different phases. When elastic stresses are considered, we observe bending and splitting of the phase layers for mechanically constrained, partially constrained and relaxed systems. The interface remains planar in the absence of elastic stresses. In addition, we study the role of volume fraction of the phases and finite size of the system on the microstructure evolution.

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

[SY-F7] Symposium F-7

Chair: Tomohiro Takaki(Kyoto Institute of Technology, Japan)
Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3

[SY-F7] A Cosserat crystal plasticity and phase field theory for grain boundary migration

○Benoit Appolaire[1,2], Anna Ask[3], Samuel Forest[3], Kais Ammar[3] （1.Institut Jean Lamour, Univ. de Lorraine, France, 2.LEM, CNRS-Onera, France, 3.Centre des Materiaux, Mines ParisTech, France）

[SY-F7] Phase-field modeling of precipitation growth and ripening during heat-treatment conditions in Ni-base superalloys

○Michael Fleck, Felix Schleifer, Markus Holzinger, Yueh-Yu Lin, Uwe Glatzel （Metals and Alloys, University Bayreuth, Germany）

[SY-F7] Two-dimensional Simulation of Cyclic Phase Transformation in Fe-C-Mn-Si Alloy using Non-equilibrium Multi-Phase-Field Model

○Masahito Segawa[1], Nomoto Sukeharu[1], Akinori Yamanaka[2] （1.ITOCHU Techno-Solutions Corporation, Japan, 2.Division of Advanced Mechanical Systems Engineering, Institute of Engineering, Tokyo University of Agriculture and Technology, Japan）

[SY-F7] Prediction of the microstructure evolution in Electron Beam Melting Alloy 718 through phase field modelling

○Chamara Kumara[1], Dunyong Deng[2], Johan Moverare[2], Per Nylén[1] （1.Department of Engineering Science, University West, Sweden, 2.Department of Management and Engineering, Linköping University, Sweden）

[SY-F7] Phase-field simulation of solidification morphology in laser powder deposition of Fe-B alloys

○Xiaoxia Li, Xiangge Qin （School of Materials Science and Engineering, Jiamusi Univ., China）

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3)

[SY-F7] A Cosserat crystal plasticity and phase field theory for grain boundary migration

Invited

○Benoit Appolaire[1,2], Anna Ask[3], Samuel Forest[3], Kais Ammar[3] （1.Institut Jean Lamour, Univ. de Lorraine, France, 2.LEM, CNRS-Onera, France, 3.Centre des Materiaux, Mines ParisTech, France）

Elaborating a unified field framework to model concurrent viscoplastic deformation and recrystallization and grain growth in metal polycrystals has remained a formidable issue. In this work, we will present such a unified framework relying on the enhancement of a Cosserat crystal plasticity model with an order parameter to account for diffuse, mobile grain boundaries in analogy with phase field models. The Cosserat directors are taken to represent the lattice orientation of the grains. In order to introduce an evolution law for reorientation during grain boundary migration, the skew-symmetric part of the Cosserat deformation tensor is associated with a dissipative stress. The formulation in terms of the Cosserat deformation provides a natural way to couple reorientation due to deformation and reorientation due to grain boundary migration. In the absence of displacements and for a particular choice of free energy function the model can be considered a generalization to three dimensions of the Kobayashi-Warren-Carter (KWC) orientation phase field model (2000, 2003).

The proposed 3D anisotropic constitutive framework couples the changing orientation at a material point due to migrating grain boundaries (which is essential to the KWC model) to the lattice reorientation due to displacements and plastic slip. Due to the coupling of the Cosserat directors and the elastic reorientation, the bulk rotation of the grains which is inherent to the KWC model (and considered an artefact here although it can nevertheless be desirable in certain cases) can be controlled and even suppressed.

In this contribution, we will explain the main features of this framework and we will illustrate its capabilities with several cases that could not be handled convincingly by other models.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3)

[SY-F7] Phase-field modeling of precipitation growth and ripening during heat-treatment conditions in Ni-base superalloys

○Michael Fleck, Felix Schleifer, Markus Holzinger, Yueh-Yu Lin, Uwe Glatzel （Metals and Alloys, University Bayreuth, Germany）

We develop a phase-field model for the simulation of chemical diffusion limited microstructure evolution, with a special focus on precipitation growth and ripening in multi-component alloys. Further, the model accounts for elastic effects, which result from the lattice-misfit between the precipitate particles and the parent matrix-phase. To be able to simulate particle growth and ripening in one dimension, we introduce an extra optional driving-force term, which mimics the effect of the curved particle/matrix interface in one dimension. As a case study, we consider the gamma'-precipitation growth and ripening under the influence of realistic heat treatment time-scales in the multi-component Ni-base single crystalline cast alloy CMSX-4. The respectively required temperature-dependent thermodynamic and kinetic input parameters are obtained from CALPHAD calculations using the commercial software-package ThermoCalc. The required temperature-dependent elastic parameters are measured in-house at the chair of Metals and Alloys, using resonance ultrasound spectroscopy for the anisotropic and inhomogeneous stiffness-tensor and high temperature X-ray defraction for the lattice misfit.

We study the kinetics of growth and ripening of statistically many interacting precipitated particles as function of the temperature and time in one and two dimensions, with the explicit consideration of up to 8 independent chemical components. Furthermore, the model is applied to calculate the detailed shape-evolution of a few interacting gamma'-particles in two and three dimensions with periodic boundary conditions. Relations to the shapes of gamma'-particles in respectively heat treated experimental microstructures are discussed.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3)

[SY-F7] Two-dimensional Simulation of Cyclic Phase Transformation in Fe-C-Mn-Si Alloy using Non-equilibrium Multi-Phase-Field Model

○Masahito Segawa[1], Nomoto Sukeharu[1], Akinori Yamanaka[2] （1.ITOCHU Techno-Solutions Corporation, Japan, 2.Division of Advanced Mechanical Systems Engineering, Institute of Engineering, Tokyo University of Agriculture and Technology, Japan）

Multi-phase-field (MPF) method incorporating CALPHAD database has attracted much attention as a powerful numerical tool for simulating microstructure evolutions in various metallic materials. Transformation modes and diffusion behavior of substitutional solute atoms strongly depend on temperature and chemical compositions of the alloy especially in multi-component steels, i.e. an Fe-C-Mn ternary alloy. Therefore, we need to use a robust MPF model which can simulate the transition of transformation mode and the complex diffusion behavior. Recently, the MPF model with finite interface dissipation has been proposed (Hereafter, the MPF model is called as the non-equilibrium MPF (NEMPF) model). The attractive advantages of the NEMPF model are its computational efficiency and flexibility for simulating microstructure evolutions under strong non-equilibrium interface condition without the equal chemical potential assumption. In the previous study, we investigated the cyclic $\gamma \rightarrow \alpha$ and $\alpha \rightarrow \gamma$ transformations in Fe-C-Mn-Si alloys using the NEMPF model coupled with CALPHAD database. The one-dimensional simulations of the cyclic phase transformation revealed that the switching of the polarities of Mn and Si spikes formed at the α / γ interface caused the stagnant stage where the phase transformation was suppressed. In this study, the two-dimensional simulation of cyclic phase transformation in Fe-C-Mn-Si alloy is performed using the NEMPF model in order to gain a deeper understanding of the mechanism of the stagnant stage and the transition of transformation modes.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3)

[SY-F7] Prediction of the microstructure evolution in Electron Beam Melting Alloy 718 through phase field modelling

○Chamara Kumara[1], Dunyong Deng[2], Johan Moverare[2], Per Nylén[1] （1.Department of Engineering Science, University West, Sweden, 2.Department of Management and Engineering, Linköping University, Sweden）

Electron Beam Melting (EBM) is a powder bed additive manufacturing process where powder material is being melted selectively by a layer-by-layer approach using an electron beam. It has some unique features when it comes to manufacturing of components in high-performance superalloys such as alloy 718 that are commonly used in gas turbines. EBM has high deposition rate due to high beam energy and speed, comparatively low residual stresses and limited problems with oxidation. However, due to the layer-by-layer melting approach and high powder bed temperature, the resultant microstructure of as-built EBM Alloy 718 is observed to have a microstructure gradient starting from the top of the sample. The aim of this study was to use modelling to create a deeper understanding of microstructure development during EBM and the homogenization that occurs during manufacturing in Alloy 718. A multi-component phase field modelling approach combined with thermodynamic modelling was used to predict the experimentally observed microstructure gradient. Of particular interest was to study the element segregation during the solidification and the subsequent “ in-situ” homogenization heat treatment that occur due to the elevated powder bed temperature. The predicted element composition was then used in thermodynamic modelling to predict the changes in the CCT and TTT diagrams for Alloy 718. This helps to explain the observed phase evolution within the microstructure. The results indicate that the approach can be a valuable tool both for creating process understanding and for process development including subsequent homogenization and heat treatment.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3)

[SY-F7] Phase-field simulation of solidification morphology in laser powder deposition of Fe-B alloys

○Xiaoxia Li, Xiangge Qin （School of Materials Science and Engineering, Jiamusi Univ., China）

Laser melting deposition is a complicated physical and chemical metallurgical process. In this paper, the phase field model of alloy solidification is coupled to laser melting deposition process, and a finite element model of heat transfer is established. By studying the variation of the spacing of dendrite Fe_2B of Fe-B alloy powder under the conditions of laser melt deposition, the robustness and accuracy of the coupled model were verified. Experiments show that under different temperature gradient conditions, the size and spacing of the dendrite Fe_2B of the cross-section morphology of the Fe-B alloy deposited by laser melting deposition have changed significantly. The quantitative phase field simulation of the heat transfer finite element model under local steady state conditions confirms this behavior. This work demonstrates the potential of the phase-field method to simulate laser melting deposition techniques and analyze the potential of alloy solidification under complex heat transfer conditions.

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

[SY-F8] Symposium F-8

Chair: Martin Diehl(Max-Planck-Institut fuer Eisenforschung GmbH, Germany)
Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3

[SY-F8] From state parameter-based microstructure modeling to temperature and strain rate-dependent yield stress

○Ernst Kozeschnik （Institute of Materials Science and Technology, TU Wien, Austria）

[SY-F8] **Modelling of grain boundary segregation and precipitation in multi-component Al alloys subjected to heat treatment**

○Dongdong Zhao[1], Sylvain Gouttebroze[2], Jesper Friis[3], Yanjun Li[1] （1.Norwegian University of Science and Technology (NTNU), 7491, Trondheim , Norway, 2.SINTEF Materials and Chemistry, 0314 Oslo, Norway, 3.SINTEF Materials and Chemistry, 7491 Trondheim, Norway）

[SY-F8] Modeling the microstructure and electrical conductivity evolution during aging of Al-Mg-Si alloys

○Yijiang Xu, Yanjun Li （Norwegian University of Science and Technology , Norway）

[SY-F8] Thermo-kinetic modeling of long-term precipitate evolution in heat-resistant alloys

○Jae-Hyeok Shim[1], Magdalena Speicher[2], Mahesh Chandran[3], Woo-Sang Jung[1] （1.Korea Institute of Science and Technology, Korea, 2.Materials Testing Institute, Germany, 3.Indo-Korea Science and Technology Centre, India）

[SY-F8] **Simultaneous Transformation Kinetics Model for Additive Manufacturing**

○Narendran Raghavan, Srdjan Simunovic, John Turner （Oak Ridge National Laboratory , United States of America）

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3)

[SY-F8] From state parameter-based microstructure modeling to temperature and strain rate-dependent yield stress

Invited

○Ernst Kozeschnik （Institute of Materials Science and Technology, TU Wien, Austria）

In the past 20 years, significant progress has been made in the development of state parameter-based modeling approaches for the simulation of microstructure evolution, in particular, with respect to precipitation kinetics, recrystallization, recovery, grain growth, dislocation density evolution in the course of thermo-mechanical treatment, as well as the mutual interactions of all mechanisms. Once, the relevant state parameters and their evolution are known, it is straightforward, however not trivial, to deduct from these the stress strain response of the microstructure as a function of temperature and strain rate. In this presentation, an overview of these models is given as well as some implementation details in the thermokinetic software package MatCalc. Finally, an example is discussed, where the precipitation microstructure and its interaction with deformation in the course of compression testing is simulated and compared to corresponding experimental data.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3)

[SY-F8] **Modelling of grain boundary segregation and precipitation in multi-component Al alloys subjected to heat treatment**

○Dongdong Zhao[1], Sylvain Gouttebroze[2], Jesper Friis[3], Yanjun Li[1] （1.Norwegian University of Science and Technology (NTNU), 7491, Trondheim , Norway, 2.SINTEF Materials and Chemistry, 0314 Oslo, Norway, 3.SINTEF Materials and Chemistry, 7491 Trondheim, Norway）

A newly developed modelling framework which accounts for grain boundary (GB) segregation and precipitation in multi-component Al alloys subjected to cooling and subsequent heat treatments is presented. Within this framework, both the equilibrium and non-equilibrium segregation mechanisms are considered to predict the solute and vacancy segregations towards GBs. In the model of non-equilibrium segregation, GBs are considered as ideal sinks for vacancy annihilation. The CALPHAD (CALculations pf PHAse Diagrams) approach is implemented to supply the important thermodynamic and kinetic data of multi-component Al alloys as input for the model. The present framework is expected to predict the solute and vacancy segregations at GBs in multi-component Al alloys during typical heat treatment (e.g. quenching, ageing) processes. It is shown that the variation of vacancy and solute segregation behavior at GBs as a function of heat treatment or microstructure variables, i.e. solution/ageing temperature, cooling rate, grain size, can be well described within the present model. Based on the segregation of solute elements, preliminary precipitation behavior at GBs and bulk are predicted using the Kampmann-Wagner numerical approach. The simulation results have been compared with experimental observations. This work is supposed to provide a preliminary theoretical understanding towards the GB segregation and precipitation in multi-component Al alloys subjected to various cooling and subsequent heat treatment processes.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3)

[SY-F8] Modeling the microstructure and electrical conductivity evolution during aging of Al-Mg-Si alloys

○Yijiang Xu, Yanjun Li （Norwegian University of Science and Technology , Norway）

Aging is commonly performed after forming process to obtain better mechanical properties and electrical conductivity of Al-Mg-Si alloys (AA6xxx series) applied in the electrical wire. In this work, the nucleation, growth, coarsening and dissolution of different precipitate phases (Mg_xSi_y) during aging treatment is simulated based on a Kampmann-Wagner Numerical (KWN) type precipitation model. By coupling with the CALPHAD, the thermodynamics of the metastable precipitate phases is well treated. Furthermore, the precipitation model is linked to an electrical conductivity model to predict the evolution of electrical conductivity based on the volume fraction, size and spatial distribution of different precipitates, solid solution level, etc. The modeling results are compared to the transmission electron microscopy (TEM) experimental results and electrical conductivity measurements. It is revealed that the present model can well address the influence of alloy composition, aging temperature and aging time on the microstructure and electrical conductivity of Al-Mg-Si alloys.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3)

[SY-F8] Thermo-kinetic modeling of long-term precipitate evolution in heat-resistant alloys

○Jae-Hyeok Shim[1], Magdalena Speicher[2], Mahesh Chandran[3], Woo-Sang Jung[1] （1.Korea Institute of Science and Technology, Korea, 2.Materials Testing Institute, Germany, 3.Indo-Korea Science and Technology Centre, India）

There is an urgent need to improve the thermal efficiency of fossil fuel power plants by raising the operation temperature and pressure in order to reduce CO_2 emission as well as the cost of fuel. Plant operation at higher temperatures inevitably requires the development of heat-resistant alloys with a higher creep strength. There has recently been an increasing interest in applying advanced heat-resistant alloys to fossil fuel power plants in order to raise their operation temperature. The important role of precipitation in the achievement of good creep properties of heat-resistant alloys has long been recognized. One of the most effective ways for improving the creep properties is to uniformly distribute fine precipitates with a good long-term stability at elevated temperatures. The experimental investigation of the long-term precipitate evolution behavior in heat-resistant alloys have not often been performed, although it is important in understanding the creep properties. In addition to experimental approaches, there have recently been a few attempts to simulate the precipitation kinetics in heat-resistant alloys. The purpose of this study is to simulate the long-term precipitate evolution in various heat-resistant alloys such as ferritic/martensitic and austenitic steels and nickel alloys using the MatCalc software, which operates based on the classical nucleation theory and evolution equations derived from the thermodynamic extremum principle that maximizes the dissipation rate of the total Gibbs energy of the system. The simulation results, such as the precipitation sequence and the precipitate size, will be compared with experimental observations.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3)

[SY-F8] Simultaneous Transformation Kinetics Model for Additive Manufacturing

○Narendran Raghavan, Srdjan Simunovic, John Turner （Oak Ridge National Laboratory , United States of America）

Metal additive manufacturing is disrupting the traditional approaches in the manufacturing sector. However, there are uncertainties associated with the qualification of fabricated components owed to the difficulty in predicting the process-structure relationship in the PSPP linkage. Understanding the process-structure linkage includes understanding the (a) liquid-solid phase transformation and (b) solid-solid phase transformation. Previously solidified layers are affected by the thermal cycles during the melting of the subsequent layers. During processing in AM, the conditions are highly non-isothermal, non-equilibrium and understanding this highly transient condition is crucial to understand the precipitation kinetics. The temperature of the substrate can also be varied in the machine. This affects the solid-state phase transformation of a given alloy system. Multiple phases can simultaneously precipitate from the product phase as a function of thermal cycle. In this work, we develop a model based on simultaneous transformation kinetics theory and the developed phenomenological model is then coupled with the numerical thermal model to predict the solid-state phase transformation and volume fraction of multiple phases as a function of thermal cycles and processing conditions. Numerical thermal model is used to predict the thermal cycles as a function of input processing conditions. The thermal cycle is then discretized into set of small isothermal steps. The extent of simultaneous precipitation/dissolution of the phases will be calculated at each of the discretized time step. Volume fraction of each of the phases is then updated and similar procedure is repeated for rest of the discretized isothermal time steps. Appropriate thermodynamic framework, database will be used to calculate the thermodynamic properties as a function of alloy system and is used as the input to the model. It is a semi-empirical model and the input from experimental results are used to calibrate the model. Some of the other calibration parameters include nucleation site densities and surface energies. Advantages and limitations of this approach will be discussed in detail.

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

[SY-N1] Symposium N-1

Chair: Danny Perez(Los Alamos National Laboratory, United States of America)

Wed. Oct 31, 2018 9:45 AM - 10:45 AM Room4

[SY-N1] Increasing the power of accelerated molecular dynamics methods and plans to exploit the coming exascale

○Arthur F Voter （Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, United States of America）

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

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

(Wed. Oct 31, 2018 9:45 AM - 10:45 AM Room4)

[SY-N1] Increasing the power of accelerated molecular dynamics methods and plans to exploit the coming exascale

Invited

○Arthur F Voter （Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, United States of America）

Many important materials processes take place on time scales that far exceed the roughly one microsecond accessible to molecular dynamics simulation. Typically, this long-time evolution is characterized by a succession of thermally activated infrequent events involving defects in the material. In the accelerated molecular dynamics (AMD) methodology, known characteristics of infrequent-event systems are exploited to make reactive events take place more frequently, in a dynamically correct way. For certain processes, this approach has been remarkably successful, offering a view of complex dynamical evolution on time scales of microseconds, milliseconds, and sometimes beyond. We have recently made advances in all three of the basic AMD methods (hyperdynamics, parallel replica dynamics, and temperature accelerated dynamics (TAD)), exploiting both algorithmic advances and novel parallelization approaches. I will describe these advances, present some examples of our latest results, and discuss what should be possible when exascale computing arrives in roughly four years.

(Wed. Oct 31, 2018 9:45 AM - 10:45 AM Room4)

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

Invited

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

Obtaining atomistic insight into the fundamental processes during phase transformations and their dynamical evolution up to experimental timescales remains one of the great challenges in materials modelling. In particular, if the mechanisms of the phase transformations are governed by so-called rare events the timescales of interest will reach far beyond the applicability of regular molecular dynamics simulations. In addition to the timescale problem the simulations provide a vast amount of data in the high-dimensional phase space. A physical interpretation of these data requires the projection into a low-dimensional space and the identification of suitable reaction coordinates.

In this presentation, I will give an example of our analysis of the atomistic processes at a complex phase boundary during a solid-solid phase transformation. The migration of the phase boundary proceeds via concerted multi-atom processes on a complex energy landscape. Here, we employ an adaptive kinetic Monte Carlo (AKMC) approach together with driven adiabatic free energy dynamics (d-AFED) to investigate such processes at the interface between the body-centered cubic and A15 phase in molybdenum.

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

[SY-N2] Symposium N-2

Chair: Erik Bitzek(FAU Erlangen-Nuernberg, Germany)
Wed. Oct 31, 2018 11:15 AM - 12:15 PM Room4

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

○Nikolas Provatas （McGill University, Canada）

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

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

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

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

(Wed. Oct 31, 2018 11:15 AM - 12:15 PM Room4)

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

Invited
○Nikolas Provatas （McGill University, Canada）

This talk will study several closely connected density functional type theories that employ both short and long range, rotationally invariant, multi-point particle interactions. Collectively, these models give rise to a class of *structural phase field crystal* (*XPFC*) models. These XPFC models allow for numerous microstructural phenomena to be studied that couple important physics emergent at the atomic scale with phase transformation kinetics occurring on diffusional time scales. Results from recent solidification studies conducted using XPFC modelling in pure materials and alloys will be presented and compared to experiments and other theory. These include multi-step nucleation in solidification, void formation in nano-confined liquid pools during rapid cooling, solute drag, and dislocation-assisted nucleation in solid-state precipitation in alloys. Coupling of the base phase field theory with heat transfer will also be demonstrated for the study of latent heat effects in solidification. We close by discussing coarse graining methods for deriving practical phase field theories from phase field crystal models for meso-scale modelling applications.

(Wed. Oct 31, 2018 11:15 AM - 12:15 PM Room4)

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

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

Phase field crystal (PFC) method allows the atomic scale motion and defect formation to be determined on diffusive timescales. A major challenge with the method is to devise free energy functions that can yield complicated crystal structures. We introduce a phase-field crystal model that creates an array of complex three- and two-dimensional crystal structures via a numerically tractable three-point correlation function. This approach successfully yields energetically stable simple cubic, diamond cubic, simple hexagonal, graphene layers, and CaF2 crystals, as well as the particularly complex and technologically important perovskite crystal structure. Highly anisotropic interfaces play an important role in the development of material microstructure. We examine the capability of the PFC model to quantitatively describe faceted interfaces by coarse graining the PFC model to attain both its complex amplitude formulation, and its corresponding phase field limit. Using this formulation, we find that the model yields Wulff shapes with missing orientations, the transition to missing orientations, and facet formation. We demonstrate, in two dimensions, how the resultant model can be used to study the growth of crystals with varying degrees of anisotropy in the phase-field limit.

(Wed. Oct 31, 2018 11:15 AM - 12:15 PM Room4)

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

Invited

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

The fracture response of bcc metals is known to be controlled by dislocation mobility, which in turn is dependent on the slow, thermally activated nucleation of kink pairs on screw dislocations. We present a general, efficient scheme to calculate free energy barriers in large crystalline systems[1] which we apply to the kink nucleation process, finding significant anharmonic contributions at low homologous temperatures. A statistical mechanical approach is then used to study kink-limited dislocation motion through a field of obstacles[2]. We identify a crossover obstacle density below which the activation energy for plastic flow is half the free energy barrier for kink pair nucleation. Our results show striking agreement with fracture experiments across a wide range of bcc metals and are applied to interpret experimental data on irradiation induced embrittlement.

[1] TD Swinburne and M-C Marinica, Physical Review Letters 120 (13), 135503

[2] TD Swinburne and SL Dudarev, Physical Review Materials 2 (7), 073608

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

[SY-N3] Symposium N-3

Chair: Arthur F. Voter(Los Alamos National Lab, United States of America)
Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room4

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

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

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

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

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

○Ivan Novoselov[1,2], Alexey Yanilkin[1] （1.Dukhov Research Institute of Automatics, Russia, 2.Moscow Institute of Physics and Technology, Russia）

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

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

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room4)

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

Invited

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

There has been significant emphasis recently on the synthesis of fivefold-twinned Ag and Cu nanowires, which are considered to be excellent candidates for transparent conductors in flexible and stretchable electronic devices. A fundamental understanding of nanowire growth is important in achieving optimal syntheses. Nanowires grow from fivefold-twinned seeds and our work shows that likely shapes for these structures include {111} end facets and “notches”, {100} side facets, and {110} facets between the notches and the ends. We find that the density of islands on the {111} facets of growing wires is lower than that on {100} facets and that islands are likely to nucleate on {111} facets near {110}-{111} facet boundaries. Our climbing-image nudged-elastic band calculations of diffusion barriers based on embedded-atom method potentials indicate that diffusion in the {111} notches and on the {110} “steps” is significantly faster than diffusion on {100} facets. Thus, these structures become “superhighways” that channel atom diffusion to the wire ends to increase wire aspect ratios. Small islands facilitate trapping of atoms on {111} facets. We use finite Markov chains to model nanowire growth and to predict net atom fluxes from nanowire sides to the ends. These simulations predict anisotropic nanowires similar to those seen experimentally.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room4)

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

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

Atomistic simulations are a key component to understand reaction chemistry in materials; for instance, the detonation chemistry of energetic materials under pressure, which is characterized by rapid breaking and remaking of covalent bonding, and where intermediate products and reaction rates are difficult to characterize in experiments.

While accurate methods exist to study systems of relevant size with explicit electronic contributions critical to the description of bonds, e.g. density functional tight-binding (DFTB), the timescale of the simulation is often limited to a few hundreds of picoseconds. This restrains the study to systems in which reactions occur relatively quickly. In the case of detonation chemistry, this implies high pressure and temperature. In order to consider less extreme conditions, one can benefit from the rare occurrence of chemical reactions to use accelerated molecular dynamics methods such as parallel replica dynamics (PRD).

In this work, we describe efforts to combine the DFTB code LATTE, developed at LANL, with the PRD method, in order to perform accelerated QMD (AQMD) simulations of reactive chemistry. AQMD was first applied to the study of liquid benzene, a prototypical reactive hydrocarbon that has been studied both experimentally and theoretically. AQMD allowed to perform simulations reaching several nanoseconds, and thus the observation of reactions at pressures below 20 GPa. Importantly, these simulations unraveled the precursor reaction to polymerization: the formation of Diels-Alder dimers.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room4)

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

○Ivan Novoselov[1,2], Alexey Yanilkin[1] （1.Dukhov Research Institute of Automatics, Russia, 2.Moscow Institute of Physics and Technology, Russia）

TiH_x is of practical interest due to high volume concentration of hydrogen, and for many applications its diffusion properties should be established with confidence. We investigate the mechanisms of diffusion, and calculate corresponding rates in the framework of quantum molecular dynamics (QMD). However, time scales accessible to conventional QMD are very limited. It therefore can be employed only at very high temperatures, where no experimental data is available. In order to explore diffusion at lower temperatures, we accelerate QMD simulations via parallel replica dynamics algorithm (PRD). Application of PRD allows to reveal different mechanisms of hydrogen diffusion in TiH_x, and also makes it possible to perform direct comparison with experiment

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(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room4)

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

Invited

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

Metallic nanoclusters are functional materials with many applications owing to their unique physical and chemical properties, which are sensitively controlled by their shapes and structures. An in-depth understanding of their morphology stability is therefore of crucial importance. It has been well documented by transmission electron microscopy (TEM) studies that metallic nanoclusters can interconvert between different isomers. However, the relevant mechanisms remain elusive because the timescales of such shape fluctuations are too short to be resolved experimentally and yet too long for conventional atomistic simulations. By employing a recently introduced Accelerated Molecular Dynamics method, Parallel Trajectory Splicing, we present simulations that reached timescales of milliseconds and thus provide a clear description of the dynamic process of the experimentally observed shape fluctuation in metallic nanoclusters. We observe transformations back and forth between face-centered-cubic (fcc) and structures with five-fold symmetry (decahedron or icosahedron). These transitions occur following either by a partial-dislocation-mediated twinning mechanism or by a surface-reconstruction driven process. The identified pathway is in remarkable agreement with the existing microscopy results and serves as further evidence that shape fluctuation can occur directly through thermal activation, without involving melting or other external factors.

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

[SY-N4] Symposium N-4

Chair: Laurent Karim Beland(Queen's University, Canada)

Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room4

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

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

[SY-N4] Accelerated Quantum Molecular Dynamics

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

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

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

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room4)

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

Invited

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

In many problems of interest to materials scientists and engineers, the evolution of crystalline extended defects (dislocations, cracks, grain boundaries, interfaces, voids, precipitates) is controlled by the flow of point defects (interstitials/substitutional atoms and/or vacancies) through the crystal into the extended defect. Accurate modeling of this process requires atomistic methods in and around the extended defect, but the flow of point defects into and out of the extended defect region can be treated by coarse-grained methods. This talk presents a multiscale algorithm to provide this coupling, which was first documented in the manuscript "Multiscale diffusion method for simulations of long-time defect evolution with application to dislocation climb," published in 2016 in the *Journal of the Mechanics and Physics of Solids*, Number 92, pages 297-312. Specifically, direct accelerated molecluar dynamics (AMD) of extended defect evolution is coupled to a diffusing point defect concentration field that captures the long spatial and temporal scales of point defect motion in the presence of the internal stress fields generated by the evolving extended defect. The algorithm is applied to study vacancy absorption into an edge dislocation in aluminum where vacancy accumulation in the core leads to nucleation of a double-jog that then operates as a sink for additional vacancies; this corresponds to the intial stages of dislocation climb modeled with explicit atomistic resolution. The method is general, so it can be applied to many other problems associated with nucleation, growth, and reactions due to accumulation of point defects in crystalline materials.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room4)

[SY-N4] Accelerated Quantum Molecular Dynamics

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

The accurate study of the long-term evolution of rare events is extraordinarily challenging as computations are arduous and quantum-based molecular dynamics simulation times are limited to, at most, hundreds of ps. Here, the Extended Lagrangian Born-Oppenheimer molecular dynamics formalism is used in conjunction with Parallel Replica Dynamics to obtain an accurate tool to describe the long-term dynamics of reactive benzene. Langevin dynamics has been employed at different temperatures to calculate the first reaction times in a periodic benzene sample at different pressures. We have also studied the long-term behavior of vacancy complexes, which compare satisfactorily with experimental observations. Our coupled engine runs for times on the order of ns (two to three orders of magnitude longer than traditional techniques) and is capable of detecting reactions characterized by rates significantly lower than we could study before.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room4)

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

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

Although it is widely recognised that even small amounts of hydrogen (H) can cause embrittlement in iron (Fe) and in (high strength) steels, the fundamental mechanisms that cause it are not yet completely understood. To contribute to a better understanding of the fundamental behaviour of hydrogen in metals, in the present work we used parallel replica dynamics (PRD) to study the effect that different amounts of atomic H have in the diffusion of a single vacancy in body centred cubic (BCC) Fe. Using PRD we calculated, for the first time, the diffusion of hydrogen vacancy complexes at temperatures and time scales that are not reachable using classical methods. These calculations showed that the diffusivity of a vacancy-H complex is not only dependent of the migration barriers, but also that the addition of one H atom reduces the diffusivity of a vacancy in BCC Fe and the subsequent addition of more H atoms has the opposite effect.

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

[SY-O5] Symposium O-5

Chairs: Hitoshi Washizu(University of Hyogo, Japan), Sophie Loehle(TOTAL Marketing &Services, Solaize, France)

Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room5

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

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

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

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

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

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

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

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

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room5)

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

Invited

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

Ultralubricity and superlubricity has been observed for diamond and tetrahedral amorphous carbon (ta-C) coatings lubricated with water and unsaturated organic friction modifiers, respectively. Although spectroscopic characterization suggests that lubricity is connected to the formation of oxygen-containing surface layers, the underlying tribo-chemical mechanisms and the detailed structures of these layers remain elusive. This talk presents atomistic calculations on various scales that elucidate the mechano-chemical processes for the formation of oxygen functional groups and aromatic protective layers [1,2].

In the first part of this talk, quantum molecular dynamcis calculations are presented that shed light on friction regimes for diamond lubricated by water and the different characteristic layers in the different regimes [1]. We find four universal friction regimes that are active on all low-index diamond surfaces: cold-welding&amorphisation, ether cold-welding without amorphisation, H/OH-termination, H/OH-termination with water layer coverage. In addition four special regimes are found: aromatic Pandey surface reconstruction for (111), ether/keto passivation for (110) and (001) as well as two mild cold-welding regimes for (110).

In the second part, combined experiments and multiscale simulations are presented that unveil the tribochemical mechanism leading to superlubricity of ta-C/ta-C tribopairs lubricated by unsaturated fatty acids [2]. Experiments show that superlow friction can be achieved by lubrication with unsaturated fatty acids. Atomistic simulations reveal that, due to the simultaneous presence of a carboxylic group and a C=C double bond, unsaturated fatty acids can concurrently chemisorb on both ta-C surfaces and bridge the tribogap. The resulting, sliding-induced mechanical strain triggers a cascade of molecular fragmentation reactions that release passivating hydroxyl, keto, hydrogen and olefinic groups to the ta-C surfaces. These findings provide design principles for novel organic friction modifiers that promote the formation of superlubricious amorphous carbon layers.

[1] T.Kuwahara, G.Moras, M.Moseler, **Phys. Rev. Lett.** 119 096101 (2017)

[2] T.Kuwahara, P.A.Romero, S.Makowski, V.Weihnacht, G.Moras, M.Moseler, under consideration (2018)

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room5)

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

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

Epoxy resin is commonly used as an adhesive for bonding metals. Recent industrial demands, e.g., light-weight multi-material cars and highly reliable pressure sensors, motivate researchers to improve the reliability and durability of bonded materials. One critical issue regarding adhesive bonding is the weakening of its bonding strength by the water that migrates from a moist environment along the interface. When bonding naturally surface-oxidized aluminum with epoxy resin, the adhesion strength reduces by about 40 % in a moist environment. Surface treatment techniques, such as sealing with polyvinyl chloride, only delay such adhesion weakening.

Despite the importance of this issue, adhesion weakening is not well understood. To understand the mechanisms at the electronic structure level, we perform atomic dynamics simulations on various Al and epoxy resin interface systems with water molecules inserted in the contact region. In accordance with experimental conditions, the Al layer is surface oxidized to a depth of 10 Åwhile the bisphenol-A type epoxy molecule has both OH and ether groups. Shear deformations are simulated using the hybrid quantum-classical method in which about 1,500 atoms at the contact region are treated with density-functional theory.

For the first time, calculated adhesion strengths compare well with the experimental values. Former simulations gave one order of magnitude larger adhesion strength than the experimental value. Three types of chemical reactions that affect the adhesion strength are found to occur depending on the terminal functional groups of the Al oxide surface and the water layer formation. Separate calculations confirm small barrier energies for all the reaction processes.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room5)

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

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

Relating to recent rapid advancement in substrate-decoration technique such as the one using the Self-Assembled Monolayers, there exist strong demands to predict the adhesion free energy between a complex liquid and polymer-grafted substrate. In principle, the adhesion free energy can be evaluated through the molecular simulation by integrating the work required to separate the liquid from the substrate. In former methods for the work of adhesion, a planar shape potential is introduced and the work of adhesion is calculated through integrating the force exerted on the potential from liquid molecules when liquid molecules are separated from the solid surface by gradually shifting the potential origin. These methods work well for sufficiently flat solid substrate. However, they are inefficient for a polymer-grafted substrate because it becomes necessary to shift the potential over a long distance.

Motivated by that, we propose a novel method to efficiently evaluate the work of adhesion of the interface between a liquid and a polymer-grafted surface. In the present method, a set of spherical potentials whose centers are set at the atomic positions of either polymer or substrate are introduced instead of a planar potential. It enables efficient separation of the liquid molecules from the polymer-grafted substrate. Moreover, potential-parameter update schemes are carefully chosen to suppress sharp variation in the force exerted on the potential and thereby to minimize the number of integration points.

The present method is applied to the interface between a water and a gold substrate on which poly(ehtylene oxide)s (PEOs) are grafted. Then, we find that the work of adhesion tends to become large at the intermediate density of PEO. This tendency is related to the number of water molecules accessible to oxygen atoms in PEO.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room5)

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

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

In order to control energy losses in mechanical systems, the study of friction in lubricated contacts has to be approached. Depending on the operating conditions and its chemical nature, the confined fluid can exhibit a limiting shear stress at high pressure [1, 2]. The physical origins of this phenomenon and its implications to friction are currently not completely understood [3]. In this study, an extensive Molecular Dynamics analysis of the shearing behavior of different types of molecules is performed. The behavior of the confined sheared system is explored and compared to the fluid bulk state. One of the main conclusion is that flow profile results from two competing forces in the molecular system, which is linked to the weakest interfaces being sheared. Additionally, the saturated shear stress response is found to be related to the concept of atomic mobility. With increasing pressure, the relaxation time of the material is increased. Thus, atomic mobility can be saturated for a range of high pressures, diffusion would not be allowed, and a solid-like behavior is displayed. Finally, a link between flow and friction behavior is discussed.

[1] Martinie, L. and Vergne, P., “ Lubrication at extreme conditions: a discussion about the limiting shear stress concept”, Tribol. Lett., 63, 2016.

[2] Ewen, J. P., Gattinoni, C., Zhang, J., Heyes, D. M., Spikes, H. A. and Dini D., “ On the effect of confined fluid molecular structure on nonequilibrium phase behaviour and friction”, Phys. Chem. Chem. Phys., 2017.

[3] Ndiaye, S. N., Martinie, L., Philippon, D., Devaux, N. and Vergne, P., “ A Quantitative Friction-Based Approach of the Limiting Shear Stress Pressure and Temperature Dependence”, Tribol. Lett., 65, 2017.

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

[SY-O6] Symposium O-6

Chairs: Yoshitaka Umeno(The University of Tokyo, Japan), Yoshinori Shiihara(Toyota Technological Institute,Japan)

Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room5

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

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

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

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

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

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

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

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

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room5)

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

Invited

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

When rough bodies are pressed against each other, a small contact area has to support all the load. This is why plastic deformation occurs even at moderate nominal contact pressure. Although indentation of elastic bodies by self-affine rough indenters has been studied extensively, little attention has so far been devoted to plasticity. This is mostly because capturing plasticity as well as contact with a self-affine rough surface is computationally quite challanging. Here, we succeed in achieving this goal by using Green's function dislocation dynamics, a modeling technique that combines discrete dislocation plasticity (DDP) with Green's function molecular dynamics (GFMD). As usual in DDP, plasticity is studied by tracking the nucleation and glide of each dislocation in the metal crystal. The dislocation image fields are instead calculated with GFMD, which allows to describe the self-affine rough surface using wavelenghts spanning from 5 nanometers to 100 micrometers.

Simulations are performed varying various parameters of the surface roughness, including the Hurst exponent and the root-mean-square height. Results show that the plastic response is size-dependent. An important implication of the size-dependence is that, when bodies deform plastically, it is not possible to scale observables such as contact pressure and contact area with crystal size or root-mean-square height, as typically done for elastic contact problems.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room5)

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

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

Liquid crystals (LC) - well-known for their application in LC-displays - have recently raised interest also for lubrication applications: favorable friction properties (specific friction of the order 0.005) have been experimentally observed in different systems [1]. The special behavior is attributed to the anisotropic viscosity and compressibility, which LC exhibit in semi-ordered phases (i.e. nematic or smectic phase). The LC molecules' elongated shape allows them to align with the shear, which could simultaneously reduce friction and increase load support. Moreover, the complex phase behavior and dynamic properties might also be exploited to design novel tribological systems with tunable or self-regulating friction, so-called ‘smart’ lubricants [2,3].

Here, we present a molecular dynamics simulations study of different LC lubricated model tribo-systems with the aim to characterize the LC rheological properties and investigate possible tuning mechanisms on a microscopic level. Shearing simulations of LC lubricating films with different structure characteristics, i.e. preferential molecule orientation, were performed for varying loads and shear rates. The response of the systems (velocity profiles, local viscosity and shear force) was evaluated and correlated to the fluid film structure, which is influenced by the flow. Of particular interest are situations, where the inherent equilibrium structure of the LC film (induced by surface boundary conditions or external fields) is different from the shear direction, due to the competing forces for aligning the LC molecules in different directions.

[1] T. Amann, C. Dold and A. Kailer, Tribology International 65 (2013), p. 3
[2] C. Tadokoro, T. Nihira and K. Nakano, Tribol Lett 56 (2014), p. 239
[3] S. Itoh, Y. Imura, K. Fukuzawa andH. Zhang, Langmuir 31 (2015), p. 11360

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room5)

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

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

In solution, amphiphilic surfactants can form physisorbed boundary films on immersed surfaces. A film’s structure and thereby its lubrication performance depend on numerous properties of all involved substances, such as the surface’s potential, as well as surfactant and background electrolyte concentration. We investigate the dependency of the coefficient of friction on adsorption film topography in exemplary contact systems by means of classical all-atom molecular dynamics. For this purpose, the present study focuses on cationic CTAB at idealized aqueous solution-gold interfaces. Recent parametrizations of CTAB, originally intended for micelle modeling in bulk solution, are combined with representations of simple gold surfaces. The stability of differently shaped pre-assembled surface aggregates at various effective surfactant concentrations are compared against expected behavior as documented by abundant experimental contributions. We finally present friction tests in simple shear geometries of surfaces covered with pairwise identical CTAB film morphologies.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room5)

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

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

Amines molecules can be used as organic friction modifiers OFM in a
lubricated contact working under in mixed/boundary regime.
Several experimental studies have been already done using steel against
steel contact. Our aim is to propose
a computational simulation protocol to have a better understanding of
what happens at atomic scale in the contact.
We study some physical properties (density, diffusivity) of amines
blended in Poly Alpha Olephin PAO using
molecular dynamics MD simulations employing the OPLS force field.
Green-Kubo formalism gives us access to diffusion coeficients of amines
in the oil.
Then, we present ab-initio (DFT+U based) study of the adsorption of

this OFM on alpha-hematite Fe2O3 surface {01-12}.
The interactions between the amine molecule and the surface will be analysed and used to fit Lennard-Jones potential
to model the interaction and open the way to new simulations using molecular dynamics.
We will conclude presenting simulations of the friction process applying stress and shear and computing a
numerical coefficient of friction.

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

[SY-O7] Symposium O-7

Chairs: Lucia Nicola(Delft University of Technology, Netherlands), Shuji Ogata(Nagoya Institute of Technology, Japan)

Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5

[SY-O7] Toward Exascale Atomistic Simulations of Interfaces

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

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

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

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

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

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

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

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

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

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5)

[SY-O7] Toward Exascale Atomistic Simulations of Interfaces

Invited

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

Under the U.S. Department of Energy, Aurora/A21 early science program, our group will be one of the 10 initial users of the Nation's first exaflop/s computer that can perform 10^{18} mathematical operations per second, when it is introduced in 2021. To make quantum molecular dynamics (QMD) and reactive molecular dynamics (RMD) simulations exa-scalable, we have developed an extension of the divide-and-conquer algorithmic framework called divide-conquer-recombine. On today's supercomputing platform, for instance, the framework has achieved over 98% of the perfect speedup on 786,432 IBM Blue Gene/Q processors for 40 trillion electronic degrees-of-freedom QMD in the framework of density functional theory and 68 billion-atom RMD. Production simulations include (1) 16,616-atom QMD simulation of rapid hydrogen production from water using metallic alloy nanoparticles, (2) 6,400-atom nonadiabatic QMD simulation of photoexcitation dynamics for efficient solar cells, and (3) 112 million-atom RMD simulation of metacarbon synthesis by high temperature oxidation of SiC nanoparticles. We will discuss tribology and interfacial applications such as frictional heating of energetic molecular crystals.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5)

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

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

It is known that silicon-based materials such as silicon carbide have low friction coefficients in water lubrication system. A tribofilm formed at a sliding interface is considered to reduce the friction coefficient, however detailed mechanism is still unclear because in-situ observation of the atomic scale sliding interface is difficult. Therefore, in this work, we investigated the structure, role and formation mechanism of the tribofilm of silicon-based materials by using molecular dynamics method. We performed sliding simulations of a SiO_2 substrate, which is a model of a native oxide layer of silicon-based materials, in water environment. We found that hydrolysis reaction of Si-O bond in SiO_2 surfaces occurred at contact areas of the surfaces as, Si-O + H_2O →Si-OH + OH. The hydrolysis reaction was mediated by proton transfer process. Since the hydrolysis reaction dissociated Si-O bonds, Si-O bond network of the SiO_2 surfaces became sparse, and then, several SiO_2 clusters were removed from the surfaces as wear debris. The wear debris were dissolved in the water layer between two surfaces, forming a colloidal silica layer. On the other hand, the water molecules penetrated into the sparse SiO_2 surfaces and hydrate the surfaces, forming a hydrophilic silica gel layers on the SiO_2 surfaces. Therefore, at the sliding interface, the colloidal silica layer was sandwiched by two silica gel layers. The colloidal silica layer prevents the contact of the surfaces and reduces a friction force, whereas the hydrophilic silica gel layer holds the colloidal silica layer at the sliding interface. Thus, the colloidal silica and silica gel layer that formed by hydrolysis reaction reduces the friction coefficient of silicon-based materials in water lubrication systems.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5)

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

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

Diamond-like carbon (DLC) has excellent friction properties such as low friction and high wear resistance. Thus, it is used as a solid lubricant material for engine parts. For this application, it is expected that DLC is used with the MoDTC friction modifier. When MoDTC is used as additives, a tribo-film of MoS_2 layers is formed at a sliding interface during friction, leading to low friction. It is known that frictional property of this system depends on many factors such as composition of additives, a structure of DLC, and so on. Thus, to improve the friction property, it is required to understand effects of these factors on friction behavior of the tribo-film. However, the friction behavior is unknown because *in situ* observation of the sliding interface is difficult. Thus, in order to investigate the friction behavior, we performed molecular dynamics simulation by using reactive force field, which takes into account the chemical reactions. In this study, we analyzed the influence of the defects in the MoS_2 layers on friction behavior of DLC by using a DLC/MoS_2 layers/DLC model. Here, we investigated the influence of the defects by comparing the friction behavior of the MoS_2 layers with and without grain boundaries. The friction simulation of the model without grain boundaries shows that the DLC/MoS_2 interface is the sliding interface. On the other hand, the simulation of the model with grain boundaries shows that the MoS_2/MoS_2 interface is the sliding interface since C-S bonds is formed between DLC and MoS_2 around grain boundaries. In addition, the MoS_2 layers with grain boundaries show higher friction force because the sliding between the MoS_2 layers is inhibited when a grain boundary attacks another grain boundary in neighboring layers. Then, we found that these friction behaviors caused by grain boundaries in the MoS_2 are major factors that increase friction force in this system. We will report the influence of other defects at the conference.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5)

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

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

Silicon and diamond are brittle materials with the same crystal structure but opposite density change upon melting. Using molecular dynamics simulations, we show that both crystals can respond to shear deformation by undergoing mechanical amorphization. The resulting amorphous material has liquid-like structure, is denser than the crystal in silicon and less dense than the crystal in diamond. As a result, as normal pressure

increases, amorphization, which is often related to nanoscale wear, is enhanced in silicon but suppressed in diamond. Moreover, shear-induced amorphization of silicon yields a high-density, ductile amorphous material at pressures much lower than the polyamorphic transition (~14 GPa) observed upon hydrostatic compression. These results are potentially relevant for the friction properties of other crystals that densify upon melting and show polyamorphism, like germanium and ice.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5)

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

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

Simulations of materials and structures submitted to wear, machining, forming, forging, and impacts, to name but a few, often involve large deformations, damage, and failure. These phenomena are challenges for usual computational tools such as finite element modeling. When large deformations occur, finite element methods have limitations due to the need to remesh which is computationally expensive and sometimes fails. Therefore, mesh-free methods such as Smooth Particle Hydrodynamics (SPH) are more suitable for these applications.

The use of SPH for the simulations of wear, tribology, and impacts problems in solids has recently gained momentum as large deformations and instability phenomena such as damage and fracture could be easily handled. However, little work exists on the implementation of damage in SPH. This is thought to be due to the approximation problems around surfaces. As damage and fracture develops in solids, this creates new surfaces around which the SPH approximation breaks down.

In this presentation, we present the results of simulations of wear response to show case a new implementation of damage in SPH that solves some of the problems due to the approximation break-downs close to surfaces. This implementation is built as an upgrade of the SPH package for solids available within LAMMPS called Smooth Mach Dynamics.

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

[SY-O8] Symposium O-8

Chairs: Tianbao Ma(Tsinghua University, China), Yang Wang(Institute for Materials Research, Tohoku University, Japan)
Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room5

[SY-O8] Friction mechanism of nanostructured steel in lubricant: A coarse-grained molecular dynamics study

○Yoshitaka Umeno Umeno, Atsushi Kubo, Yuta Sudo （The University of Tokyo, Japan）

[SY-O8] Coarse-Grained Molecular Dynamic Simulation on the Wear Mechanism of Polymer Brush with Different Chain Topologies

○Zhongmin Liu, Shuichi Uehara, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Material Research,Tohoku Univ., Japan）

[SY-O8] Molecular Dynamics Simulation Study on Friction of Bottlebrush Polymer with a Cationic Anchor Block Adsorbed on Substrate

○Shuichi Uehara, Zhongmin Liu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Materials Research, Tohoku Univ., Japan）

[SY-O8] Temperature dependent dynamics simulation of traction fluid by molecular dynamics method

○Eiji Tomiyama[1,2], Takeshi Iwasaki[3], Hitoshi Washizu[2] （1.Research Organization for Information Science and Technology, Japan, 2.Graduate School of Simulation Studies, Univ. of Hyogo, Japan, 3.Lubricants Research Laboratory, Idemitsu Kosan Co., Ltd., Japan）

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room5)

[SY-O8] Friction mechanism of nanostructured steel in lubricant: A coarse-grained molecular dynamics study

○Yoshitaka Umeno Umeno, Atsushi Kubo, Yuta Sudo （The University of Tokyo, Japan）

Intensive studies have been dedicated to the problem of boundary lubrication in recent years. Experimental studies have demonstrated a significant reduction in friction coefficients of steel that has nanostructured surfaces. It is conjectured that nanostructured metals have a large density of sites with strong attraction to lubricant molecules, resulting in reduced friction. The detailed mechanism of the phenomenon however remains unclear.

To reveal the mechanism of lubrication between metal surfaces, atomic- or molecular-level investigations are required for the effect of metal-molecule interaction on boundary lubrication. Coarse-grained molecular dynamics (CGMD) is a useful and efficient simulation method to tackle such problems. Indeed, a CGMD study of shear flow of lubricant molecules between metal surfaces showed that the more molecules were adsorbed on the surfaces, the lower the friction coefficient became. Nevertheless, molecular-level mechanisms are not fully understood regarding the experimentally presented effect of the surface nanostructure on the friction coefficient or the nature of structural ordering in shear flow.

In this study, we performed CGMD simulations with the aim to reveal the molecular-level friction mechanism in boundary lubrication between nanostructured steel surfaces. As lubricant molecules, polyethylene (nonpolar) and fatty acid (polar) were modeled by the coarse-grained method representing methylene (CH2) and carboxyl (COOH) groups by individual particles. The effect of the surface nanostructure was mimicked by distributing atoms producing stronger attraction with the molecular groups. The effect of alignment of the strong potentials on the friction coefficient is apparent in the case of polar molecules. In both polar and nonpolar lubricants, the nanostructure enhances critical shear stress for separation of adsorbed lubricants from the surface. These results suggest salient influence of the surface nanostructure on the friction coefficient.

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room5)

[SY-O8] Coarse-Grained Molecular Dynamic Simulation on the Wear Mechanism of Polymer Brush with Different Chain Topologies

○Zhongmin Liu, Shuichi Uehara, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Material Research,Tohoku Univ., Japan）

As a low friction material, polymer brush has attracted attention in many areas because of its good frictional properties and biological compatibility. The frictional properties of polymer brush are improved by different chain topologies. However, the effects of the chain topologies on the wear of polymer brush are still not clear. To reduce the wear of the polymer brush, it is required to understand the wear behaviors and mechanism of different topological polymer brush. However, in-situ observation of the sliding interface at the molecular scale is difficult. Thus, we investigated the wear mechanism of polymer brush with different topological chain by using coarse-grained molecular dynamics (CGMD) method.

We perform friction simulations of linear polymer brush, cyclic polymer brush where the polymer chains have cyclic structure, and crosslinked polymer brush where the polymer chains are connected with the neighboring polymer chain with crosslinker to understand the effect of chain topologies on the wear. We found that cyclic polymer brush and crosslinked polymer brush had smaller number of dissociation than linear polymer brush because the cyclic polymer brush and crosslinked polymer brush showed smaller frictional forces than that of linear polymer brush. We found that the cyclic polymer brush and crosslinked polymer brush had less interpenetrating beads than that of linear polymer brush. Therefore, the cyclic polymer brush and crosslinked polymer brush have smaller entanglements, leading to the low frictional force. We conclude that chain topologies of polymer brush can improve the wear resistance because they suppress the interpenetration at the sliding interface.

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room5)

[SY-O8] Molecular Dynamics Simulation Study on Friction of Bottlebrush Polymer with a Cationic Anchor Block Adsorbed on Substrate

○Shuichi Uehara, Zhongmin Liu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Materials Research, Tohoku Univ., Japan）

In recent years, concentrated polymer brush (CPB), which is constructed by grafting polymer chains onto a substrate with high density, has been developed. CPB has attracted much attention for application to low friction materials as artificial joints because of its high wear resistance and biocompatibility. However, the graft of polymer chains onto substrate is complicated and takes much cost. As an alternative method analogous to CPB, bottlebrush polymer (BBP) known as macromolecules with polymeric side chains is candidate for low friction materials. Previous studies have revealed that BBPs with a cationic anchor block adsorbed on a negatively charged surface swell, which produces low friction force. However, the detail of friction mechanism of BBP is not clear. Furthermore, the effects of sliding speed and side chain length on friction properties are also unknown because the in-situ observation of the sliding interface is difficult. Thus, computational simulation is required. Herein, to reveal the mechanism during friction of BBP consisting of a cationic anchor block, we developed a coarse-grained molecular dynamics code which can consider chemical specificity of each monomer, and performed friction simulation in water solvent. The low friction coefficient was observed at the low load, but friction coefficient was increased at high load. We found that, at low load, water beads which coordinate to the side chain of BBP suppressed contact between BBPs on the counter surfaces, because side chains of BBP prefer to interact with the water beads. This swelling state of BBP facilitates shear between the opposite substrates. With high load, water beads were removed from the sliding interface, which reduces the number of water beads around BBP. Therefore, the contact between BBPs on a counter surface leads to high friction coefficient. The effects of side chain length and sliding speed on the friction properties will be discussed on the day.

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room5)

[SY-O8] Temperature dependent dynamics simulation of traction fluid by molecular dynamics method

○Eiji Tomiyama[1,2], Takeshi Iwasaki[3], Hitoshi Washizu[2] （1.Research Organization for Information Science and Technology, Japan, 2.Graduate School of Simulation Studies, Univ. of Hyogo, Japan, 3.Lubricants Research Laboratory, Idemitsu Kosan Co., Ltd., Japan）

Traction drive is a mechanism that transmits power by a rotor and lubricating oil. In order to evaluate the characteristics of the fluid molecules in the traction drive, we construct a simulation method to apply shear to the fluid confined between solids using LAMMPS, a molecular dynamics simulator.

In this simulation, conditions are set as follows. The boundary condition of the system is a periodic boundary condition in the horizontal direction. Fluid is composed of a single hydrocarbon compound and the number of atoms is about ten thousand. The solids are a model metal surface imitating (100) plane of α-iron, and thier atomic motion is frozen. The force field parameter of fluid molecules uses the Dreiding force field. Apply a pressure of 0.8 GPa to 1.24 GPa in the direction perpendicular to the solid atoms. Furthermore, a constant slip of relative sliding speed 1 m/s to 50 m/s is applied. Then, the simulation time on the order of nanoseconds is passed and the steady state is set. With the above setting, an ensemble of constant pressure / constant shear state is created.

The temperature dependency of the coefficient of traction is evaluated by changing the temperature of the fluid from -20 ˚C to 140 ˚C. The coefficient of traction also change with the change of temperature, and the tendency is at least qualitatively consistent with the experimental values.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A5] Symposium A-5

Chair: Sinisa Dj Mesarovic(Washington State University, United States of America)
Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room6

[SY-A5] Parameters to consider in the modelling of dislocation boundary evolution

○Grethe Winther Winther （Technical University of Denmark, Denmark）

[SY-A5] Data Mining of Indentation Induced Dislocation Microstructures

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

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

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

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room6)

[SY-A5] Parameters to consider in the modelling of dislocation boundary evolution

Invited

○Grethe Winther Winther （Technical University of Denmark, Denmark）

An essential part of the development of theory and simulations of microstructure evolution is the parameters used as input as well as the output, which should be comparable to experimental observations. An overview of the experimentally observed dislocation boundary evolution in metals of medium to high stacking fault energy are presented with emphasis on such parameters. In particular, the spatial distribution of boundaries in terms of boundary planes, spacings and misorientation angles are considered as a function of crystallographic grain orientation, deformation mode and strain. Based on the experimental observations relations to crystal plasticity and the Burgers vectors available for boundary formation are discussed.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room6)

[SY-A5] Data Mining of Indentation Induced Dislocation Microstructures

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

In general, data mining is the process of discovering patterns in large data sets, with the most common tasks being, anomaly detection, association rule learning, clustering, classification, regression and summarization. Within materials science, the most popular application so far is materials discovery, one of the goals of the well-known Materials Genome Initiative (https://www.mgi.gov).

In order to understand the convoluted interactions of dislocations that define the mechanical properties of metals to a large degree, a lot of data has been and is being generated, be it via experiments or simulations. Due to the complexity of the dislocation microstructure and its discrete nature aforementioned algorithms can not be applied ad-hoc. Thus, developing methods that enable their use are highly desirable.

In this presentation we want to outline the key aspects of the data mining framework for dislocation microstructures that we are currently developing. Among others, we will show examples of how quantitative comparisons of dislocation data—be it from experimental or computational methods—can be done. Aforementioned framework will be applied to a dataset consisting of hundreds of realizations of a numerical indentation experiment realized with discrete dislocation dynamics. Rate coefficient beneath the indenter will be extracted for the dislocation densities commonly found in continuous dislocation dynamics models. The resulting microstructures will be analyzed for common patterns and their correlation with the intially emerging structure to enable predicting the characteristics of the final state from the first initial steps.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room6)

[SY-A5] Lattice continua for polycrystal grains: Climb and glide of

dislocations, diffusion and grain boundary kinematics.

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

At high temperatures, the interior of each grain in a polycrystal suffers: (1) dislocation glide, (2) climb, and (3) diffusion of vacancies. Grain boundaries undergo: (4) growth/disappearance, as a result of vacancy diffusion, and, (5) crystallographic reorientation/mismatch, as a result of dislocations arriving to the boundaries either by glide or by climb. All the above deformation mechanisms are naturally described in the lattice continuum framework, whereby the lattice represents the material. Climbing edge dislocations are lattice sink/source which must be reflected in the continuity equation and the transport theorem. The interacting kinematics of dislocation glide and climb requires dual definition of crystallographic slip fields: the true slip and the apparent slip. The transport theorem for grains with lattice growing or disappearing lattice at different grain boundary faces results in the direct formulation of the boundary condition for vacancy diffusion flux in terms of the boundary velocity (different from the lattice velocity). The field equations for each grain are derived by means of the principle of virtual power. Additional boundary conditions result from the relative motion of the adjacent crystal faces: Change of tilt and twist angle and surface elastic mismatch are derived from the geometry of dislocations arriving to the boundary. The resulting polycrystal initial/boundary value problem consists of elasticity-plasticity-diffusion field equations in each crystalline domain with moving boundaries, coupled through the boundary conditions.

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Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A6] Symposium A-6

Chair: Emma Griffiths(University of Cape Town, South Africa)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room6

[SY-A6] Design of patchy nanoparticles via the self-assembly of triblock terpolymers in selective solvents

○Eliot Fried, Nicolás Moreno （Okinawa Institute of Science and Technology, Japan）

[SY-A6] Nanoporous Composites: Giving Polymers Strength and Helping Metals Move

○Emma Griffiths[1], Jana Wilmers[2], Swantje Bargmann[2], BD Reddy[1] （1.University of Cape Town, South Africa, 2.University of Wuppertal, Germany）

[SY-A6] Multiscale modeling of advanced materials for hybrid organic-inorganic solar cells

○Alexander E. Kobryn （Nanotechnology Research Center, National Research Council Canada, Canada）

[SY-A6] **From cellulose and lignin to kerogen: molecular simulations of a geological process**

○Roland PELLENQ[1], Pierre-Louis Valdenaire[1], Christophe Bichara[3], Franz Ulm[1], Jean-Marc Leyssale[2] （1.<MSE>2, MIT- CNRS - AMU, United States of America, 2.ISM, CNRS - Bordeaux U., France, 3.CINaM, CNRS - Aix-Marseille U., France）

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room6)

[SY-A6] Design of patchy nanoparticles via the self-assembly of triblock terpolymers in selective solvents

Invited

○Eliot Fried, Nicolás Moreno (Okinawa Institute of Science and Technology, Japan)

The hierarchical self-assembly of triblock terpolymers in solution is a successful bottom-up methodology for constructing functional patchy nanoparticles with prescribed topology and shape. Currently, the design of such nanoparticles requires an iterative process to identify the experimental phase parameters needed to produce any target pattern. The broad use of this technology is therefore cumbersome and limited by an incomplete understanding of the mechanisms underlying patch transition. A detailed understanding of how thermodynamics and kinetics influence the topology of the assemblies is also missing. In this work, we present a set of rules for programming desired shapes of the nanoparticles and predicting the pathways by which they assemble. We investigate systematically the interplay between entropic and enthalpic parameters governing the self-assembly of ABC triblock copolymers in a selective solvent for the C block. We use a computational modeling at the mesoscale and thereby encompass the length and time scales associated with the motion and assembly of the polymer coils, while accurately approximating the chemically driven interactions. The phase diagram predicted by our model is consistent with experimentally identified characteristic nanoparticle shapes. We find that the effective volume fraction of the soluble block determines the size of a particle and the distribution of its patches via steric interactions. Moreover, we find that the relative fraction of the patch-forming block and its affinity with the core of a articles dictates the number and shape of its patches. As a major outcome, we construct a morphologically-based library of nanoparticles. That library can be used to hierarchically design mesoscale aggregates with specific morphologies. Our results provide insight regarding the mechanisms that determine nanometer scale objects in synthetic and naturally occurring systems.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room6)

[SY-A6] Nanoporous Composites: Giving Polymers Strength and Helping Metals Move

○Emma Griffiths[1], Jana Wilmers[2], Swantje Bargmann[2], BD Reddy[1] (1.University of Cape Town, South Africa, 2.University of Wuppertal, Germany)

An important benefit of electroactive polymers is their large strain response due to certain stimuli such as an electric current. However, for sufficient mechanical use in electrochemical systems, they lack the necessary strength and stiffness. Metals on the other hand have sufficient strength and stiffness but are unable to function as piezoelectric materials [1]. By creating a metal-polymer composite, however, a stronger material with large strain capacity is created that can withstand larger actuation forces. Specifically, using polymer impregnated nanoporous structures, with their exceptional mechanical properties providing a reinforcing base [2,3], creates a composite material with superior actuator properties by having both sufficient strength and strain capabilities.

This work presents the chemoelectromechanical response of a gold-polymer nanocomposite model. A representative volume element is modelled using a linear version of the chemoelectromechanical theory developed by Wilmers et al. [4] and is implemented through a staggered explicit-implicit finite element

simulation in ABAQUS. Additionally the theory is enhanced by introducing an implicit solvent model to capture the effects of the crowding of ions due to saturation within the material. The micromechanical response of the composite is explored under an imposed electric field and thus providing information to be used in the optimization of microstructures for sensory and actuation applications.

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(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room6)

[SY-A6] Multiscale modeling of advanced materials for hybrid organic-inorganic solar cells

○Alexander E. Kobryn （Nanotechnology Research Center, National Research Council Canada, Canada）

When it comes to talk about alternatives to non-renewable sources of energy, photovoltaics is one of the most promising choices for converting solar light into electricity with the use of solar cells. At present, there is wide variety of solar cell devices on the market and this variety will continue to grow because of the race for better conversion efficiency and the final product sustainability. Within recent years, the seemingly clear boundaries between photovoltaics of inorganic and organic solar cells have started to fade by the advent of metal-halide hybrid organic-inorganic perovskites (OIP). They are very promising candidates for future photovoltaic applications because they have wide-direct band gap, which can be tuned by either changing the organic cation, the metal atom, or the halide. Their power conversion efficiency now reached over 22%. At the same time, the level of our understanding of the origin of such performance is still insufficient. We believe that thin film morphology is a key factor determining the performance of bulk heterojunction organic solar cells, because of its influence on charge separation, charge transport and recombination losses in donor-acceptor blends. With this respect, we present both descriptive and predictive multiscale modeling of electronic and structural properties of blends of PCBM or hybrid OIP of the type $CH_3NH_3PbX_3$ (X=Cl, Br, I) with P3HT, P3BT or squaraine SQ2 dye sensitizer, including adsorption on TiO_2 clusters. Here, the multiscale nature of modeling means that in a set of simple hierarchical approaches we combine different methods for different scales (quantum mechanical, microscopic, mesoscopic) interpreted independently and that the information obtained at one level is transmitted to the next level as a required input. If necessary, new information is sometime transmitted back to the previous level for a feedback control. As the result, we arrive at a very reliable methodology that allows computing the microscopic structure of blends on the nanometer scale and getting insight on miscibility of its components at various thermodynamic conditions. The calculated nanoscale morphologies serve as an instrument in rational design of hybrid OIP. They are used in collaboration with experts who actually make prototypes or devices for practical applications.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room6)

[SY-A6] From cellulose and lignin to kerogen: molecular simulations of a geological process

○Roland PELLENQ[1], Pierre-Louis Valdenaire[1], Christophe Bichara[3], Franz Ulm[1], Jean-Marc Leyssale[2]
（1.<MSE>2, MIT- CNRS - AMU, United States of America, 2.ISM, CNRS - Bordeaux U., France, 3.CINaM, CNRS - Aix-Marseille U., France）

The process by which organic matter decomposes deep underground to form petroleum and its underlying kerogen matrix has so far remained a no man’ s land to theoreticians, largely because of the geological (Millions of years) timescale associated with the process. Using a replica exchange accelerated molecular dynamics method initially developed in the context of the micro- to milli-second timescale for protein folding, we simulate the full transformation of cellulose and lignin (the main components of wood) into kerogen under prevailing geological conditions. We observe in sequence (i) the fragmentation of the cellulose crystal and production of water, (ii) the development of an aliphatic macromolecular phase, (iii) its aromatization, and (iv) its aggregation into a stiff porous aromatic carbon upon expulsion of the fluid phase. The composition of the solid residue along the maturation pathway strictly follows what is observed for natural type III kerogens and for artificially matured samples under closed conditions, providing further evidence of a kinetically controlled, irreversible, decomposition process in which the aliphatic (immature) phase is a metastable intermediate.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A7] Symposium A-7

Chair: Michael Zaiser(FAU University of Erlangen-Nuremberg, Germany)
Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6

[SY-A7] Mathematical challenges for a mesoscale theory of dislocations

○Thomas Hochrainer (TU Graz, Austria)

[SY-A7] **Dislocation multiplication in the discrete-continuum transition regime**

○Katrin Schulz[1], Markus Sudmanns[1], Kolja Zoller[1], Peter Gumbsch[1,2] (1.Karlsruhe Institute of Technology, Germany, 2.Fraunhofer Institute for Mechanics of Materials, Germany)

[SY-A7] The fundamental instability of dislocation transport equations

○Michael Zaiser, Ronghai Wu (FAU University of Erlangen-Nuremberg, Germany)

[SY-A7] 2D continuum theory of dislocations

○Istvan Groma (Eotvos Lorand University, Hungary)

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

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

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6)

[SY-A7] Mathematical challenges for a mesoscale theory of dislocations

Invited

○Thomas Hochrainer (TU Graz, Austria)

During the last two decades, dislocation research saw a revival driven by new experimental techniques for small scale testing, high resolution characterization and the rise of large scale discrete dislocation simulations. This also stimulated intensive research in mesoscale theories of dislocations. Great advances were achieved on continuum models of dislocation interactions for strongly simplified straight-dislocation systems and continuum dislocation dynamics of single slip deformation. However, a transfer of the employed averaging methods to fully three-dimensional multiple slip deformation remains a challenge for various reasons.

In the current talk we shall highlight some challenges appearing on different levels of continuum dislocation modelling. At the most fundamental level it is yet unclear what continuum measures are suited for characterizing 3D networks of dislocations. The alignment tensors successfully used for dislocation distributions in single slip seem to be of limited value in networks consisting mostly of junctions and reaction products. It is likewise an open question how to describe the kinematics of dislocation networks, where reactions and junction formation or break-up imply permanent changes in the topology of the network and the characteristics of dislocations. Closely related is the challenge of capturing the averaged energetics, kinematics and dissipation of these dislocation interactions.

To overcome the named challenges possibly requires new mathematical tools or at least the adoption of concepts from other areas of physics and mathematics which were not yet (fully) exploited in dislocation theory. We shall discuss several ideas where we might find new impulses and promising tools for further successes in developing a mesoscale theory of dislocations. Expected key areas include discrete and differential topology, gradient flows, rough energy landscapes, and temporal and spatial statistics.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6)

[SY-A7] **Dislocation multiplication in the discrete-continuum transition regime**

○Katrin Schulz[1], Markus Sudmanns[1], Kolja Zoller[1], Peter Gumbsch[1,2] (1.Karlsruhe Institute of Technology, Germany, 2.Fraunhofer Institute for Mechanics of Materials, Germany)

The striving for advanced materials with well-defined microstructures has led to an increasing effort towards a physically based description of the motion of dislocations as the cause of plastic deformation. Several dislocation based continuum theories have been introduced, but only recently rigorous techniques have been developed for performing meaningful averages over systems of moving, curved dislocations, yielding evolution equations for a dislocation density tensor, see [1].

Regarding a self-consistent coarsening of dislocation modeling in order to construct an efficient numerical implementation, several issues have to be solved including calculation of the stress field of a system of dislocations, representation of dislocation interactions and reactions as well as boundary conditions. Accurate solutions have been found for one and two dimensional systems [2, 3]. However, the analysis and understanding of dislocation networks in three dimensions involves additional challenges such as the representation of dislocation multiplication.

In this presentation, we discuss the implications of a homogenization of dislocation interactions and reactions in the discrete-continuum transition regime. Based on the analysis of 3d discrete dislocation structures, we present a coarse-grained continuum formulation for dislocation multiplication due to cross-slip and glissile reaction events. The formulation is validated by the comparison with discrete dislocation dynamics simulations and discussed in the context of a continuum limit as lower application limit of a continuum approach.

[1]Hochrainer, T.; Sandfeld, S.; Zaiser, M.; Gumbsch, P.: Continuum dislocation dynamics: Towards a physical theory of crystal plasticity. *J. Mechan. Phys. Solids.* 63 (2014), p. 167-178.

[2] Schmitt, S., Gumbsch, P., Schulz, K.: Internal Stresses in a Homogenized Representation of Dislocation Microstructures. *J. Mechan. Phys. Solids*, 84 (2015), p. 528-544.

[3] Schulz, K., Sudmanns, M., Gumbsch, P.: Dislocation-Density based Description of the Deformation of a Composite Material. Modell. Simul. Mater. Sci. Eng., 25 (2017), 064003.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6)

[SY-A7] The fundamental instability of dislocation transport equations

○Michael Zaiser, Ronghai Wu （FAU University of Erlangen-Nuremberg, Germany）

We analyze the stability of transport equations which describe dislocation dynamics in terms of fluxes of dislocation densities defined on scales above the dislocation spacing. We demonstrate that such transport equations exhibit a generic instability which emerges as soon as a dislocation flux function, which in the simplest case is identical with the shear strain rate on a given slip system, has a negative derivative with respect to the flowing dislocation density. The criterion for instability is equivalent to the condition that the stress required to sustain plastic flow at a given rate is an increasing function of dislocation density. We conclude that dislocation patterning of some kind is an almost trivial, and practically unavoidable, consequence of dislocation transpoort in conjuction with work hardening. Implications for the theory and interpretation of different types of dislocation patterns, and for density-based simulations of plastic flow in general, are discussed.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6)

[SY-A7] 2D continuum theory of dislocations

○Istvan Groma （Eotvos Lorand University, Hungary）

During the past 20 years, by a systematic course graining of the equation of motion of straight parallel edge dislocations a 2D continuum theory of dislocation has been developed. It is able to account for many important feature of the collective properties of dislocations, like size effect, hardening due to precipitates, dislocation density distribution next to boundaries, and dislocation patterning. The predictions of the theory

are directly compared to discrete dislocation dynamics simulations.

In spite of the success of the theory there are several open issues need to be addressed for further developing the current theory. In the talk the problems "blocking" the extension of the theory are discussed:

1. Do we need a continuum theory?

2. Why still in 2D? What we can learn from it?

3. Should we course grain the equations of motion of the dislocations or the energy of the discrete system to derive the continuum theory?

3. Numerical determination of the dislocation dislocation correlation function. Problems related to the the finite size effect observed.

4. What to do next to boundaries?

5. Phase field approach. Issues related to the nontrivial mobility function one has to introduce.

6. Slow, power law relaxation of the dislocation system.

7. How to incorporate stochastic effects.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6)

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

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

Many dislocation dynamics simulation models were developed to understand plastic deformation of metals most of which are based on small deformation kinematics. In this talk, I will present a density-based dislocation dynamics model within the framework of finite deformation of crystals, focusing on crystal mechanics and the dislocation transport equations at finite deformation. The geometric coupling and non-linearity of the dislocation transport on various slip systems will be explained. The relevant crystal mechanics, thermodynamics, and constitutive closure questions will also be discussed. Collaboration: Giacomo Po, University of California-Los Angeles; Grethe Winther, Technical University of Denmark.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A8] Symposium A-8

Chair: Thomas Hochrainer(TU Graz, Austria)
Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room6

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

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

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

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

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

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

[SY-A8] A Sharp Phase Field Method

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

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room6)

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

Invited

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

Pattern formation in thin elastic shells has attracted increasing interest in both fundamental studies and practical applications. Examples include biological systems and engineering applications, such as the fabrication of flexible microelectronics. In this talk we explore the mechanical instabilities of an intrinsically curved thin shell deposited on a liquid surface. Here, the pattern formation is not a direct result of externally imposed strain, but is due to the geometric incompatibility between a curved, stiff membrane and an (initially flat) liquid substrate. We observe several types of instabilities, including a wrinkle-to-fold transition from periodic sinusoidal solutions to morphologies that combine sinusoidal wrinkles and folds; a transition from dimples (geometric inversions) to periodic sinusoidal solutions; and a transition from flat bands with zero Gaussian curvature, to dimpled periodic patterns. We show that whe wrinkling patterns can be described via an effective theory of liquid crystalline smectics at intermediate length scales. This insight allows better understanding of the wrinkling patterns seen in such systems, with which we explain pattern breaking into domains, the properties of domain walls and wrinkle undulation. We compare our predictions with numerical simulations and experimental observations. We investigate how the global geometry of the curved shells and their elastic properties control the transitions between the various morphologies. Last, we discuss various new strategies for creating and controlling patterns in thin elastic shells with natural curvature.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room6)

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

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

Domain structures consisting of multiple off-phase variants are generally formed in ordering process in binary alloy systems. The $L1_0$ type order is formed in AB type alloys on the basis of an *fcc* lattice. The crystal structure is tetragonal. Therefore three orientational variants can be formed depending on which of <100> directions corresponds to c-axis and two translational variants are possible for each of them; six distinct crystallographic variants exist in this type of order. The present authors previously developed a phase-field formulation for ordering process of $L1_0$ type in binary alloys, taking into account the symmetry of the crystal structure. In the $L1_0$ structure the *fcc* lattice is divided into four simple cubic sublattices. The atomic occupation probabilities on the sublattices are represented by three independent order parameters and a composition parameter. If the state of order of atomic arrangement is represented by a point in the three dimensional Euclidean space spanned by the three order parameters, the six equivalent variants are defined by the six tips of a regular octahedron centered on the origin for the disordered state. A mean-field free energy is defined in a form of Landau type expansion with the order parameters and the composition parameter. In this presentation we further consider the effect of the lattice distortion. An elastic energy is introduced with eigen strains according to Khachatrian's method. The interface energy automatically reflects the direction of c-axis and satisfies symmetries of cubic, tetragonal and orthorhombic structures. Kinetic equations for time-evolution of the order parameters and the concentration are derived from the Ginzburg-

Landau type thermodynamical potential. Formation of domain structures was simulated by treating the kinetic equations numerically in a three-dimensional cell scheme. The microstructures obtained are compared with experimental results of TEM observation.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room6)

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

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

An important focus in creating more realistic phase field models is the incorporation of the thermodynamic driving forces in multicomponent multiphase-field models by coupling to thermodynamic databases. This coupling, which aims at retrieving Gibbs energies and chemical potentials, becomes increasingly intricate as the number of components/chemical elements in the system increases. This is caused by the fact that the number of elements in a tensor increases exponentially with the number of dimensions, and so do the computational and memory requirements. The exponential dependency (and the problems that are caused by it) is called the curse of dimensionality.

Alternatives need to be investigated for the storage and handling of the thermodynamic data required for the phase field simulations. A possible solution for this might be the use of a canonical polyadic decomposition on the tensors containing the thermodynamic data. In this way, the huge tensors are approximated well by compact multilinear models or decompositions. Tensor decompositions are more versatile tools than the linear models resulting from traditional matrix approaches.

This solution promises to be suitable for this challenge and has been applied to a quaternary and quinary metal-oxide system in a multicomponent multiphase-field model which incorporates facetted and dendritic growth and can also treat the boundaries as an open boundary where the melt is locally in equilibrium with the atmosphere at a certain partial oxygen pressure. The results and improvements in computational requirements are compared for various methods to couple to a thermodynamic database.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room6)

[SY-A8] A Sharp Phase Field Method

Invited

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

Phase field modelling offers an extremely general framework to predict microstructural evolutions in complex systems. However, its computational implementation requires a discretisation scheme with a grid spacing small enough to preserve the diffuse character of the theory. We present a new formulation in which the interfaces are resolved with essentially one grid point with no pinning on the grid and an accurate rotational invariance, allowing to multiply the accessible linear dimensions by an order of magnitude or, conversely, to reduce the computational time by almost three orders of magnitude. We show that this Sharp Phase Field Method (S-PFM) reproduces interfacial kinetic properties with a very high accuracy. Then, we apply the model to a situation where conserved and non-conserved fields are coupled. Finally, to couple S-PFM to elastic fields, we propose a new elastic solver that efficiently treats strong elastic heterogeneities and that is mathematically stable.

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

[SY-I5] Symposium I-5

Chairs: Stephen M Foiles(Sandia National Laboratories, United States of America), Mitra L Taheri(Drexel University, United States of America)

Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room7

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

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

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

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

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

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

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room7)

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

Invited

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

In specific conditions, grain boundary (GB) migration occurs in polycrystalline materials as an alternative vector of plasticity compared to the usual dislocation activity. The shear-coupled GB migration, the expected most efficient GB based mechanism, couples the GB motion to an applied shear stress. The migration of the GB occurs through the nucleation and motion of disconnections.

We report a detailed theoretical study of the elementary mechanisms occurring during heterogeneous disconnections nucleation. Using molecular simulations, the absorption of a $1/2[110]$ edge bulk dislocation in a symmetric $\Sigma{17}(410)$ $[001]$ tilt GB generates an immobile disconnection in the GB. We show that the shearing of this GB induces its migration and reveals a new GB migration mechanism through the nucleation of a mobile disconnection from the immobile one. Energy barriers and yield stress for the GB migrations are evaluated and compared to the migration of a perfect GB. As expected, the migration of imperfect GB is easier than the one of perfect GB. An immobile disconnection in a BG can thus operate as a source of disconnections driving the GB migration.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room7)

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

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

We propose a novel approach to simulate the evolution of polycrystalline microstructures based upon a disconnection model for grain boundary (GB) kinetics. The model incorporates surface tension, applied stress, and jumps in chemical potential across GBs. The model also includes disconnection nucleation and mobility. Disconnections are line defects that lie solely with GB and are characterized by both a Burgers vector and a step height, as set by the GB bicrystallography. We first derive a continuum equation of motion for individual GBs and then for GB triple junctions (TJ) within a polycrystalline microstructure that rigorously accounts for conservation of disconnection Burgers vectors and step heights and couples the GBs meeting at the TJ. We then implement this model in a continuum simulation of GB dynamics without TJs, with TJs and in a polycrystalline microstructure. The resultant simulations provide clear demonstrations of the importance of including a crystallography-respecting microscopic model of microstructure evolution and the intrinsic coupling between stress, capillarity, and microstructure connectivity in microstructure evolution.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room7)

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

Invited

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

In the current work, mechanisms for dislocation-mediated motion of and deformation at coherent boundaries in fcc materials is investigated along with the resulting mechanical behavior.
On the modeling side, molecular dynamics (MD) simulations are carried out on bulk single and bi-crystal Cu, the latter containing two Σ3(111) boundaries. These are subject to loading conditions varying between shear loading parallel to the boundaries and perpendicular uniaxial loading. In the case of pure shear loading, MD results demonstrate that <112> shearing on Σ3(111) results in monotonic flow depending on the shear sign, whereas <110> shearing leads to oscillatory flow. As it turns out, this difference in behavior can be related to corresponding changes in the coincidence site lattice (CSL). In particular, in the case of <112> shearing, new potential boundary positions in the CSL occur every three atomic layers. Depending on the shear sign, however, one of these positions is closer to the current boundary position than the other. Since less energy is required for the boundary to shift to the closer position, the boundary moves to this position. In contrast, <110> shearing results in new potential boundary positions in the CSL having the same distance to the current boundary. Consequently, none of these is favored energetically, resulting in oscillatory motion of the boundary between these.
On the experimental side, nano-indentation experiments with 2m sized spherical indenter tips are used to study the impact of coherent Σ3(111) boundaries on the yield strength distribution in copper. The indents are performed either inside a grain or close to a coherent Σ3(111) boundary aligned normal to the sample surface. The force-displacement curves show elastic loading following Hertz´s predictions until a sudden displacement burst - a “pop-in” - is observed. The maximum shear stress beneath the indenter tip at the pop-in force is interpreted as yield stress. The statistical behavior of the yield stress is analyzed via cumulative probability (CP) plots. The CP plots show a significantly lower average yield stress at the boundary with respect to the single grains and an extremely narrow distribution at the boundary. The later finding suggests that the mechanism responsible for dislocation source activation is omnipresent at the boundaries.

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

[SY-I6] Symposium I-6

Chairs: Garritt Tucker(Colorado School of Mines, United States of America), Chuang Deng(University of Manitoba, Canada)

Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room7

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

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

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

○Shuyang Dai[1], Yang Xiang[2], David Joseph Srolovitz[3] （1.Wuhan University, China, 2.Hong Kong University of Science and Technology, Hong Kong, 3.University of Pennsylvania, United States of America）

[SY-I6] The influence of normal stress on the structural transformation and migration of grain boundaries

○Chuang Deng, Mohammad Aramfard （University of Manitoba, Canada）

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room7)

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

Invited

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

We report molecular dynamics simulations and their analysis for grain boundaries vicinal to the Sigma 7 symmetric tilt boundary of the type {1 2 3} in aluminium. When minimized in energy at 0K a grain boundary of this type exhibits nano-facets that contain kinks. We observe that at higher temperatures of migration simulations, given extended annealing times, it is energetically favorable for these nano-facets to coalesce into a large terrace-facet structure. Therefore we initiate the simulations from such a structure and study as a function of applied driving force and temperature how the boundary migrates. We find the migration of a faceted boundary can be described in terms of the flow of steps. The migration is dominated at lower driving force by the collective motion of the steps incorporated in the facet, and at higher driving forces by the step detachment from the terrace-facet junction and propagation of steps across the terraces. The velocity of steps on terraces is faster than their velocity when incorporated in the facet, and very much faster than the velocity of the facet profile itself, which is almost stationary. A simple kinetic Monte Carlo model matches the broad kinematic features revealed by the molecular dynamics. Since the mechanisms seem likely to be very general on kinked grain boundary planes, the step flow description is a promising approach to more quantitative modeling of general grain boundaries.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room7)

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

○Shuyang Dai[1], Yang Xiang[2], David Joseph Srolovitz[3] （1.Wuhan University, China, 2.Hong Kong University of Science and Technology, Hong Kong, 3.University of Pennsylvania, United States of America）

We present a multiscale model to describe the structure and the energetics for various grain boundaires. The model incorporates both the anisotropy elasticity in each grain and the first-principle calculation informed interaction between two grains across the grain boundary, i.e., the generalized stacking-fault energy based upon the disregistry. The force balance between these two contributions determines the structure. We apply this approach to determine the structure and energetics of several twist grain boudnaries and tilt grain boundaries in FCC metals such as Cu, Al and Ni.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room7)

[SY-I6] The influence of normal stress on the structural transformation and migration of grain boundaries

Invited

○Chuang Deng, Mohammad Aramfard （University of Manitoba, Canada）

It is now widely accepted that stress plays important roles on the kinetics of grain boundaries. Past studies on grain boundary kinetics by atomistic simulation mainly focused on those under shear deformation by recognizing that shear coupling is one of the most fundamental modes of grain boundary motion. However, grain boundaries in polycrystalline materials under realistic loading conditions rarely experience pure shear deformation and stresses with both shear and normal components are more common. In this work, we used molecular dynamics simulations to investigate (1) how normal stress would influence the ground state structures of a few types of special CSL grain boundaries and (2) how such structural change would further influence the modes and energy barrier for migration in those grain boundaries.

We found that while both constant and cyclic normal stresses can facilitate the transition in grain boundary structure among its metastable states, the influences of tension and compression are not the same and vary among different types of grain boundaries. It is also found that the macroscopic strain caused in the materials due to the structural transformation in grain boundaries under cyclic stress can be well described by Coble creep, which implies a possible new mechanism of Coble creep that has been overlooked before. Furthermore, the grain boundary structural transformation can either lower or raise the energy barrier for grain boundary migration depending on the grain boundary type, which can be explained by the relative easiness of atomic shuffling in each grain boundary based on their DSC lattice.

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

[SY-I7] Symposium I-7

Chairs: Nicolas Combe(CEMES Toulouse, France), Brandon Runnels(University of Colorado Colorado Springs, United States of America)
Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room7

[SY-I7] Insights into recrystallisation: atomistic simulations of the properties of grain boundaries in heavily deformed material

○Chris P Race （University of Manchester, UK）

[SY-I7] Continuum Dislocation Dynamic Based Grain Fragmentation Modeling for Severe Plastic Deformation in FCC Metals

○Ali Al-Hadi I. Kobaissy[1], Georges Ayoub[2], Mu'Tasem Shehadeh[1] （1.Department of Mechanical Engineering, American University of Beirut, Lebanon, 2.Department of Industrial and Manufacturing Systems Engineering, University of Michigan-Dearborn, United States of America）

[SY-I7] Atomistic Investigation on Interaction of Stress-Assisted Grain Boundary Motion with Crack

○Mohammad Aramfard, Chuang Deng （Univ. Manitoba, Canada）

[SY-I7] **Effect of grain boundary structure on its Dynamic Response using Molecular Dynamics**

○Saryu Fensin[1], Timothy Frolov[2] （1.Los Alamos National Lab, United States of America, 2.Lawrence Livermore National Laboratory, United States of America）

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room7)

[SY-I7] Insights into recrystallisation: atomistic simulations of the properties of grain boundaries in heavily deformed material

Invited

○Chris P Race （University of Manchester, UK）

A critical process in the development of a desirable microstructure in polycrystalline metals is that of recrystallisation, in which new grains of defect-free material nucleate and grow within the defect-laden microstructure of deformed material.

Thus, recrystallisation involves the creation and migration of grain boundaries between pristine and highly defective crystal. The structure and properties of these grain boundaries will be strongly affected by the plastic deformation in the defective grain. Furthermore, the driving force for their migration will be the elimination of the deformation defects. This force will be larger in magnitude and different in character to the driving forces present in other cases of grain boundary migration, such as grain growth. Grain boundary properties under these conditions have, however, received comparatively little attention.

Here we present insights from atomistic models of grain boundaries between cold-worked and defect-free grains which begin to uncover trends in their static and dynamic properties under conditions of recrystallisation.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room7)

[SY-I7] Continuum Dislocation Dynamic Based Grain Fragmentation Modeling for Severe Plastic Deformation in FCC Metals

○Ali Al-Hadi I. Kobaissy[1], Georges Ayoub[2], Mu'Tasem Shehadeh[1] （1.Department of Mechanical Engineering, American University of Beirut, Lebanon, 2.Department of Industrial and Manufacturing Systems Engineering, University of Michigan-Dearborn, United States of America）

In this work, the mechanical response as well as the microstructural features of face-centered cubic (fcc) metals subjected to severe plastic deformation (SPD) are investigated. A multi-scale framework that couples crystal plasticity (CP) scheme with continuum dislocation dynamics (CDD) model is proposed to mimic the loading conditions during Equal Channel Angular Pressing (ECAP) processes. Several aspects of the deformation process have been considered including texture evolution, the evolution of statistically stored dislocations (SSDs) and geometrically necessary dislocations (GNDs), and the fragmentation of the grains and its effect on the overall mechanical response. The framework is applied to a reference volume element (RVE) in which the grains are distributed and assigned a position. Within the model, each grain is allowed to split into 1024 new smaller grains which subsequently lead to strain hardening and grain refinement. The latter is modeled by accounting for the grain-grain interaction, for which the concept of the GNDs is incorporated into the mean free path of the dislocations. GNDs are assumed to be induced by grain boundaries that restrict the free deformation of a grain and result in an increase of stresses leading to the grain size reduction. The grain refinement procedure is triggered when the misorientation threshold between subgrains is exceeded. The calibration of the model parameters is performed using torsion test of pure copper material. The simulations results of generated texture and grain size reduction are in very good agreement with experimental data available in the literature.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room7)

[SY-I7] Atomistic Investigation on Interaction of Stress-Assisted Grain Boundary Motion with Crack

○Mohammad Aramfard, Chuang Deng （Univ. Manitoba, Canada）

Stress-assisted grain boundary motion is a prominent phenomenon in crystalline materials. On the other hand, crack/voids are common features in physical materials, thus the interaction of a moving grain boundary mediated by stress with such features are important to study the microstructural evolution of crystalline materials under severe plastic deformation. In this work three major behaviors are studied using atomistic simulations when a stress-mediated moving grain boundary interacts with crack, i.e., crack healing, crack propagation and sub-grain formation. The underlying macromechanism is described using atomistic configurations for each case and the effect of loading type, i.e., monotonic or cyclic is described. It is shown that metastable phases are the main reason for crack heal-ability of grain boundaries. The effect of material type which is in terms of stacking fault energy is also explored.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room7)

[SY-I7] **Effect of grain boundary structure on its Dynamic Response using Molecular Dynamics**

Invited

○Saryu Fensin[1], Timothy Frolov[2] （1.Los Alamos National Lab, United States of America, 2.Lawrence Livermore National Laboratory, United States of America）

Grain boundaries (GBs) can play an important role in governing the mechanical behavior and damage evolution of a material during both quasistatic and dynamic loading. However, the general consensus of the shock physics community has been that minute details about the GB structure should not affect the response of a material to dynamic loading. In this paper, we present results of molecular-dynamics simulations investigating whether or not small changes in boundary structure are 'recognized' by the shock wave and can in turn affect the spall strength of a material. As a test case, we will study grain boundaries in both Copper and Tungsten with similar orientation relationships but varying local structures. Specifically, we propose to use grand-canonically optimized structures for grain boundaries that retain their ordered structure even at elevated temperatures.

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

[SY-I8] Symposium I-8

Chair: Srikanth Patala(North Carolina State University, United States of America)
Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room7

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

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

[SY-I8] **Grain Boundary Sliding: the best supporting role in ductile localization**

○Alexandre Dimanov[1], Jean Raphanel[1], Michel Bornert[2], Eva Héripré[3], Mathieu Bourcier[1], Ababacar Gaye[2], Alexandre El Sabbagh[1], Wolfgang Ludwig[4], Andrew King[5] （1.LMS, CNRS-UMR7649, Ecole Polytechnique, France, 2.Laboratoire Navier, CNRS-UMR8205, Ecole des Ponts, France, 3.MSSMAT, CNRS-UMR8579, Centrale-Supélec, France, 4.MATEIS, UMR5510, INSA-Lyon, France, 5.SOLEIL Synchrotron, Beam line Psiché, France）

[SY-I8] Polycrystal plasticity with anisotropic grain boundary energy described on the five-dimensional grain boundary space

○Nikhil Chandra Admal[1], Javier Segurado[2,1], Jaime Marian[1] （1.University of California Los Angeles, United States of America, 2.IMDEA, Spain）

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room7)

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

Invited

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

Engineering interest in nanocrystalline (NC) materials has been founded on the potential to improve mechanical properties such as increased strength/hardness, while scientific interest stems from the alternative fundamental mechanisms that are operative. Compared to their coarser-grained counterparts, the influence of interfaces (i.e., grain boundaries (GB)) becomes more significant in NC materials. Current simulation techniques for understanding NC mechanics rely on non-physical microstructures, first-order grain boundary descriptors that poorly capture the complexity of interfacial structure-property relationships, and a lack of quantitative approaches that can accurately capture the specific contribution of different deformation mechanisms. In this study, we propose utilizing higher-order GB descriptors to improve interfacial understanding, while determining polycrystalline behavior through networks connecting bulk and boundary behaviors. We perform atomistic modeling (e.g., Molecular Dynamics) studies of both favored CSL and general high-angle GBs for analyzing empirical and structural descriptors from atomic-scale behavior at the interfaces. These descriptors then aid in our GB network modeling to understand larger-scale polycrystalline behavior by unraveling the complexity surrounding the competition/cooperation between different deformation mechanisms. The importance of choosing physically-based atomistic microstructures and proper equilibration techniques in such simulations are also discussed. Finally, by utilizing continuum-based kinematic metrics, which can resolve the individual contribution of various deformation mechanisms such as GB and dislocation-mediated deformation to the total strain in the material, we help to further unravel the complex microstructural deformation behavior in NC metals.

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room7)

[SY-I8] **Grain Boundary Sliding: the best supporting role in ductile localization**

○Alexandre Dimanov[1], Jean Raphanel[1], Michel Bornert[2], Eva Héripré[3], Mathieu Bourcier[1], Ababacar Gaye[2], Alexandre El Sabbagh[1], Wolfgang Ludwig[4], Andrew King[5] （1.LMS, CNRS-UMR7649, Ecole Polytechnique, France, 2.Laboratoire Navier, CNRS-UMR8205, Ecole des Ponts, France, 3.MSSMAT, CNRS-UMR8579, Centrale-Supélec, France, 4.MATEIS, UMR5510, INSA-Lyon, France, 5.SOLEIL Synchrotron, Beam line Psiché, France）

Viscoplastic deformation of polycrystalline materials conditions many aspects of our everyday life from industrial hot forming of metallic items and durability of engineered structures, to glacier flow or plate tectonics powered by convection of Earth’s mantle rocks. Usually, polycrystalline viscoplastic deformation is largely based on crystal slip plasticity (CSP). However, grain boundary sliding (GBS) may become a dominant mechanism at high temperatures, small grain sizes and low strain rates. Both mechanisms are often considered to act in parallel and to contribute independently to the global behaviour. We considered different classes of polycrystalline materials, such as Silicates, NaCl and Aluminium, combining high temperature rheological investigations and micromechanical testing with *in situ* SEM multi-scale

observations. In the latter case, we performed full field strain measurements, based on digital image correlation (DIC). For NaCl we could perform micromechanical tests *in situ* synchrotron X-ray microtomography and obtain both 2D and 3D strain fields. We show that for all of the considered materials CSP and GBS are not independent, but co-operative. Depending on microstructure and loading conditions, each one may be either the dominant strain cumulative mechanism, or a secondary mechanism, allowing for accommodation of the local strain incompatibilities related to the previous one. Both are necessary to ensure macroscopically homogeneous flow. We show examples of minor but crucial contribution of GBS to ductile localization phenomena and strain propagation throughout the microstructure.

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room7)

[SY-I8] Polycrystal plasticity with anisotropic grain boundary energy described on the five-dimensional grain boundary space

○Nikhil Chandra Admal[1], Javier Segurado[2,1], Jaime Marian[1] （1.University of California Los Angeles, United States of America, 2.IMDEA, Spain）

At high temperatures, grain boundaries are not static entities but can migrate in response to thermo-mechanical forces brought about by temperature, external stresses, and internal microstructure. This gives rise to a wide array of dynamic behavior, including recovery, recrystallization, grain growth, etc.

In this talk, we present a recently developed three-dimensional polycrystal plasticity model driven by a single energy functional that captures both grain boundary (GB) energy and bulk elastic energy in response to plastic deformation. The model represents any arbitrary grain boundary using geometrically necessary dislocations (GNDs), and the GB energy is constructed as a function of the GNDs. Moreover, in contrast to previous phase-field approaches for grain boundary evolution, our model’s energy functional is described on the entire five-dimensional grain boundary space allowing the consideration of both misorientation and inclination in the grain boundary energy.

The model is parameterized using grain boundary energy data from atomistic simulations, after which it is used to simulate the microstructure evolution of polycrystalline samples. The framework is used first to simulate the recrystallization process in a three dimensional polycrystal without external loads. Finally, the deformation of polycrystals under external loads is simulated for a few selected cases.

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

[SY-G1] Symposium G-1

Chairs: Byeongchan Lee(KyungHee Univ., Korea), Keonwook Kang(Yonsei University, Korea)
Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room8

[SY-G1] A systematic method to develop a potential model for harsh environments

○Takuji Oda, Sehyeok Park, Woonghee Cho （Dept. of Nuclear Engineering, Seoul National Univ., Korea）

[SY-G1] Molecular dynamics study of the bulk cascades in W-Re alloy

○Hyunggyu Lee[1], Byeongchan Lee[2], Keonwook Kang[1] （1.yonsei university, Korea, 2.kyung hee university, Korea）

[SY-G1] Defect Energetics in W-Based Transition-Metal Ternary Systems

○Younggak Shin, Byeongchan Lee （KyungHee Univ., Korea）

[SY-G1] A numerical study of channel deformation and fracture in irradiated stainless steel single crystals

○Jean-Michel Scherer[1,2], Samuel Forest[2], Jacques Besson[2], Benoit Tanguy[1], Jérémy Hure[1] （1.DEN-Service d'Etudes des Matériaux Irradiés, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette cedex, France, France, 2.MINES ParisTech, PSL-Research University, Centre des matériaux, CNRS UMR 7633, 63-65 rue Henri Auguste DesbruèresBP 87 91003 Evry Cedex, France, France）

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room8)

[SY-G1] A systematic method to develop a potential model for harsh environments

Invited

○Takuji Oda, Sehyeok Park, Woonghee Cho （Dept. of Nuclear Engineering, Seoul National Univ., Korea）

Molecular dynamics (MD) calculation is an important computational method for materials science and engineering. To obtain meaningful results from MD simulations for harsh environments, one has to prepare a quality potential model that works appropriately not only in equilibrium states but also in non-equilibrium states. We have recently developed a systematic method to construct (i) two-body potentials [T. Oda, W.J. Weber, H. Tanigawa, Comp. Mater. Sci. 111 (2016) 53] and (ii) embedded-atom method (EAM) potentials [T. Oda, submitted]. In this method, potential functions are expanded with cosine/sine series in reference to energies, forces and stresses evaluated by first-principles calculations. In the present study, using this method, we aim to construct potential models of a metal (bcc-Fe) and a metal oxide (Li_2O) for radiation environments. For this aim, results of first-principles molecular dynamics calculations of several atomic collision events are included in the reference data. MD simulation results with the constructed potential models show a reasonable agreement with available experimental data on fundamental material properties and threshold displacement energies. It is indicated that the method can effectively construct a potential model for MD simulations of harsh environments.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room8)

[SY-G1] Molecular dynamics study of the bulk cascades in W-Re alloy

○Hyunggyu Lee[1], Byeongchan Lee[2], Keonwook Kang[1] （1.yonsei university, Korea, 2.kyung hee university, Korea）

Tungsten is widely used as a facing material, because it has a high thermal conductivity and low sputtering yield. However, under the neutron irradiation, pure tungsten transmutes into the Re and Os. This causes degradation of material properties due to the formation of defect clusters, such as precipitates, that caused by irradiation. Therefore, it is important to understand the formation mechanism of defect clusters for preventing the degradation of material properties. In this study, for knowing the formation mechanism of defect clusters, we conducted irradiation simulation of bulk W-Re alloy using molecular dynamics simulation. To describe the neutron irradiation, we choose the certain atom that is hit by neutron, which is called PKA (Primary Knock-on Atom) and shot the PKA with certain kinetic energy. We analyze the defects formation of bulk system as changing the initial energy of PKA.

Acknowledgement

This research was supported by Nuclear Fusion Research Program through the National Research Foundation of Korea(NRF) (2017M1A7A1A01016221)

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room8)

[SY-G1] Defect Energetics in W-Based Transition-Metal Ternary Systems

○Younggak Shin, Byeongchan Lee （KyungHee Univ., Korea）

W has been considered as a potential core element for plasma facing material of fusion reactors for ITER thanks to its outstanding high-temperature properties. However, studies so far on W and W-based binary alloys show precipitation and defect clustering under neutron irradiation. In this talk, we report the first principles calculations of the defect energetics in ternary W alloys. W-Ta-Re systems are chosen for extensive calculations on interstitial defect structures around solute atoms.

Overall, as in pure W or W binary alloys such as W-Re, the most preferable defect type is found to be the bridge interstitial, followed by <111> interstitials. With negative solute-solute binding energy, Ta and Re atoms prefer to make a solute pair in the system and the solute pair strongly attracts W self-interstitial atom, forming a solute-interstitial complex. The binding between a Ta-Re solute pair and a W self-interstitial atom can be stronger in this ternary alloy than in binary systems, and plays a role in slowing down the W interstitial diffusion as a primary dissociation barrier. The defect energetics in the alloys can be understood as the combined results of both strain-relief effect and electronic effect, but the former, which is related with atomic size of elements and local pressure felt by each atom in lattice, seems dominant.

To summarize, the defect complexes in W-Ta-Re alloys are expected to trap W self-interstitial atoms, preventing self-interstitial atoms from escaping to the surface or grain boundary. The reduction in the number of disappearing self-interstitial atoms increases the odds for Frenkel defects to annihilate, reducing residual void concentration and hence void formation. It is also expected that, at elevated temperature, the rise in configuration entropy increases the interaction energy between solute pair and self-interstitial atom, and hence further slows interstitial migration.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room8)

[SY-G1] A numerical study of channel deformation and fracture in irradiated stainless steel single crystals

○Jean-Michel Scherer[1,2], Samuel Forest[2], Jacques Besson[2], Benoit Tanguy[1], Jérémy Hure[1] （1.DEN-Service d'Etudes des Matériaux Irradiés, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette cedex, France, France, 2.MINES ParisTech, PSL-Research University, Centre des matériaux, CNRS UMR 7633, 63-65 rue Henri Auguste DesbruèresBP 87 91003 Evry Cedex, France, France）

Stainless steels are widely used as structural materials for nuclear core internals. Due to their proximity with the nuclear fuel, these materials are subjected to high level of irradiation doses. In the last decades, irradiation effects on structural materials’ mechanical properties have been heavily investigated in order to ensure structures’ reliability over nuclear plant lifetime. Irradiation induced defects - such as Frank dislocation loops and nanocavities - can lead to significant mechanical properties changes, as for example a significant hardening due to pinning of dislocations on defects. Under mechanical loading, gliding dislocations may incorporate sessile defects lying in their gliding plane, leaving behind a reduced defect density path. These zones, typically bands or channels of 10-100 nm width, beeing therefore softened by the "defects cleaning” , may localize strain and lead to highly heterogeneous deformation at the grain scale. This process is called dislocation channelling. A peculiar fracture mode called channel fracture is oberved in austenitic stainless steels irradiated at high temperature to high doses, leading to transgranular facets on fracture surfaces. It has been hypothesized [1] that channel fracture is due to nanovoids coalescence in dislocation channnels. Channel fracture is therefore assessed numerically in this study using a strain gradient crystal plasticity model that has been developped in order to take into account irradiation defect densities in the hardening/softening behaviour of the material and that has been implemented in a Finite Element solver [2]. Such model allows to regularize strain localization, and is used to model dislocation channelling. Single crystal porous unit-cells are subjected to simple shear, and the effect of void sizes and dislocation channels widths are systematically investigated. Numerical results are finally used to assess the hypothesis proposed in [1] regarding channel fracture in irradiated stainless steels.

[1] Margolin B. et al. (2016) The radiation swelling effect on fracture properties and fracture mechanisms of irradiated austenitic steels. Journal of Nuclear Materials
[2] Ling C. et al. (2017) Void growth and coalescence in triaxial stress fields in irradiated fcc single crystals. Journal of Nuclear Materials

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

[SY-G2] Symposium G-2

Chairs: Seunghwa Ryu(Korea Advanced Institute of Science and Technology, Korea), Keonwook Kang(Yonsei University, Korea)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8

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

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

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

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

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

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

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

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

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

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

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8)

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

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

Aluminum honeycombs are widely used as sandwich cores in the protective component in transport industry. For example, they are involved in the bird strike shielding as well as in the crashworthiness design, etc. Under impact loading, testing results showed a significant enhancement of the out-of-plane crushing strength of honeycombs with respect to the quasi-static case, which cannot be explained by the rate sensitivity of aluminum alloy.

This paper firstly presents the quasi-static and impact testing results for a series of aluminium honeycombs of different cell sizes (3003 and 5052 alloys). A significantly different strength enhancement of 3003 honeycombs is found from the 5052 ones. In order to understand and model this strength enhancement, a comprehensive numerical investigation with rate insensitive constitutive laws is performed to reproduce the experimental results for different cell size/wall thickness/base materials. In fact, due to the lateral inertia effect under impact buckling, larger strain under impact loading than quasi-static case in the element nears intersectional line is observed. Different ratios of the strain hardening stress over the yield stress of the 3003 alloy from the 5052 alloy lead to the different honeycomb strength enhancements. Finally, aluminum 5052 and 3003 honeycombs are studied under combined shear-compression loading. It was focused on the interaction between the additional shear loading and the lateral inertia effect under the impact loading. It was found that the expansion of the crush envelopes from the quasi-static loading to the dynamic loading was almost homogeneous for the two honeycombs.

Hou B., Zhao H., Pattofatto S., Liu J.G., Li Y.L., 2012, Inertia effects on the progressive crushing of aluminium honeycombs under impact loading, Int. J. Solids &Struct.,, 49 (19-20), 2754-2762.
Hou B., Pattofatto S., Li Y. L., Zhao H., 2011, Impact behavior of honeycombs under combined shear-compression, Part II Analysis, Int. J. Solids &Struct.. 48, 698-705

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8)

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

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

The mechanical issues on high capacity electrode materials, such as silicon, tin, and silicon oxide, prevents their usage for lithium ion batteries. So, the oxides (i.e. silicon dioxide) are the prevalent materials used for a high-expected capacity and strong mechanical stability during cycles. Although tremendous efforts have devoted to the study of the electro-chemo-mechanical behaviors of high-capacity electrode materials, the mechanical behavior of amorphous SiO_2 during electro-chemical reaction remains largely unknown. Here we systematically investigate the inelastic stress evolution, the electronic structure and the mechanical deformation of lithiated silicon dioxide through first-principles computation and finite element method. The structural and thermodynamics analysis was performed to predict electrochemistry characteristics Si and Si-O system. The mechanical strength and brittle behavior of SiO2 due to strong Si-O bonds are also compared with Si. Although both Si and SiO2 experience mechanical softening during lithiation, the clearly distinguishable relaxation kinetic of SiO_2 inducing deviatoric inelastic strains due to mechanical constraints is found by density functional theory calculation. These results would provide fundamental perspectives on the chemo-mechanical behavior of silicon and silicon oxide electrode for the practical use.

ACKNOWLEDGMENT
This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (No. 2017R1C1B5017837).

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8)

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

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

Coatings suffer dramatic deterioration and premature damage in the deep-sea environment, in sharp contrast to the good protective performance in typical marine environments. Hydrostatic pressure (HP), which varies with ocean depth, has pronounced impact on coating performance when compared with other factors, such as oxygen level and pH value. The idea that loss of wet adhesion is the first step towards coating failure seems to be raising some controversy, with some researchers suggesting that the loss of adhesion results from the pressure relief process in the experiment rather than from hydrostatic pressure itself. AHP decreased the protective properties of coatings more rapidly than HP via a “ push-and-pull” effect, which promotes bubbles formation at the interface between coatings and base metal.

Compared to other simulation methods, the finite element method (FEM) is capable of providing a multi-physical field to solve complex engineering problems more effectively. The interface is most susceptible to corrosion and the coating failure can be affirmed when the corrosion products are visible on there.

In this study, we attempt to develop a model of the growth of a bubble and the change of the stress distribution at the coating/substrate interface under AHP by means of FEM. The results show that the impacts of alternating hydrostatic pressure and hydrostatic pressure on the interface were compared with a precondition of bubbles inducing the coating failure.

1. Hydrostatic pressure cannot mechanically destroy the coating/metal interface because it acts as a compressive stress on the dry bubbles. If the bubbles turn into wet, the pressure loaded on the bubble will disappear.

2. Alternating hydrostatic pressure can provide tensile stress on the wet bubbles during every immersion period, so it accelerates disbonding of the coating.

3. The maximum stress on the bottom of wet bubbles is able to be minimized to less than the stable adhesion value if the lag time is large enough. In this case, alternating hydrostatic pressure cannot accelerate disbonding any more. The lag time will be different if the period of alternating pressure is changed. Thus, the lag time of a coating should be considered when it is designed to serve under alternating hydrostatic pressure.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8)

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

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

Designing high energy-efficiency structural materials with superior mechanical properties is a key challenge for scientists and engineer. Among these properties, strength versus mass density and strength versus ductility are amongst the most important factors that affect component design, and thus structure weight. Ideal structural materials are the ones that may retain high strength with low mass density and excellent ductility. However, current state-of-the-art materials have a drastic tradeoff between these properties. In this work, a multiscale modeling approach is developed and used to design a new class of high-strength-ductility material system. It is shown that by integrating the effects of nanoparticle, nanolaminate and gradient structure on strength and ductility, it is possible to design and manufacture 3D-architectured lightweight metamaterial systems. The system is made of interconnected microscale metallic ligaments reinforced by nanolaminate metallic layers and have superior mechanical properties (strength-density, strength-ductility) compared to their bulk counterparts.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8)

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

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

We propose a method for efficiently coupling the finite element method with atomistic simulations like molecular dynamics or kinetic Monte Carlo. Our method enables to dynamically build an unstructured mesh with optimized density that follows the geometry defined by atomistic data. On this mesh, multiphysics problems can be solved to obtain distribution of physical quantities of interest, which can then be fed back to the atomistic system. The simulation flow is optimized to maximize computational efficiency while maintaining good accuracy.

We use this method to simulate the evolution of nanostructures under high electric field. By solving Poisson equation, we obtain the 3D distribution of electric field around the nanostructure. Using the field, we calculate electron emission currents, surface and space charge and electrostatic forces for surface atoms. By

taking Joule and Nottingham heating into account and solving 3D heat equation, we also obtain atomistic velocity perturbation.

Our method has shown remarkable overlapping with an analytical solution and has proved to be efficient and robust enough to simulate large-scale thermal runaway processes. Using those simulations, we demonstrated for the first time the disintegration of Cu nanotip in extreme field conditions. This process is widely believed to lead to the formation of plasma and cause vacuum arcing in high gradient structures.

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

[SY-G3] Symposium G-3

Chairs: Seunghwa Ryu(Korea Advanced Institute of Science and Technology, Korea), Keonwook Kang(Yonsei University, Korea)

Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8

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

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

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

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

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

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

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

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

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

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

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8)

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

Invited

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

Some special numerical techniques are desired when simulating the behavior of matters in extreme conditions, and in particular, the chemical-thermal energy release from the combustion of explosives and propellants must be carefully addressed when capturing the high strain rate deformation of metals and polymeric binders interacting with the energetic elements of the system. In this talk, selective research accomplishments associated with modeling of both energetic and inert matters exposed to high pressure conditions are discussed. Models are developed for addressing the problems of shock-induced ignition and multi-scale hot spot initiation of metalized energetic components from the shock compression system.
To do so, one needs to adapt a stable interface tracking algorithm for severely transient fluid-structure interaction problems. We have developed a multi-material hydrodynamic shock physics code with a hybrid particle level set method for simulating the shock induced chemical reaction of energetic materials and volumetric deformation of metals. The experimental measurements are obtained to validate the simulated results presented in this talk.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8)

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

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

Shock compression is an effective means of probing the mechanical and thermodynamic properties of solids. The majority of shock compression studies to date have reported principal Hugoniot curves, for which the material ahead of the shock is conveniently chosen to be in the quiescent state ($P = 0$ and $u = 0$). However, studies of branched Hugoniots (that emanate from non-quiescent states) are relatively rare, although branched Hugoniots are equally important for accurate description of shock wave physics involving interaction. In this talk, we discuss a sophisticated modeling scheme for shock hydrodynamics, accompanied by a full deck of principal and branched Hugoniots obtained with molecular dynamics computations. The system is a single-crystalline aluminum impacted at velocities ranging from 0.1 to 3.0 km/s, as described in the companion paper. Simulations show that branched Hugoniots should be used for accuracy in predictions, especially when there are material boundaries causing reflection and interaction of shocks.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8)

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

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

Two different embedded-atom method(EAM) potentials were used in single crystalline FCC Al : WKG (J.M. Winey, Alison Kubota, and Y.M. Gupta), and FWYD (Qin-Na Fan, Chong-Yu Wang, Tao Yu, Jun-Ping Du). A 300k single crystalline Al system is inflicted planar shock at an adiabatic condition of 0.1 to 3.0 km/s. Pressure, volume and temperature profiles are obtained after shock as impact velocity. We extract the principle Hugoniot curve in averaged value of profiles. Branch points are selected on the principle Hugoniot curve. We made an isentropic equilibrium system that approximates branch points. The isentropic equilibrium system is inflicted planar shock to impact at an adiabatic condition of 0.1 to 3.0 km/s to obtain the branched Hugoniot curve. It is observed that either stacking fault formation or phase transformation from FCC to HCP or FCC to BCC occurs depending on the potential model. This study shows how the branched Hugoniot curve of single crystalline aluminum differs from the principle Hugoniot curve in strong shock. In addition, by analyzing the differences according to potential models, we show that the potential model must be carefully selected in the strong shock simulation.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8)

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

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

In this work we study shock-induced plasticity in Mo single crystals, using a method to relate information of dislocations from the atomic to the continuum scale [1]. We use molecular dynamics (MD) simulations to simulate the shock propagation along the <110> crystal orientation. Shock waves with compressive axial stresses of about 120 GPa are simulated. These stresses induce homogeneous nucleation of dislocations but barely lead to a phase transition. Using the Dislocation Extraction Algorithm (DXA) and the newly developed Discrete to Continuum (D2C) technique, the atomistic information is turned into continuous dislocation fields. In conjunction, we extract from the MD simulations thermo-dynamical macroscopic quantities such as macroscopic strain, density, temperature and stress tensor during the propagation of the shock wave. Correlating the stress evolution and the evolution of the continuous dislocation fields, we analyze the attenuation of the sharp elastic jump at the front of the shock wave and the plastic deformation behind it. Analyzing the MD simulations, we show that the initially an elastic precursor wave overshoots the dislocation nucleation stress, after which dislocations on a specific group of slip planes (which we denote as out-of-plane) are nucleated, slightly lagging behind the elastic front. As dislocations are nucleated in the out-of-plane direction, the resolved shear stress on these planes is relaxed, but the principal lateral stresses increase. This leads to an increase in the shear stresses on a plane parallel to the shock wave (denoted as in-plane), resulting in an additional retarded front of dislocation nucleation on planes parallel to the shock front. Finally, the two-stage process of plasticity results in close to isotropic stress state. Interestingly, the DXA-D2C analysis shows that non-zero contributions in the Kroener-Nye tensor appear only in the first stage of plasticity, right behind the shock front. The MD simulation results are employed to calculate the dislocation densities on specific slip planes and the plastic deformation behind the shock, bridging the gap between the information on the atomic scale and the continuum level.

[1] Kositski, et al. Computational Materials Science 149 (2018): 125-133.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8)

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

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

Graphene and other 2D materials with superior mechanical properties have been widely proposed as effective reinforcement for stronger and tougher nanocomposites [1] to realize structures capable to sustain extreme mechanical conditions, such impact loads. However current studies are limited to constitutive properties in the quasi-static regime [1] or to the impact properties of stand-alone 2D materials armors [2] without considering the behavior of the resulting nanocomposite under real hypervelocity shock conditions, where second order effect occur, such as elastic-plastic shock wave propagation or induced phase transformation. We present a molecular dynamics (MD) simulation study on shock behavior of graphene-reinforced single crystal copper (Cu), investigating the role of graphitic inclusion on the shock Hugoniot of such nanocomposites. Our results give insights of the failure behavior of graphene-metal nanocomposite under hypervelocity shock load and the consequent implications to their engineering applications.

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[1] Y. Kim, J. Lee, M. Yeom, J. Shin, H. Kim, Y. Cui, J.W. Kysar, J. Hone, Y. Jung, S. Jeon, S. Han. Strengthening effect of single-atomic-layer graphene in metal-graphene nanolayered composites. *Nature Communications* 4:2114, 2013.
[2] S. Signetti, S. Taioli, N.M. Pugno. 2D Materials Armors Showing Superior Impact Strength of Few Layers. *ACS Applied Materials &Interfaces* 8:40820-40830, 2017.

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

[SY-G4] Symposium G-4

Chairs: Keonwook Kang(Yonsei University, Korea), Byeongchan Lee(KyungHee Univ., Korea)
Wed. Oct 31, 2018 4:00 PM - 4:45 PM Room8

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

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

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

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

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

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

(Wed. Oct 31, 2018 4:00 PM - 4:45 PM Room8)

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

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

Despite the significance of surface effects on the deformation behaviors of small-scale metallic glasses, systematic investigations on surface states are lacking. In this work, by employing atomistic simulations, we characterize the distributions of local inhomogeneity near surfaces created by casting and cutting, along with internal distributions in pristine and irradiated bulk specimens, and investigate the effects of inhomogeneity on the mechanical properties. The cast surface shows enhanced yield strength and degrees of shear localization, while the cut surface shows the opposite effects, although the fraction of vibrational soft spots, known to indicate low-energy barriers for local rearrangement, is high near both surfaces. Correspondingly, plastic deformation is initiated near the cut surface, but far from the cast surface. We reveal that improved local orientational symmetry promotes strengthening in cast surfaces and originates from the effectively lower quenching rate due to faster diffusion near the surface. However, a significant correlation among vibrational soft spots, local symmetries, and the degree of shear localization is found for the pristine and irradiated bulk materials. Our findings reveal the sensitivity of the surface state to the surface preparation methods, and indicate that particular care must be taken when studying metallic glasses containing free surfaces.

(Wed. Oct 31, 2018 4:00 PM - 4:45 PM Room8)

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

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

Voronoi tessellation technique, or also called as Voronoi analysis, has been quite widely adopted to describe the internal structure of materials from molecular level such as short-range order of icosahedra on metallic glasses to centimeter-order powder level such as occupied volume on powder packing. Especially, Voronoi tessellation technique is applied to the investigations by molecular dynamics or discrete element method. In the ordinary Voronoi tessellation technique, a face is placed halfway between equal-sized atoms or particles. However, as the size of particles or atoms in single material are not same, bisection cannot depict the exact plane to represent a convex polyhedron including an atom or a particle. Moreover, packed particles in an vessel usually has a Gaussian particle size distribution for natural powders and a Rosin-Rammler particle size distribution for pulverized powders. It is not just a problem for size distribution. It makes a huge difference on estimation of occupied volume and number of faces by atoms or particles. Therefore, we suggest an alternative way, Radical Plane Method, to solve these problems in this paper. It shows that the error of results could reach up to 60% differences.

(Wed. Oct 31, 2018 4:00 PM - 4:45 PM Room8)

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

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

The hydrated cement paste has complex microstructures. The pore and solid phase distribution characteristics within microstructures affect the material responses significantly. Material microstructure and its responses have been correlated with porosity [1]. However, porosity might not be sufficient to describe the complex microstructures. In this study, the relation between microstructure characteristics and material properties is investigated using a statistical method. To extract the microstructural characteristics of cement paste, micro-CT images are used. Pore and solid phase are separated from micro-CT images using the Powers’ model. A lineal-path function [2], one of the low-order probability functions, is selected for estimating the microstructure characteristics. Particularly, the area of lineal-path function [3] is used as a quantitative parameter related to the material property in this study. Virtual specimens obtained from synchrotron micro-CT are used to evaluate material mechanical properties. The phase field fracture model is applied to evaluate stiffness and strength of cement paste with complex microstructures. From this study, it is concluded that the area of lineal-path function has a potential to be an alternative parameter for correlating material characteristics and properties.

[1] C. Miehe, M. Hofacker, F. Welschinger, A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits, Comput. Meth. Appl. Mech. Eng. 199 (2010) 2765-2778.
[2] B. Lu, S. Torquato, Lineal-path function for random heterogeneous materials, Phys. Rev. A 45 (1992) 922-929.
[3] T. S. Han, X. Zhang, J. S. Kim, S. Y. Chung, J. H. Lim, C. Linder, Area of lineal-path function for describing the pore microstructures of cement paste and their relations to the mechanical properties simulated from μ-CT microstructures. Cem. Concr. Compos. 89 (2018) 1-17.

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

[SY-H3] Symposium H-3

Chair: Hansohl Cho(Los Alamos National Laboratory, United States of America)
Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room9

[SY-H3] Polydomain liquid crystal elastomers1

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

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

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

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

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

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room9)

[SY-H3] Polydomain liquid crystal elastomers1

Invited

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

Liquid crystal elastomers are rubbery solids with liquid crystal mesogens incorporated into their main chains. They display an isotropic to nematic phase transformation accompanied by a large spontaneous deformation. Depending on how these liquid crystal elastomers are synthesized, they can either be a mono domain (uniform liquid crystal order) or polydomain (nonuniform liquid crystal order). This talk will describe various phenomena and modeling questions related to the effective behavior of polydomain liquid crystal elastomers1

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room9)

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

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

Because of their emissions free of carbon dioxyde, polymer electrolyte fuel cells (PEFCs) are of great interest for energy production respectful of the environment. The transport of charges between the electrodes of the fuel cell is insured by a hydrated polymer membrane such as perfluorosulfonic acid (PFSA) membrane. The durability of the fuel cell is still limited by the chemical and mechanical degradation of the polymer membrane after cycles of utilization. This work focuses on the study of the mechanical behavior of PFSA membrane at nanoscale. The understanding of the relation between structure and mechanical properties is the key point to improve the resistance of the membrane against mechanical degradation.

Molecular Dynamics (MD) simulations are performed using a Coarse-Grained model to generate samples of PFSA membranes. The results obtained from structural characterization are compared with data from previous atomistic models and experiments. After validation of the nanostructures, mechanical tests are performed on the hydrated polymer membrane. With an increasing level of hydration, the results for elastic properties are in good agreement with experimental values and a similar trend as experiments is observed for early plastic behavior. The computation of the local mechanical properties of the samples allows to discuss the void nucleation and the influence of water content on the rupture behavior.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room9)

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

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

We employ a novel coarse-graining approach[6], to study star-chain mixtures[1-4], in the limit of long chains. The coarse-grained approach is based on the calculation of the effective interaction between a star polymer and a short chain of length N_c =10 at infinite dilution. A multi-blob-like approach is then employed to coarse-grain chains of arbitrary length N_c . We study mixtures of star polymer and linear chains in the protein limit, i.e. when $q = R_h^c/R_h^s > 1$. We find that the addition of linear chains makes the star fluid more structured, confirming experimental observation obtained through rheological measurements.

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[6] Locatelli, B.Capone and C.N. Likos. Journal of Chemical Physics (2016)

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

[SY-H4] Symposium H-4

Chair: Meredith Silberstein(Cornell University, United States of America)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room9

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

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

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

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

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

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

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

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

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room9)

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

Invited

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

Liquid-crystalline elastomers (LCEs) are soft stimuli-responsive materials that exhibit remarkable mechanical and optical properties. LCEs consist of stiff mesogens, bound in a network of flexible polymer chains, which can self-organize into crystalline order while retaining liquid-like properties. The directional ordering of the mesogens changes in response to external stimuli and the director coupling between the mesogens and network chains brings about unusual behaviors. These include large reversible actuation in response to temperature or light and soft-elasticity. LCEs also exhibit enhanced dissipation behaviors, including a high *tan delta* 0.5-1.0 for wide range of frequencies and temperatures, spanning the glass and nematic transition temperatures, and large hysteresis in the stress response that increases with the strain rate [1]. We hypothesize that the enhanced dissipation behavior arises from the relative motions of the mesogens within the network and set out to measure the effect of mesogen ordering and network orientation on the enhanced dissipation behavior of LCEs. Experiments were performed to measure the rate-dependent hysteresis and frequency dependent dynamic properties for main-chain LCEs in the nematic state with different network structures, including an unoriented and macroscopically isotropic polydomain as well as monodomains with different degrees of mesogens and chain alignment. Oriented monodomains with an aligned or unaligned network can be synthesized by applying a second-stage crosslinking or exchangeable bond reaction to a stretched LCE sample. In this presentation, I will briefly describe the experimental methods, then compare the dissipative behavior of the different network structures, and discuss how the results will be applied to develop a rate-dependent constitutive model for the main-chain LCE networks.

[1] A. Azoug, V. Vasconcellos, J. Dooling, M. Saed, C. M. Yakacki and T. D. Nguyen (2016) *Polymer* 98:165-171.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room9)

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

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

Polymers are largely used in everyday life; however, their large strain behavior is still not well understood because of the complexity of the mechanisms involved in their deformation. To improve the current knowledge on these materials, extensive experimental and theoretical researches have been performed leading to development of constitutive numerical models to predict their large strain behavior. Most of models based on polymer physics have been developed for amorphous polymers. The few ones predicting the mechanical behavior of semi-crystalline polymers do not consider the important evolution of microstructure occurring during the plasticity. This is especially true for ultra-high molecular weight semi-crystalline (UHMWSC) polymers. Because their microstructure exhibits very long macromolecular chains, one chain belongs at the same time at the crystal network and macromolecular network. During the plastic deformation of the polymers, fibrillation process occurs leading to the progressive collapse of the crystalline network and inducing strong variations in the material mechanical properties. Thus, to accurately predict the mechanical behavior of UHMWSC polymers, the mechanical coupling between crystallites and fibrils and its evolution during the deformation has to be taken into account. From the expression of the mechanical coupling for the elastic modulus given by Humbert et al. [1] (non-parallel/non-series configuration), Deplancke et al. [2] developed a one-dimensional model for the prediction of the mechanical behavior of Ultra High Molecular Weight PolyEthylene (UHMWPE). However, to extend its possible range of applications, transformation into a three-dimensional model is needed. Therefore, we have developed a 3D model which take into account the evolutive mechanical coupling, between crystals and fibrils, as a function of the deformation. The model is based on series configuration with consideration of the crystal ratio in the definition of the deformation gradients. Good agreement is found between the experimental results and 3D numerical predictions during loading and unloading.

[1] Humbert et al., *Polymer* **52** (2011) 4899-4909

[2] Deplancke et al., on going

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room9)

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

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

Matrix-free polymer-grafted nanocrystals, called assembled hairy nanoparticles (aHNPs), can significantly enhance the thermomechanical performance of nanocomposites by overcoming nanoparticle dispersion challenges and achieving stronger interfacial interactions through grafted polymer chains. However, effective strategies to improve both the mechanical stiffness and toughness of aHNPs is lacking given the general conflicting nature of these two properties and the large number of molecular parameters involved in design of aHNPs. Here, we propose a computational framework that combines multi-response Gaussian process metamodeling and coarse-grained molecular dynamics simulations to establish design strategies for achieving optimal mechanical properties of aHNPs within a parametric space. Taking poly(methyl methacrylate) grafted to high-aspect ratio cellulose nanocrystals as a model nanocomposite, our multi-objective design optimization framework reveals that the polymer chain length and grafting density are the main influencing factors governing the mechanical properties of aHNPs, in comparison to the nanoparticle size and the polymer-nanoparticle interfacial interactions. In particular, the Pareto frontier marking the upper-bound of mechanical properties within the design parameter space can be achieved when the weight percentage of nanoparticle is above around 60% and the grafted chains exceed the critical length scale governing transition into the semi-dilute brush regime. We show that theoretical scaling relationships derived from the Daoud-Cotton model capture the dependence of the critical length scale on graft density and nanoparticle size. Our established modeling framework provides valuable insights into the mechanical behavior of these hairy nanoparticle assemblies at the molecular level and allows us to establish guidelines for nanocomposite design.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room9)

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

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

Extrusion in fused filament fabrication is typically fast enough to produce significant chain alignment that may change the weld strength of 3D printed objects in several ways. Some studies suggest that alignment may enhance interdiffusion because of the entropic force driving chains towards unaligned conformations or by reducing entanglement density. Alignment of strong backbone bonds along the interface may also change the mechanical properties of material near the joint. As part of a multiscale study of 3D printing, we have used molecular dynamics simulations of a generic polymer model to examine the effect of alignment on the dynamics of welding and evolution of weld strength. Entropy drives chain retraction in the tube, but this does not speed interdiffusion since the tubes are aligned along the interface. There is also no indication of accelerated interdiffusion due to entanglement loss. The ambiguities in recent real space methods for identifying entanglements will be discussed. Alignment does reduce the strength of bulk material adjacent to the weld. At intermediate times this greatly enhances weld strength by moving failure away from the interface. The dependence of the bulk strength on alignment is presented for different thermal histories.

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

[SY-H5] Symposium H-5

Chair: Alexey Lyulin(Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands)
Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room9

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

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

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

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

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

○Sumit Basu （Indian Institute of Technology Kanpur, India）

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

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

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room9)

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

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

Polymeric foams materials can have various applications in engineering. We consider in this work the effect of the foam microstructure in the homogenized response of a random 3D structural polymeric foam under high dynamic mechanical loading conditions (shock). In the analysis, the microstructure of the foam is extracted from 3D computed micro-tomography. The mechanical response of the solid part of the foam is described in terms of deviatoric and pressure response. Using Direct Numerical Simulations (DNS), Finite Element Method (FEM) and the concepts of Micromechanics the average foam response to shock is determined. The results are compared with the 1D-shock equations for the homogenized case to determine the effect of fluctuating fields of physical quantities due to the randomness of the foam microstructure.

LA-UR-18-22612

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room9)

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

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

Crystalline thermoplastic polymers have a complicated hierarchical structure consisting of lamellae of amorphous phases with a random coil structure and crystalline phases in which molecular chains are regularly arranged. The lamellae grow radially repetition of secondary nucleation on a surface of growing lamellae and spherulite structures are generated. Peculiar mechanical characteristics of the crystalline thermoplastic polymers, such as nonlinear elasticity, strain softening after yielding, propagation of necking, and orientation rehardening cannot be seen in the case of metals. Mechanical properties of crystalline thermoplastic polymers depend on the complicated microstructures, and the microstructures varies depending on molding conditions. A theoretical model predicting the microstructure and reproducing the mechanical properties are expected in the field of industrial CAE to enhance formability and reliability of the crystalline thermoplastic polymers. Phenomenological models on macroscopic crystallinity or crystallization rate are popular in terms of industrial availability. Such models cannot investigate effects of sizes, shapes, and distribution of spherulites. In this study, we construct a model expressing generation of spherulite structures for prediction of microstructures of crystalline thermoplastic polymers depending on thermal conditions. A spherulite growth are represented by initial nucleation in an amorphous phase and secondary nucleation on surfaces of spherulites. Rates of the both nucleation are identified by experimental observations of spherulites growth under different thermal conditions. Monte Carlo simulations are performed using the constructed method to reproduce the generation and growth of spherulites in an amorphous phase. In addition, we evaluate effects of crystallization temperature on the nucleation rate and the growth rate by comparison of experiment and analysis results.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room9)

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

○Sumit Basu （Indian Institute of Technology Kanpur, India）

Polymers, by virtue of being synthetic, microscopically tailorable and light materials, are finding uses in challenging new technological situations. These new applications, involving high temperatures, harsh environments, impact, sustained dead loading and others, often demand changes in the macromolecular architecture. The ability to predict the effects of an architectural alteration on the ultimate mechanical behaviour of a bulk polymer is therefore, useful. Coarse grained molecular dynamics provide a route to conducting large and long simulations to establish structure property relationships in these materials. However, a wide variety of coarse graining methodologies exist and their suitability for obtaining mechanical properties needs to be systematically established before they can become effective predictive tools. In this talk, we will focus on our experience with coarse grained molecular dynamics simulations on long chained and crosslinked polymers. In particular, we will discuss, coarse graining strategies that rely on Boltzmann inversion based techniques for calibrating bonded interactions, and a variety of heuristic techniques targetting specific physical properties for the non-bonded. We will highlight the problems associated with simultaneously targetting multiple end properties like density, total energy and atomic virial. Moreover, the mismatch in time scales between detailed atomistic and coarse grained simulations and their influence on the rate dependent behaviour of properties like the glass transition temperature and uniaxial stress-strain response will also be discussed. Finally, we will demonstrate a few case studies on polystyrene and a group of crosslinked polyimides to show that coarse grained molecular dynamics simulations of polymers have good predictive capability and sometimes can provide useful insights into material behaviour.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room9)

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

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

Non-covalent cross-linking interactions such as metal ligands can be used to tailor stiffness and structure of linear polymers while enabling interesting features like self-healing, energy dissipation, and extended stretching capability. Here we present a novel system of copper(II) carboxylate bonds used to crosslink a low Tg acrylic backbone. These crosslinks behave in a covalent manner to form novel materials with increased stiffness, strength, and dissolution resistance, and decreased ductility. It was found that substitution of the copper cation with different ligands imparts a dynamic nature to the crosslinks, thereby enabling dissolution and regeneration of the initial linear polymer. These ligands also strongly influence behavior in the solid-state polymer, increasing ductility with minimal stiffness and strength reduction, and enabling self-healing behavior. The polymer was characterized under monotonic uniaxial tensile loading at different temperatures and strain rates. This experimentally observed mechanical behavior is then considered in the context of topological and mechanochemical elastomer models. The mechanochemical model highlights how modulation of the dynamic cross-link strength within an otherwise linear elastomer can modulate bulk mechanical behavior.

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

[SY-H6] Symposium H-6

Chair: Alexey Lyulin(Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands)

Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9

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

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

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

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

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

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

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

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

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

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

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9)

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

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

Filler morphology, radius, and strength of the filler-polymer interaction impact the physical properties of filled rubber. It is crucial to understand relationships between them so as to improve tire performances. Four large-scale coarse-grained molecular dynamics models were created. The first model is a reference model in which filler particles are distributed in a lattice pattern. The second model is an aggregated model including a non-homogenous filler distribution. The third model is a small particle size model in which small particles are distributed with identical morphology and volume fraction with the reference model. The forth model is a weak interaction model. The polymer-filler interaction is weaker than the reference model, even though the morphology and the particle size match the reference model.

Comparing stress-strain curves, we confirmed that effects of them which are observed in experimental results; filler aggregates, small particles, and strong interaction make modulus and hysteresis greater, were reproduced qualitatively. Measuring a polymer density distribution and a change of polymer chains bridging fillers, it was found that an increase of polymer density around fillers induced by the polymer-filler attractive interaction grows the modulus of the polymer phase and irreversible changes of polymer chains cause hysteresis. We determined that these changes observed in all models are fundamental mechanisms of filled rubber. Comparing the stress-strain curves of the reference model and the aggregated model, we found that the differences are attributed to filler stress. Fillers are to be contacted with another filler particle during deformation and filler stress grows when fillers are aggregated. Comparing the reference model and the weak interaction model, we found that the number and force per a bond of extended chains in the reference model, which are main sources of polymer stress, are greater than the weak interaction model, even though length of the extended chains are much the same. These differences of polymer stress make modulus and hysteresis greater.
Last, a significant increase of the number of extended chains grows polymer stress, when fillers are small and the volume fraction of filler is identical with the reference model. Thus the modulus and hysteresis become greater.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9)

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

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

Rubbers are frequently used in vibration isolation, e.g. as the material for engine mounts or tram wheel suspension segments. These parts are subjected to periodical mechanical loading and to the effects of the environment, such as temperature or chemical reactions. Depending on the nature of the structure changes induced by the environment, physical or chemical ageing may be distinguished (see e.g. [1]). Chemical ageing is governed by the consumption of oxygen, which in turn depends on its transport by diffusion.

Both damage and ageing lead to changes in mechanical properties, each of the phenomena, however, takes place at a different length scale. This contribution is focused on the influence of fatigue damage on the diffusion of oxygen. The central assumption is that the formation and growth of microcracks influence the paths of the gas molecules, which manifest itself as the coefficient of diffusivity on the macroscopic scale. We present various examples of crack geometries and the resulting oxygen flux and concentration computed by the finite element method (FEM). These results will be further used to derive a phenomenological model of coupled fatigue damage and diffusion-limited oxidation (DLO). This model will be an extension of an existing model [2], in which, however, no explicit relation for the coupling between fatigue damage and diffusivity is considered.

[1] Herzig, A. , Johlitz, M. and Lion, A. Consumption and diffusion of oxygen during the thermoxidative ageing process of elastomers. *Mat.-wiss. u. Werkstofftech*, 47: 376-387, 2016.
[2] Heczko, J., Kottner, R. Modelling of ageing and fatigue under large strains. In *Computational Mechanics - EXTENDED ABSTRACTS*, 2017.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9)

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

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

A molecular dynamics approach to calculate general tensile properties of real rubber is developed to alleviate lengthy experimental procedures for the determination of the strain energy function of the rubber material. In this presentation, first, the general framework for the calculation of tensile properties of rubber using molecular dynamics simulation will be illustrated. The overview on the molecular modeling for the real rubber is followed and some pilot calculations are performed to obtain the tensile properties for carbon black filled styrene-butadiene rubbers.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9)

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

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

Thermosets have outstanding mechanical strength and solvent resistance due to their permanently cross-linked networks. They cannot flow upon heating and cannot be reshaped and recycled. The recently developed reversible networks provide opportunities to recycle thermoset polymers. For example, the covalent adaptable networks (CANs; also known as vitrimers) can rearrange their network topology through reversible bond exchange reactions (BERs). It was recently reported that CANs can be dissolved in solvents. At high temperature, small solvent molecules can break long polymer chains into short segments via BERs. In this study, molecular dynamics simulations are used to investigate the dissolution of an epoxy CAN in alcohol solvents due to the transesterification type BER. The diffusion of solvent molecules and the decomposition of epoxy networks are analyzed. It is found that the dissolution proceeds in a surface erosion mode, which is consistent with experimental observations.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9)

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

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

The static elastic behaviour of biophysical networks comprising cross-linked semi-flexible filaments is well characterised due to extensive theoretical, computational and experimental studies of in-vitro materials. The dynamic response of these networks, however, still holds several mysteries, including the peculiar variation of the loss modulus with frequency, G’’（ω）. For example, entropic effects can explain the increase of G’’ with frequency at high frequencies, but not the minimum in G’’（ω）at intermediate frequencies. The latter feature has been suggested to be governed by the cross-linker dynamics, but the experimental trends are yet to be predicted by theory in a phenomenologically consistent manner. Here, we present a minimal micromechanical description, consisting of two semi-flexible filaments coupled by cross-linkers, whose dynamics is described through a Grand Canonical Monte Carlo scheme.

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

[SY-B1] Symposium B-1

Chair: Lorenzo Malerba(CIEMAT, Energy, Environment and Technology Research Centre, Spain)
Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10

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

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

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

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

[SY-B1] **Properties of interstitials in concentrated Fe-Cr alloys from first principles**

○Marcin Roland Zemla[1], Jan Stanislaw Wrobel[1], Marek Muzyk[1], Tomasz Wejrzanowski[1], Duc Nguyen-Manh[2], Sergei L. Dudarev[2], Luca Messina[3], Par Olsson[3], Christophe Domain[4] （1.Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland, 2.CCFE, Culham Centre for Fusion Energy, Abingdon, Oxon OX14 3DB, UK, 3.KTH Royal Institute of Technology, Nuclear Engineering, 106 91 Stockholm, Sweden, 4.Département Matériaux et Mécanique des Composants, EDF-R&D, Les Renardières, F-77250 Moret sur Loing, France）

[SY-B1] **Defect production in cascade overlap with defect clusters in iron and tungsten**

○Jesper Byggmastar[1], Fredric Granberg[1], Andrea E Sand[1], Kai Nordlund[1] （1. Department of Physics, University of Helsinki, Finland）

[SY-B1] Multiscale modelling of radiation damage evolution in Fe and Fe-based alloys

○Fredric Granberg[1], Haixuan Xu[2], Kai Nordlund[1] （1.Department of Physics, University of Helsinki, Finland, 2.Department of Materials Science and Engineering, University of Tennessee, United States of America）

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10)

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

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

Many industrially important alloys and steels are intentionally processed and explored, as metastable microstructures comprising a supersaturation of crystal defects in various forms of aggregation. Even though it is well understood that this microstructural complexity governs the material performance, the defects composition, thermal stability, how they are distributed and in which concentrations are not yet resolved experimentally. Hardened ferritic steels are important example where the lattice defects play deterministic role in their deformation behavior..

While it is long-known that carbon atoms dispersed in the matrix of iron and steels have an influence on the type of defects produced, it is only recently that atomistic simulations have clearly and quantitatively revealed that carbon atoms bind very strongly to vacancies, giving rise to the formation of a whole fauna of carbon-vacancy (mCnV) complexes. These complexes may act as traps for other defects, which suggests that hardening in iron and its alloys will be the consequence of the interaction of dislocations with complex defects formed by not only point defects but also carbon atoms. In this context, the formation of mCnV clusters is the triggering mechanisms for the growth of other complex defects.
In this study, the focus is given on the examination of relaxation processes which occur in the internal friction spectra of a variety of iron alloys and steels with different carbon concentrations, and out-of-equilibrium vacancy concentrations, achieved either by fast cooling (quenching) or plastic deformation. The relaxation peaks are analyzed on the basis of the Debye relaxation model and their activation energies and integrated intensities are determined. By comparing the results with theoretical calculation, positron annihilation spectroscopy results, and magnetic after effect measurements, the observed relaxation processes are assigned to the dissolution of carbon-vacancy (mCnV) clusters [1]. Dissolution energies and relaxation strengths (concentrations) of various mCnV clusters are found to be in the correct energy range according to density functional calculations.

[1] M. J. Konstantinović and L. Malerba, Phys. Rev. Mat. **1,** 053602 (2017).

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10)

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

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

Phosphorus(P) causes Grain-boundary(GB) embrittlement that is considered as one factor of ductile-brittle transition in reactor pressure vessel steels. While the prediction of GB P segregation is desired, the detailed process of P segregation to GB is still unclear. We studied the process of P segregation to GB by simulating the migration of a mixed interstitial dumbbell, an octahedral interstitial P atom and a P-vacancy complex using a molecular dynamics method. As a result, it was found that the P atom of them becomes a substitutional atom before they reach the GB. The self-interstitial atom (SIA) or vacancy of them was absorbed by the GB. This phenomenon was also confirmed partially by first-principles calculations. In addition, it was found that the P atom left behind approaches the GB by successively interacting with an SIA or a vacancy coming to its nearest neighbor site. We think that the conventional understanding of GB P segregation should be revised.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10)

[SY-B1] Properties of interstitials in concentrated Fe-Cr alloys from first principles

○Marcin Roland Zemla[1], Jan Stanislaw Wrobel[1], Marek Muzyk[1], Tomasz Wejrzanowski[1], Duc Nguyen-Manh[2], Sergei L. Dudarev[2], Luca Messina[3], Par Olsson[3], Christophe Domain[4] (1.Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland, 2.CCFE, Culham Centre for Fusion Energy, Abingdon, Oxon OX14 3DB, UK, 3.KTH Royal Institute of Technology, Nuclear Engineering, 106 91 Stockholm, Sweden, 4.Département Matériaux et Mécanique des Composants, EDF-R&D, Les Renardières, F-77250 Moret sur Loing, France)

Point defects, for example self-interstitials and vacancies, play an important part in controlling properties of materials and their kinetic evolution. As a consequence, proper understanding and modelling of materials properties require precise knowledge of point defect behaviour and their characteristics, in particular their formation and migration energies. In magnetic alloys such as FeCr, the investigation of point defects is complicated, because their properties strongly depend on various parameters such as Cr composition, alloy short-range ordering and the defect local environment [1-3].

In this work, we have investigated properties of dumbbell-type defects in FeCr with a large dataset of density functional theory calculations, for Cr concentrations ranging from low to approx. 35%. Analysis shows that properties of self-interstitial and interstitial (IA) defects in concentrated bcc FeCr alloys fluctuate significantly as functions of the above parameters. These fluctuations are observed to a lesser or greater extent for the lattice parameter, chemical potentials, bulk moduli, relaxation volumes, magnetic moments, and migration energies of dumbbells. We conclude that the formation energy of dumbbells depends on the Cr content and also on the number of Cr atoms in the local environment of a defect. For each chemical composition the average migration energies of Cr IA defects (Cr-Cr, Cr-Fe dumbbells) moving to the first nearest-neighbour (1NN) position, are significantly smaller than those of Fe-Fe exchanging with the 1NN Fe atom. The relaxation volumes of dumbbells increase in the ordered structure and decrease in the disordered one with the increase of number of Cr atoms in the local environment of a defect. The trends exhibited by the mean values of the various properties have been observed and analysed, and the most stable directions of Fe-Fe, Fe-Cr and Cr-Cr dumbbells have been determined. Moreover, the energy of elastic interaction between such defects are quantitatively estimated using the suitably parametrized dipole tensors of the defects.

[1] D. Costa, G. Adjanor, C.S. Becquart, et al., J. Nucl. Mater. 452 (2014) 425-433

[2] D. Nguyen-Manh, M.Y. Lavrentiev, S.L. Dudarev, C. R. Physique 9 (2008) 379-388

[3] D. Nguyen-Manh, M.Y. Lavrentiev, M. Muzyk et al., J Mater Sci (2012) 47: 7385

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10)

[SY-B1] **Defect production in cascade overlap with defect clusters in iron and tungsten**

○Jesper Byggmastar[1], Fredric Granberg[1], Andrea E Sand[1], Kai Nordlund[1] （1. Department of Physics, University of Helsinki, Finland）

During the lifetime of a typical reactor, the radiation damage in the wall materials will reach high damage doses. Collision cascades initiated by subsequent irradiation will therefore become increasingly likely to overlap with pre-existing atomistic damage, such as dislocation loops, voids, and other defect structures. We have therefore carried out a large number of molecular dynamics simulations using well-established interatomic potentials, to build a database for the defect production in collision cascades overlapping with pre-existing defect clusters in both iron and tungsten. We primarily study cascades overlapping with dislocation loops of different size. Cascade overlap on other defect clusters leads to similar results. We find that cascades overlapping with pre-existing interstitial clusters result in a significant reduction in the number of new point defects. The overlap effect on vacancy clusters is weaker. By running cascades on different-sized clusters, with different cascade energies and at different temperatures, we obtain a database that can be used to fit a simple analytical model for the defect production bias due to the overlap effects. The data and the fitted analytical model can be transferred to larger-scale simulation methods, such as Monte Carlo techniques, to model the radiation damage accumulation at longer length and time scales.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10)

[SY-B1] Multiscale modelling of radiation damage evolution in Fe and Fe-based alloys

○Fredric Granberg[1], Haixuan Xu[2], Kai Nordlund[1] （1.Department of Physics, University of Helsinki, Finland, 2.Department of Materials Science and Engineering, University of Tennessee, United States of America）

In order to predict the behaviour of materials used in places where radiation is present, many aspects must be considered. The macroscopic effects like swelling and cracking, are a product of defect evolution starting at atomistic level. The energetic ion will, on the atomic level, transmit energy to lattice atoms, which will start collision cascades in the material. To be able to predict what the irradiation will do to the material, we must start on this level. The problem arises from that there is no single method that can accurately simulate everything from single atoms or electrons up to macroscopic parts that builds up the construction. To tackle this problem, a combination of two or more methods can be used consecutively, to be able to extend the time and/or length scale of the simulation. In this study, we focus on extending the time scale, to be able to predict the evolution of irradiation induced defects.

To study the irradiation effect in Fe and Fe-based alloys we utilize Molecular Dynamics (MD), to simulate the primary damage production on an atomistic level. The simulations are carried out by giving a recoil energy to a random atom in the simulation box. These simulations are very accurate to study the movement of all atoms, but are limited to nanoscale simulation boxes and times on the pico- or nanosecond time scale. The length scale is sufficient to accurately simulate the defect production, however the time scale is not sufficient for a long term evolution of the system. This long term evolution is needed to obtain comparable results with experiments and to compare with materials in use in these kinds of environments. To remedy the time scale problem, we utilize Kinetic Monte Carlo (KMC), to obtain longer time scales. A special version of KMC, Self-Evolving Atomistic KMC (SEAKMC), is used as no predefined and pre-calculated barriers are needed. This on-the-fly method is perfect for cases where the defects produced can have many different complicated structures. In these cases, it would be impossible to predict their structure beforehand and calculate all the barriers. A combination of MD and SEAKMC is used to both accurately predict the produced primary damage (with MD) as well as its evolution (with SEAKMC), before a second cascade will hit the same region, as in experimental cases where intensive irradiation is present.

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

[SY-B2] Symposium B-2

Chair: Davide Pizzocri(Politecnico di Milano, Italy)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room10

[SY-B2] Atomic scale calculations of nuclear fuel properties to sustain multiscale modeling of fuel behavior

○Emeric Bourasseau, Marjorie Bertolus, Michel Freyss, Gérald Jomard, Ibrahim Cheik Njifon, Martin-Stéphane Talla Noutack, Cyrille Takoukam Takoundjou （CEA/DEN/DEC, Centre CEA de Cadarache, France）

[SY-B2] Influence of vibrational entropy on the concentrations of uranium vacancies in UO_2

○Jean-Paul Crocombette[1], Fabien Bruneval[1], Aurélien Soulié[1], Mihai-Cosmin Marinica[1], Samuel Murphy[2] （1.CEA Saclay, France, 2.Lancaster University, UK）

[SY-B2] **Modelling of defect and rare gas transport properties in UO_2 from the atomic to the grain scale**

○Marjorie Bertolus, Michel Freyss, Emerson Vathonne, Emeric Bourasseau, Serge Maillard, Gérald Jomard （CEA, DEN, Département d'Etude des Combustibles, Centre de Cadarache, 13108 Saint-Paul-lez-Durance, France）

[SY-B2] **Intragranular bubble impact on nuclear fuel thermomechanical properties**

Fabienne Ribeiro[1], Mehdi Colbert[1], ○Jack Arayro[1], Guy Tréglia[2] （1.Institut de Radioprotection et de Sûreté Nucléaire/PSN-RES/SEMIA/LPTM, France, France, 2.Centre Interdisciplinaire de Nanoscience de Marseille, CNRS, France, France）

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room10)

[SY-B2] Atomic scale calculations of nuclear fuel properties to sustain multiscale modeling of fuel behavior

Invited

○Emeric Bourasseau, Marjorie Bertolus, Michel Freyss, Gérald Jomard, Ibrahim Cheik Njifon, Martin-Stéphane Talla Noutack, Cyrille Takoukam Takoundjou （CEA/DEN/DEC, Centre CEA de Cadarache, France）

Until recently, simulations of the fuel behavior during normal or accidental operation in nuclear reactor were based on rather empirical laws built from numerous experimental observations. Nowadays, simulation codes try to render the underlying physics, and are used to understand the measurements performed during irradiations or post-irradiation experiments. Thus, the fuel modelling and the laws used to predict its behavior must be improved by fundamental researches and feed by results from separate effects experiments. In support to these experiments, multi-scale modelling is an important tool, which aim is to understand the phenomena occurring at the microscopic scale to improve the modelling of the material at the macroscopic scale.

In this presentation, we will show our recent works concerning atomic scale simulations used to improve the knowledge of nuclear fuel properties before and during irradiation. Three points will be emphasized. First, we will present ab initio calculations of point defects in MOX fuels, and how they can be used to determine the elementary mechanisms of atomic diffusion in the irradiated fuel. Then, we will show a study of the energetic and structural properties of grain boundaries in UO_2 using classical molecular dynamics. In particular, an interesting correlation observed between cleavage energy and disorientation angle will be shown. And finally, we will present the results of the determination of thermodynamic properties of $(U,Pu)O_2$ through molecular Monte Carlo method. This method appears to be particularly relevant to explore the various cationic configurations available in mixed oxide.
For each examples, we will try to underline the link with experimental works, and to show how our results are included in simulations at higher scales.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room10)

[SY-B2] Influence of vibrational entropy on the concentrations of uranium vacancies in UO_2

○Jean-Paul Crocombette[1], Fabien Bruneval[1], Aurélien Soulié[1], Mihai-Cosmin Marinica[1], Samuel Murphy[2] （1.CEA Saclay, France, 2.Lancaster University, UK）

The wide deviations of the composition of UO_2 around its nominal composition are accommodated by point defects or clusters of oxygen interstitials. The formation energies of these defects have been the subject of many studies DFT calculations. In the high temperature understoichiometric regime, atomistic calculations and experiment agree on the fact that oxygen vacancies are the dominant defect. At the opposite for the overstoichiometric material the formation energies predict uranium vacancies to dominate over oxygen interstitials. This contradicts experimental facts which show that oxygen interstitials, either isolated or clustered are accommodating the overstoichiometry in UO_{2+x}. This so-called “ uranium vacancy problem” has been noticed for many years [1] and has resisted the various calculations improvements, either methodological (e.g. use of DFT+U) or numerical (e.g. calculations made on bigger boxes).

Considering the vibrational entropy of the defects enables to solve this problem. We have combined ab initio formation energies of point defects and oxygen clusters in UO_2 [2] with harmonic entropies calculated with a many body empirical potential with charge equilibration [3]. Including the vibrational contribution to the free energy of defects de-stabilizes the uranium vacancies compared to the oxygen defects. The latter are then predicted to be dominant at high temperatures or large overstoichiometry in agreement with experiments. However our calculations exhibit a composition and temperature domain where uranium vacancies may in fact be the majority defect in UO_{2+x}. Some experimental observations (dilatometry, positron annihilation spectroscopy and uranium diffusion measurements) tend to confirm this prediction.

[1] J.P. Crocombette*, et al.*, Phys. Rev. B **64**, 104107 (2001).
[2] F. Bruneval*, et al.*, Phys. Rev. Materials **2**, 023801 (2018).
[3] A. Soulié*, et al.*, Acta Mater. **150**, 248 (2018).

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room10)

[SY-B2] Modelling of defect and rare gas transport properties in UO_2 from the atomic to the grain scale

○Marjorie Bertolus, Michel Freyss, Emerson Vathonne, Emeric Bourasseau, Serge Maillard, Gérald Jomard （CEA, DEN, Département d'Etude des Combustibles, Centre de Cadarache, 13108 Saint-Paul-lez-Durance, France）

One of the challenges for the next generation of nuclear reactors is to increase significantly the efficiency in designing and qualifying innovative fuels. One way of doing this is to develop a more physically-based description of nuclear fuels to enhance the predictive capability of fuel behaviour simulation. This should enable a better selection of promising fuel systems and a reduction of the effort necessary for the design of new fuels. Basic research approaches combining multiscale modelling and separate effect experiments can bring significant insight into key phenomena involved in the evolution of nuclear fuels during their reactor life.

We will describe the multiscale modelling approach developed from the atomic to the mesoscopic scale to investigate the transport properties of defects and rare gases in nuclear fuels. We will show examples of the results obtained at atomic scale on uranium dioxide concerning the data necessary for the mesoscale models and for the interpretation of separate experiments on fuels. We will also present the application of mesoscale models, in particular cluster dynamics.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room10)

[SY-B2] Intragranular bubble impact on nuclear fuel thermomechanical properties

Fabienne Ribeiro[1], Mehdi Colbert[1], ○Jack Arayro[1], Guy Tréglia[2] （1.Institut de Radioprotection et de Sûreté Nucléaire/PSN-RES/SEMIA/LPTM, France, France, 2.Centre Interdisciplinaire de Nanoscience de Marseille, CNRS, France, France）

UO2 is used as a standard fuel in pressurized water reactors. During fission reactions bubbles of xenon are generated. The presence of these bubbles modifies the thermo-mechanical properties of the fuel. The need to characterize these effects led to an extensive work both from experimental and theoretical points of view. Our contribution belongs to the later type.

First, the variation of the thermomechanical properties of UO2 versus porosity is studied through atomistic simulations with semi-empirical potentials. A good agreement is found between the elastic properties calculated in the present simulations, and those coming from micro-mechanical modelling and experimental ones. Concerning thermal properties, an analytical model taking into account the nanoporosities is derived. This study emphasizes the importance of bubble surface effects of intragranular bubbles on the thermomechanical behavior of the matrix.

Second, to clarify this effect, we study simplified systems of xenon on UO2 surfaces. We first determine the surface relative stability according to their orientations and then to their polarities, by combining thermostatistical relaxation and analytic formulations within a simple electrostatic model. The main result is that, whereas the (111) surface appears stable with only minor reorganization, the polar (100) one is only stabilized through drastic rearrangement of the surface region. Xenon adsorption on these relaxed surfaces is then realized through Grand Canonical Monte Carlo simulation.

Finally, the pressure inside the Xenon and in the UO2 matrix is investigated. For the Xenon, we show that whatever its cristallographic structure, the pressure increases with the density, but not with the temperature for a fixed density. In the latter case, we present stress profiles through the UO2 matrix before and after xenon adsorption. The next step will be to introduce these results in a micromechanical model in order to derive a thermomechanical behavior law for the porous UO2.

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

[SY-B3] Symposium B-3

Chair: Kazuto Arakawa(Shimane University, Japan)
Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10

[SY-B3] **Formation of radiation-induced Re and Os precipitation in W and its effects on mechanical properties**

○Guang-Hong Lu, Yu-Hao Li, Hong-Bo Zhou （Beihang University, China）

[SY-B3] **Elastic fields and interaction between self-interstitial atom defects in bcc metals.**

○Sergei L Dudarev, Pui-Wai Ma （UK Atomic Energy Authority, UK）

[SY-B3] Molecular dynamics simulation study of the interaction of Re with interstitial defects in tungsten bulk

Yangchun Chen[1], Jingzhong Fang[1], Ning Gao[2], Hong-Bo Zhou[3], Wangyu Hu[4], Fei Gao[4,5], ○Huiqiu Deng[1,4] （1.School of Physics and Electronics, Hunan University, China, 2.Institute of Modern Physics, Chinese Academy of Sciences, China, 3.Department of Physics, Beihang University, China, 4.College of Materials Science and Engineering, Hunan University, China, 5.Department of Nuclear Engineering and Radiological Science, University of Michigan, United States of America）

[SY-B3] **Hydrogen super-saturated layers in plasma loaded tungsten: a global model combining Density Functional Theory data, Thermodynamic and Kinetic models**

○Yves Ferro, Etienne Hodille （Aix-Marseille University, France）

[SY-B3] Mobility of small vacancy and interstitial prismatic dislocation loops in BCC tungsten

○Jan Fikar[1], Roman Gröger[1], Robin Schäublin[2] （1.Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic, Switzerland, 2.Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, Switzerland）

(Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10)

[SY-B3] **Formation of radiation-induced Re and Os precipitation in W and its effects on mechanical properties**

Invited

○Guang-Hong Lu, Yu-Hao Li, Hong-Bo Zhou (Beihang University, China)

Tungsten (W) is one of the most promising candidates for plasma facing materials in future fusion reactors. Rhenium (Re) and Osmium (Os) are not only the typical alloying elements but also the main productions of transmutation in W. More importantly, Re and Os will aggregate and precipitate under high energy radiation, which substantially enhance the radiation hardening and embrittlement, leading to the great concerns for the life-limiting of W. So far, the formation mechanism of Re/Os-rich clusters in W as well as its influences on the mechanical properties remains to be fully elucidated.

We have investigated the interaction between Re/Os and defects in W using a first-principles method in combination with thermodynamic models in order to explore the precipitating mechanism of Re/Os under irradiation. It is found that the presence of defects can significantly reduce the total nucleation free energy change of Re/Os, and thus facilitate the nucleation of Re/Os in W. Kinetically, self-interstitial atom is shown to be easily trapped by substitutional Re/Os, and form W-Re/Os mixed dumbbell. Such W-Re/Os dumbbell combining with the substitutional Re/Os atom will transfer to high stable Re/Os-Re/Os dumbbell, which can serve as a trapping centre for subsequent W-Re/Os dumbbells, leading to the growth of Re/Os-rich clusters. Consequently, an interstitial-mediated migration and aggregation mechanism for Re and Os precipitation has been proposed.

To shed light on the effects of transmutation elements on the mechanical properties, we further have investigated the influences of Re on the motion of 1/2 screw dislocation in W. It is found that the influence of Re on the dislocation motion is directly related to the distribution of Re in W. For the state of Re dispersed distribution, the addition of Re will reduce the generalized stacking fault energy (GSFE) for both 1/2{112} and 1/2{110}, and improve the ductility. However, the influence of Re clusters (for the state of Re aggregation) on the dislocation motion is significantly different from that of dispersed Re. The presence of Re clusters will substantially increase the Peierls stress and energy, inhibiting the dislocation mobility. This will significantly exacerbate the irradiation hardening, and thus degrade the mechanical properties of W.

(Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10)

[SY-B3] **Elastic fields and interaction between self-interstitial atom defects in bcc metals.**

○Sergei L Dudarev, Pui-Wai Ma (UK Atomic Energy Authority, UK)

Strongly anisotropic self-interstitial defect configurations form spontaneously in body-centred cubic metals, like sodium or tungsten, if an extra atom is inserted in the crystal lattice and the resulting structure is relaxed into the lowest energy configuration. The equilibrium structure and modes of Brownian motion of individual SIA defects in body-centred transition metals are now well established. Yet, there is still no regular approach to modelling evolution of ensembles of such defects that would include the treatment of elastic interaction between them. The difficulty appears fundamental, illustrating the lack of a suitable mathematical formalism, linking the discrete atomistic representation of nano-scale defects with continuum elasticity. We derive an analytical expression for the dipole tensor of a dislocation loop, valid in the isotropic and anisotropic elasticity approximations, and explore it in the limit of infinitely small loop size. We discover that the prediction for the dipole tensor of a point defect that does not agree with numerical calculations even for defects in tungsten, a material that is well described by isotropic elasticity theory. We then derive an analytical formula for the dipole tensor of a defect using a two-parameter tensor form, which shows that in addition to a pure prismatic dislocation loop character, the elastic field of a SIA defect contains a significant dilatation component. We evaluate the energy of interaction between SIA defects, and between a SIA defect and a dilatation centre, e.g. a vacancy cluster. To illustrate applications of the new formalism, we compute the energy of interaction between SIA defects ordered as a periodic simple cubic super-lattice, encountered in a DFT calculation. Surprisingly, we find that the energy minimum of such a periodic configuration corresponds to the orientation of the directional unit vector of the defect collinear with a 111 direction.

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 under grant agreements No 633053 and No 755039. Also, it has been part-funded by the RCUK Energy Programme (Grant Number EP/P012450/1).

(Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10)

[SY-B3] Molecular dynamics simulation study of the interaction of Re with interstitial defects in tungsten bulk

Yangchun Chen[1], Jingzhong Fang[1], Ning Gao[2], Hong-Bo Zhou[3], Wangyu Hu[4], Fei Gao[4,5], ○Huiqiu Deng[1,4]
（1.School of Physics and Electronics, Hunan University, China, 2.Institute of Modern Physics, Chinese Academy of Sciences, China, 3.Department of Physics, Beihang University, China, 4.College of Materials Science and Engineering, Hunan University, China, 5.Department of Nuclear Engineering and Radiological Science, University of Michigan, United States of America）

Tungsten (W) and W-based alloys have been considered as promising candidates for plasma-facing materials (PFMs) in future fusion reactors. However, the neutrons generated in fusion reactions result in not only the cascade damage but also the transmutation products (mainly Re and Os) in W bulk. The irradiation defects and transmutation products will have a serious effect on the service behaviors of W PFMs under the condition of fusion irradiation. With molecular dynamics simulations and W-Re potentials developed recently in our group, we have systematically investigated the interaction between Re atom/cluster and interstitial defects in W bulk. It is found that: (1) the self-interstitial atoms (SIAs) and interstitial Re atoms are energetically favorable to align along <111> direction in the form of W-W and Re-W dumbbell/crowdion, respectively; (2) the SIA clusters and 1/2<111> interstitial dislocation loops can undergo fast migration along <111> direction and their migration barriers (< 0.1 eV) are nearly independent of defect size; (3) Re atoms inhibit the migration and growth of SIA clusters, due to their strong attractions; (4) newly formed Re-Re dumbbells and Re-W mixed dumbbell clusters are thermally stable and immobile, which can serve as the trapping center for subsequent Re-W mixed dumbbell, leading to the growth of Re clusters in W. The present work is helpful for understanding the interaction of Re with interstitial defects and dislocation loops and the initial nucleation mechanism of Re atoms in bulk W, and the results can also be used to supply more accurate inputs for larger-scale simulations such as object kinetic Monte Carlo simulations.

(Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10)

[SY-B3] **Hydrogen super-saturated layers in plasma loaded tungsten: a global model combining Density Functional Theory data, Thermodynamic and Kinetic models**

○Yves Ferro, Etienne Hodille （Aix-Marseille University, France）

In this work, we combined Density Functional Theory data, a Thermodynamic and a kinetic model to build a global model enabling to determine the total concentration of hydrogen implanted in the sub-surface of tungsten exposed to a hydrogen flux. This is achieved given a flux of hydrogen, a temperature of implantation, and the energy of the incoming hydrogen ions. This model is built step by step; an equilibrium with a molecular hydrogen gas phase is first considered and the resulting solubility is compared with experimental results. A kinetic model is subsequently used to determine a chemical potential for hydrogen in the sub-surface of tungsten. Combining both these models, two regimes are then established in which hydrogen is trapped at interstitial sites or in vacancies. The existence of these two regimes are driven by the temperature of implantation; above a temperature of implantation is the *interstitial* regime, below is the *vacancy* regime in which super-saturated layers are formed. A simple analytical and easy to use expression is work-out for the transition temperature, which allows to plot a diagram of existence of the super-saturated layer depending on the implantation temperature, the incident energy and the flux of the hydrogen ions.

(Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10)

[SY-B3] Mobility of small vacancy and interstitial prismatic dislocation loops in BCC tungsten

○Jan Fikar[1], Roman Gröger[1], Robin Schäublin[2] （1.Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic, Switzerland, 2.Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, Switzerland）

Vacancies and self interstitials produced in collision cascades often form clusters, which can further collapse into prismatic dislocation loops. In BCC metals dislocation loops with Burgers vectors 1/2 and are observed and they can be either vacancy or interstitial type. These dislocation loops usually move easily in the direction of the Burgers vector. The mobility of prismatic dislocation loops is studied by molecular dynamics. The small dislocation loops under 100 defects seem to behave more like point defect clusters and the mobility of vacancy loops is substantially lower than the one of interstitial loops. Similar effect is observed in formation energies, where the small vacancy loops have higher formation energies than the corresponding interstitial loops. At larger sizes the dislocation loops seem to behave as perfect dislocations and there is no difference between vacancy and interstitials loops mobilities and formation energies.

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

[SY-B4] Symposium B-4

Chair: Gary S Was(University of Michigan, United States of America)
Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room10

[SY-B4] **Kinetics of Precipitation in Fe-Cr and Fe-Cr-C alloys under Irradiation**

○Frederic Soisson （CEA Saclay, France）

[SY-B4] **The complex problem of the experimental validation of atomistic and microstructural evolution models**

○Lorenzo Malerba （ CIEMAT, Energy, Environment and Technology Research Centre, Spain）

[SY-B4] Physically based prediction of radiation hardening: application to steels and model alloys

○Ghiath Monnet （EDF - R&D, MMC, France）

[SY-B4] **Oxygen diffusion in bcc Fe under the influence of foreign atoms and vacancies**

○Xiaoshuang Wang, Matthias Posselt, Jürgen Faßbender （Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany）

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room10)

[SY-B4] Kinetics of Precipitation in Fe-Cr and Fe-Cr-C alloys under Irradiation

Invited

○Frederic Soisson (CEA Saclay, France)

In ferritic steels, the precipitation of the Cr-rich α' phase leads to a degradation of mechanical properties. Below 400°C, the precipitation is usually too slow to be a real concern, but it can be significantly accelerated by irradiation, due to an increase in point defect concentrations. Irradiation also produces a ballistic mixing between Fe and Cr atoms, and therefore prevent the nucleation of α' precipitates or the dissolution of existing ones.

We present a multiscale approach which models these contradictory effects by taking into account the different mechanisms of atomic transport taking place under irradiation: the creation of vacancies and self-interstitials and the ballistic mixing within displacement cascades, the thermally activated diffusion of point defects, and their elimination at sinks or by mutual recombination. The method combines DFT calculations (which provide the fundamental information on thermodynamics and point defects properties), atomistic Kinetic Monte Carlo Simulations (to model the diffusion of point defects and the α' precipitation), and Cluster Dynamics (to model the evolution of the sink density under irradiation). The simulations show that the acceleration of the α' precipitation occurs under irradiation at low or moderate dose rates, but that ballistic dissolution becomes dominant under ion irradiation at high dose rates -- due to a large density of sinks that limits the point defect supersaturation.

The results of the simulations are compared with recent experimental studies. The same multiscale approach is used to model the diffusion of carbon atoms in Fe-Cr alloys and their strong interaction with point defects. We will consider their possible effect on Fe and Cr diffusion, and on the kinetics of α' precipitation under irradiation.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room10)

[SY-B4] The complex problem of the experimental validation of atomistic and microstructural evolution models

○Lorenzo Malerba (CIEMAT, Energy, Environment and Technology Research Centre, Spain)

The development of physical models for the description of the behaviour of materials under certain conditions goes hands-in-hands with the use of advanced experimental characterization techniques. The experiments provide data and reveal phenomena that the models are expected to predict and explain. The exchange of information between models and experiments is therefore continuous and goes in two directions: models may predict results that need to be verified experimentally and experiments observe processes that the models are expected to reproduce and explain in terms of physical laws and mechanisms. This continuous interplay is often denoted as "experimental validation" of models. While this definition is somewhat restrictive, the validation of models is a discipline in itself that requires first of all the performance of experiments that may be long and expensive, and need to be carefully designed. In addition, the comparison between the results of the models, in particular computer simulations, and the observations from characterization techniques is not always straightforward, because both the experimental and the simulation outcomes need to be properly treated.

In this presentation these problems will be discussed taking the example of the comparison between models that describe the microstructural evolution of iron alloys under irradiation and the results of microstructural characterization techniques such as positron annihilation, small angle neutron scattering, atom probe and transmission electron microscopy.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room10)

[SY-B4] Physically based prediction of radiation hardening: application to steels and model alloys

○Ghiath Monnet （EDF - R&D, MMC, France）

Based on a multiscale modeling framework, it is shown that radiation hardening can be rationalized in several industrial materials and model alloys. Microstructure features of the as-received materials are first considered for the assessment of the yield stress prior to irradiation. The later can be decomposed into two contributions: short-range stresses induced by local obstacles (such as forest dislocations, precipitates, etc.) and long-range stresses resulting from sub-grain dislocation walls and grain boundaries. Introducing radiation defects as local obstacles, the same methodology can be employed to predict the yield stress of the irradiated materials. The considered radiation defects are solute clusters (SCs) and Dislocations Loops (DLs). SCs are assumed to be spherical coherent precipitates that can be sheared by dislocations with a given shear resistance, computed from atomistic simulations. This resistance is used in Dislocations Dynamics (DD) simulations to compute hardening induced by SCs. The sizes and densities implemented in DD simulations are those given by experiment (TEM, APT, SANS etc.). The contribution of DLs is computed from DD simulations. Upon interaction with mobile dislocations, small DLs are absorbed leading to strong pinning and high hardening level, while large DLs experience classical dislocation-dislocation interactions (junction, annihilation, etc.). The yield stress of the irradiated materials is predicted using the constitutive equations of radiation hardening induced by SCs and DLs.

Several FeCr, FeMnNi model alloys and some RPV steels are considered for the validation of the model. It is shown that local obstacles (present before irradiation) may have a significant effect on radiation effects on the mechanical properties: radiation hardening is not independent of the initial yield stress. With almost no adjustable parameters, the predicted increase in the yield stress is found in close agreement with experiment.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room10)

[SY-B4] **Oxygen diffusion in bcc Fe under the influence of foreign atoms and vacancies**

○Xiaoshuang Wang, Matthias Posselt, Jürgen Faßbender （Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany）

A multiscale approach including Density Functional Theory (DFT) and Atomistic Kinetic Monte Carlo (AKMC) simulations is applied to investigate the diffusion of oxygen in bcc Fe under the influence of substitutional

foreign atoms or solutes (Al, Si, P, S, Ti, Cr, Mn, Ni, Y, Mo, W) and vacancies. The solutes can be assumed to be immobile since their diffusion coefficient is much smaller than that of oxygen. On the other hand, the vacancy mobility must be considered in the calculations because it is comparable to that of oxygen. The most stable state of oxygen in pure bcc Fe is the octahedral interstitial configuration. Recently, jumps of oxygen in pure bcc Fe, between first-, second-, and third-neighbor octahedral interstitial sites were investigated by DFT. It was found that the first-neighbor jump is most relevant. The second-neighbor jump consists of two consecutive first-neighbor jumps whereas the barrier of the third-neighbor jump is too high to be significant for the diffusion process. In this work DFT is used to determine the modified migration barriers in the presence of solutes. It is found that Si, P, Ni, Mo and W have some effect on the migration barriers of oxygen and their interaction with O is mainly repulsive. Al, Cr and Mn have a significant influence on the barriers and they exhibit strong attractive interactions with O. The most important modification of the barriers is found for S, Ti, and Y where deep attractive states exist. The barriers for oxygen jumps near a vacancy and barriers for vacancy jumps in the environment of oxygen are also calculated by DFT. Based on the migration barriers obtained by DFT, AKMC simulations on a rigid lattice are employed to determine the diffusion coefficient of oxygen in a dilute iron alloy containing different substitutional foreign atoms. It is found that Si, P, Ni, Mo, and W have almost no influence on the diffusivity of O. The presence of Al, Cr, Mn, S, Ti, and Y causes a significant reduction of the mobility of oxygen. Another version of the AKMC code is applied to investigate the mutual influence of oxygen and vacancy diffusion as well as the migration of the oxygen-vacancy pair.

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

[PO-A2] Poster Session 2

Symposium A
Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-01] Multiscale model of solid state amorphization during processing of pharmaceutical materials

Chunyu Li[1], Yifei Zeng[1], Lorena Alzate-Vargas[1], Pilsun Yoo[1], Rachel Frocino[2], Jeff Brum[2], Peilin Liao[1], Marisol Koslowski[1], ○Alejandro Strachan[1] （1.Purdue University, United States of America, 2.GlaxoSmithKline, Analytical Sciences and Development, United States of America）

[P2-02] FTMP-based Modeling and Simulations of HCP Mg Single Crystal

○Takahiro Kitano, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P2-03] Nonlinear elasticity on Riemannian manifold and its application to general surface development

○Yuto Horikawa[1], Ryuichi Tarumi[2], Yoji Shibutani[1] （1.Dept. of Mechanical Engineering, Osaka Univ., Japan, 2.Grad. Sch. of Engineering Science, Osaka Univ., Japan）

[P2-04] The challenge of achieving quantitative phase field models for microstructure evolution in irradiated solids - the case of voids

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

[P2-05] A Molecular-Dynamics Study of Surface Tension: From Alloy Droplets to Bubbles in Molten Alloy

○Xiangming Ma, Hongtao Liang, Yang Yang （East China Normal Univercity, China）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-01] Multiscale model of solid state amorphization during processing of pharmaceutical materials

Chunyu Li[1], Yifei Zeng[1], Lorena Alzate-Vargas[1], Pilsun Yoo[1], Rachel Frocino[2], Jeff Brum[2], Peilin Liao[1], Marisol Koslowski[1], ○Alejandro Strachan[1] （1.Purdue University, United States of America, 2.GlaxoSmithKline, Analytical Sciences and Development, United States of America）

Processing of active pharmaceutical ingredients and excipients to reduce and control particle size involve milling and micronization which result in severe plastic deformation and fracture. The increase in free energy of the crystal during deformation can result in polymorphic transformations and amorphization and affect the physical properties of the product, including bioavailability.

In order to predict how materials properties and processing conditions affect plastic deformation and phase transitions in pharmaceutical materials we developed a multiscale model that combines electronic structure using density functional theory, large-scale molecular dynamics simulations and a phase field modeling. At the finer scale, we use DFT to predict elastic constants of the crystals and amorphous systems of interest and validate the force fields used with MD. MD simulations provide insight into the process of amorphization and enables the characterization of the difference in enthalpy between the crystal and amorphous phase and their interfacial energy, critical to describe the nucleation and growth of the amorphous phase. Finally, the materials properties from DFT and MD calculations are used to inform a phase field model that describes, self-consistently, plastic deformation, including the nucleation of crystal defects informed by dislocation dynamics, with phase transformations.

Using the multiscale model, we investigate the effect of deformation, shear, impact and particle surface roughness on the evolution of the crystallite size and the nucleation and growth of an amorphous phase in molecular crystals of interest for pharmaceutical applications.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-02] FTMP-based Modeling and Simulations of HCP Mg Single Crystal

○Takahiro Kitano, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

Extended usages of Mg and Mg alloys have been widely promoted to date, attempting to make the best use of their attractive properties, such as light weight, high specific strength, superior recyclability and excellent bio-compatibility. Modeling attempts of Mg and Mg alloys, however, often meet difficulty in the treatments of the complex plasticity, mainly stem from their highly anisotropic slip systems and intricate activities of twinning. The present study aims at enhancing the feasibility of the recently-proposed model for deformation twinning based on FTMP (Field Theory of Multiscale Plasticity) toward extended applications to HCP Mg single crystal. The major updates of the model are two fold: one is the extension to efficient 3D simulations by introducing special computational schemes, while the other is to apply modified lattice rotation based on the rotational part of the incompatibility tensor. The twinning model with the modified lattice rotation is introduced in the hardening law in the FTMP-based crystalline plasticity framework, and is further implemented into a finite element code accommodated with the above new scheme. Deformation analyses are performed based on 2D/3D FEM for pure single crystal magnesium with HCP (hexagonal close-packed) structure, and critical comparisons are made with experimental data obtained under plain-strain

compression in multiple orientations by Kelly and Hosford, particularly, with those exhibiting the unique stress-strain responses induced by deformation twinning, i.e., orientations A, E and F. Natural expression of twin-induced lattice rotation is attempted by introducing a modification based on the pure rotation part of the incompatibility tensor, spontaneously evolved during deformation. The modification is shown to allow autonomic transitions between slip and twinning modes, e.g., from twin-dominant stress response to that carried by slip, as in the orientations E and F by Kelly-Hosford.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-03] Nonlinear elasticity on Riemannian manifold and its application to general surface development

○Yuto Horikawa[1], Ryuichi Tarumi[2], Yoji Shibutani[1] （1.Dept. of Mechanical Engineering, Osaka Univ., Japan, 2.Grad. Sch. of Engineering Science, Osaka Univ., Japan）

This study aims to develop a theoretical framework to construct a three-dimensional curved surface from pieces of an elastic sheet which is embedded in two-dimensional Euclidean space. Our formulation is based on the standard nonlinear elasticity within the framework of differential geometry. We first introduce the Riemannian manifolds which equip the metrics, g[0] and g[t], for reference and current configurations. The strain energy density is defined as a quadratic form of Green strain tensor under the assumption that elastic medium is isotropic in the reference configuration g[0]. Then, the surface development problem ends up with a variational problem such that to find an embedding mapping which minimizes the strain energy functional. We solve the variational problem numerically using the isogeometric analysis (IGA). To this end, we first derive a weak form equilibrium equation from the first variation of the functional. The embedding mapping is approximated by a linear combination of non-uniform rational B-spline (NURBS) functions with the coefficients ξ. Consequently, the equilibrium equation yields a system of nonlinear algebraic equations for ξ and which is solved iteratively around a linearized solution by the Newton method. It should be noted here that present method consider in-plane deformation of the elastic sheet exclusively. It implies that two-dimensional isometric deformation, such as out-of-plane bending deformation, produces no strain energy in the medium. In this regards, present method is a fair generalization of conventional surface development method which is frequently used in the paper craft such as origami. Numerical analysis for a one-dimensional system demonstrates that present method converges to an exact solution within a sufficient accuracy.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-04] The challenge of achieving quantitative phase field models for microstructure evolution in irradiated solids - the case of voids

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

We present a thermodynamics-consistent formalism of a phase field model of void growth in irradiated solids, along with its sharp interface counterpart. Asymptotic matching of the two models was performed to yield all phase field model parameters in terms of real materials properties. In this presentation, the results of a first quantitative simulations of void growth driven by irradiation using our phase field approach will be reported. This work was performed in collaboration with Srujan Rokkam, Thomas Hochrainer, and Karim Ahmed.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-05] A Molecular-Dynamics Study of Surface Tension: From Alloy Droplets to Bubbles in Molten Alloy

○Xiangming Ma, Hongtao Liang, Yang Yang （East China Normal Univercity, China）

We present a substantial atomistic simulation study of the equilibrium surface tension for liquid-state binary alloy systems. Four types of spherical surface/interfaces are investigated: liquid Pb droplet embedded in bulk liquid Al, liquid Al droplet in bulk liquid Pb, a bubble in liquid state Pb-Bi eutectic (LBE) and a LBE droplet. The surface tension for these non-planar surfaces are calculated based on the calculation of the local pressure tensor in spherical coordinates. Several thermodynamics property (droplet size, temperature, capillary pressure, mutual miscibilities) dependencies of surface tension are obtained. Our results provide useful input data for the mesoscale simulations of the selective laser melting, advanced welding and bubble formation in nuclear coolants.

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

[PO-B2] Poster Session 2

Symposium B

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-06] Effects of rhenium on the mechanical behavior of irradiated tungsten: a molecular dynamics study using neural-network potential

○Ryo KOBAYASHI （Nagoya Institute of Technology (NITech), Japan）

[P2-07] Diffusion behavior and temperature dependence of hydrogen in tungsten and molybdenum under isotropic strain state

○QuanFu Han[1], Yue-Lin Liu[2], Ying Zhang[1], Guang-Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

[P2-08] **Diffusion of Point Defects on Tungsten Surface**

Jiannan Hao[1], ○Shuo Jin[1], Haixuan Xu[2], Xiaolin Shu[1], Guanghong Lu[1] （1.School of Physics and Nuclear Energy Engineering, Beihang University, China, 2.Department of Material Science and Engineering, The University of Tennessee, Knoxville, United States of America）

[P2-09] Influence of anisotropic strain and temperature on hydrogen dissolution in tungsten

○Ying zhang[1], Quan Fu Han[1], Yue lin Liu[2], Guang Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

[P2-10] Screw dislocation-interstitial solute coevolution in W-O alloys using atomistically-informed kinetic Monte Carlo simulations

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

[P2-11] Kinetic Monte-Carlo Simulations of Radiation Damage in W(Re,Os) Alloys

○Matthew James Lloyd[1,2], David Armstrong[1], Enrique Martinez Saez[3], Duc Nguyen-Manh[2] （1.Department of Materials, University of Oxford, UK, 2.Culham Centre for Fusion Energy, UK, 3.Los Alamos National Laboratory, United States of America）

[P2-13] **Dynamics of Magnetism in Neutron Irradiated Iron-Chromium Steels**

○Jacob B. J. Chapman, Pui-Wai Ma, Sergei L. Dudarev （Culham Centre for Fusion Energy (CCFE), UK）

[P2-14] **Atomistic insights into the grain boundaries interaction with radiation-induced point defects in bcc Fe-Cr alloys**

○Marcin Roland Zemla, Jan Stanislaw Wrobel, Tomasz Wejrzanowski （Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland）

[P2-15] Production and Process of Cascade Development in Irradiated Pure α-Zr from Molecular Dynamics Simulations

○Rongjian Pan[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Bang Wen[1], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3] （1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine）

[P2-16] Microstructure evolution of cascade annealing in irradiated pure α-Zr from molecular dynamics simulations

○Bang Wen[1], Rongjian Pan[1], Wei Zhang[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3] （1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine）

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[P2-06] Effects of rhenium on the mechanical behavior of irradiated tungsten: a molecular dynamics study using neural-network potential

○Ryo KOBAYASHI （Nagoya Institute of Technology (NITech), Japan）

Tungsten (W) is considered as a promising candidate for the plasma facing wall material at divertor in nuclear fusion reactors. In order to assess the lifetime of the divertor for safe operation of the nuclear fusion reactors, mechanical response to the irradiation of high energy neutrons and helium atoms should be precisely understood from atomistic scale. Under the irradiation of high energy neutrons, not only defects are formed but also transmutation occurs, which will produce a few percent of rhenium (Re) concentration within several-year operation of nuclear fusion reactor. Thus the effect of solute Re atoms on the mechanical behavior of host material, W, should be taken into account, such as recovering rate after cascading damage, H/D/T retention, He bubble formation, or dislcation mobility. In this study, we create a neural-network (NN) potential for quarternary system, W-Re-H-He, combined to an EAM potential for W-Re binary system. It is known that machine-learning (ML) potentials such as NN can well reproduce DFT energies of wide variety of atomic configurations, but it requires big data to learn a lot of free parameters and it is usually much slower than the classical potentials such as EAM. By combining the NN with EAM potentials, we can construct a potential with smaller number of referece data and make it much faster than fully NN potential. The properties of the potential and the effect of Re on the recovering rate after cascading damage, He bubble formation/growth rate, and dislocation punching will be discussed.

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[P2-07] Diffusion behavior and temperature dependence of hydrogen in tungsten and molybdenum under isotropic strain state

○QuanFu Han[1], Yue-Lin Liu[2], Ying Zhang[1], Guang-Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

The interaction between hydrogen and metal exhibits a great scientific and technological importance so that it has a direct impact on the design and operation of metallic materials. Here, we have carried out first-principles calculations to investigate interstitial hydrogen diffusion behaviors in tungsten and molybdenum by considering double effects of temperature and strain. The temperature and strain effects are reflected by the vibration Helmholtz free energy in the quasi-harmonic approximation and isotropic loading, respectively. The hydrogen diffusion is analyzed through two nearest neighbor tetrahedral sites. At a ground state (0-K) condition, the hydrogen diffusion activation energy can increase and decrease notably with rising compressive and tensile strain, respectively. While at each compressive/tensile strain case, the hydrogen diffusion activation energy depends distinctly on the temperature and increases with rising temperature. This is mainly originated from the contribution of vibration Helmholtz free energy induced by the larger vibration frequency of hydrogen in two metals. With the increasing temperature, the hydrogen diffusivity is shown to be dependent on the compressive/tensile strain alteration. The present study demonstrates a remarkable influence of “temperature and strain” on the hydrogen diffusion behaviors in tungsten and molybdenum.

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[P2-08] **Diffusion of Point Defects on Tungsten Surface**

Jiannan Hao[1], ○Shuo Jin[1], Haixuan Xu[2], Xiaolin Shu[1], Guanghong Lu[1] （1.School of Physics and Nuclear Energy Engineering, Beihang University, China, 2.Department of Material Science and Engineering, The University of Tennessee, Knoxville, United States of America）

Hydrogen (H) / helium (He) retention in tungsten (W) and can significantly reduce the thermal conductivity and sputtering threshold of W, and at the same time, continuous bombardment with 14.1 MeV neutron can introduce Frenkel defects (composed of self-interstitial atoms (SIAs) and vacancies), which lead to a high concentration of W impurity. The surface deformation and blisters are observed experimentally in W, in which the surface morphology is relevant to the plasma fluence and surface directions [1-2]. The near-surface atomistic configuration is changed via diffusion of frenkel defects which is driven by heat and/or bubble loop punching process. Therefore, revealing the evolution mechanism of point defects on the W surfaces under H/He irradiation is crucial for W application in future fusion reactors.

We employ the first-principles and molecular dynamics simulation to calculate the energy barriers of single adatom (AD) and vacancy (VA) diffusion on the W (100), (110) and (111) surface. The diffusion paths of defects is determined by the dimmer method built in the SEAKMC code [3]. At least three diffusion paths with high energy barriers are found for both AD and VA on the (100) surface. However, only one path with low energy barrier of both AD and VA on the (110) surface are dominated throughout the diffusion process. Moreover, the diffusion of AD and VA on the (111) surface is investigated, in which the formation energies of different surface defects are biased. Nonetheless, the symmetry of the (111) surface will break spontaneously at the certain temperature and concentration of impurity through the thermodynamic calculation, and the morphology is in good agreement with the SEM images [1]. The work will help to understand the early stage of surface morphology evolution under irradiations or in the annealing process.

Keywords: tungsten, point defects, diffusion, surface

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[P2-09] Influence of anisotropic strain and temperature on hydrogen

dissolution in tungsten

○Ying zhang[1], Quan Fu Han[1], Yue lin Liu[2], Guang Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

Tungsten (W) is an alternative candidate for a plasma facing material in the future fusion reactor due to its high melting point, high thermal conductivity and low plasma sputtering yield. The solubility of hydrogen in tungsten is a basic and crucial factor to influence the formation of hydrogen bubbles. In this work, we have investigated the effects of anisotropic strain and temperature on the dissolution of H in tungsten via the first-principles calculation in combination with thermodynamic models. The temperature and strain effects are reflected by the vibration Helmholtz free energy in the quasi-harmonic approximation and uniaxial/biaxial strain loading, respectively. It is found that the solubility of hydrogen can be enhanced by both compressive and tensile anisotropic strain, independent with of the sign of strain. This is different from the influence of isotropic strain, where the solubility of hydrogen in tungsten responds to the isotropic strain monotonically. Besides, the difference of the dissolution energy between hydrogen dissolves in tetrahedral and octahedral site constantly changes in the anisotropic strain range of -4%-4%. Further, under same anisotropic strain condition, the solution energy of hydrogen in tungsten increases with the increasing of the temperature from 300-1800 K, which can be mainly contributed to the vibration Helmholtz free energy. Our finding suggests that the local anisotropic strain and temperature can significantly influence the dissolution of hydrogen in tungsten, which may play a key role on hydrogen bubble formation.

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[P2-10] Screw dislocation-interstitial solute coevolution in W-O alloys using atomistically-informed kinetic Monte Carlo simulations

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The interaction of interstitial impurities with in-grown dislocations in metals can lead to various processes, including solute solution hardening and/or dynamic strain aging. The coevolution of solutes and dislocations occurs on length and time scales that are very challenging to resolve experimentally. The interaction of interstitial solutes with dislocation segments is highly local, however, and models must be capable of resolving the fine details of the interaction if we are to gain any understanding from the process. Here we develop a kinetic Monte Carlo model of dislocation motion in the presence of diffusing solutes. We focus on the W-O solid solution, such that the subject of our study is screw dislocations, as they control plastic flow at low temperatures in body-centered cubic metals and alloys. Solute diffusion is affected by dislocation strain fields, which we study via the elastic dipole tensor using electronic structure calculations. As well, we calculate binding energies of O atoms to screw dislocation cores, and discuss the joint structures formed, the implications of the calculated energetics, and show the effect on the dislocation velocity of solute diffusion at several temperatures.

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[P2-11] Kinetic Monte-Carlo Simulations of Radiation Damage in W(Re,Os) Alloys

○Matthew James Lloyd[1,2], David Armstrong[1], Enrique Martinez Saez[3], Duc Nguyen-Manh[2] （1.Department of Materials, University of Oxford, UK, 2.Culham Centre for Fusion Energy, UK, 3.Los Alamos National Laboratory, United States of America）

The realisation of fusion energy is dependant on the development of high performance materials that can withstand the extreme conditions that they will be subjected to. The plasma facing components of a fusion reactor will experience a combination of high thermal loading (˜10MWm^{-2}) and an intense flux of both 14MeV neutrons and high energy He/H ions (˜5-20dpa/yr), meaning they will have to operate at very high temperatures (˜1300 K). Tungsten is currently the leading candidate material due to its high melting temperature (˜3695K); good thermal conductivity (˜150Wm^{-1}K^{-1}) and resistance to sputtering (Eth=200eV). But at such a high neutron flux, transmutation of W in a fusion reactor is significant, resulting in several at.% Re, Os and Ta over the lifetime of the reactor. Precipitation of Re and Os has been observed well below their solubility limit in W, resulting in embrittlement, hardening, and a reduction in thermal conductivity.

The research presented examines irradiated W-(Re,Os,Ta) alloy systems, using a combination of DFT parametrised, multicomponent atomistic kinetic Monte-Carlo (AKMC) modelling, and high resolution nanoscale characterisation techniques such as atom probe tomography (APT). The role of interstitial defects in W-Re and W-Os is thought to play an important role in precipitation, because of the low rotation energy of the W-Re/W-Os mixed dumbbell. This enables the 3D transport of solute atoms, that would otherwise be confined to the <111> direction. We present a multicomponent kinetic Monte Carlo model, incorporating both vacancy and interstitial defects, and solute concentration dependant interactions. The predictions made by our model are supported by APT data of W-Re and W-Os alloys irradiated at high temperature, using W ions.

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[P2-13] **Dynamics of Magnetism in Neutron Irradiated Iron-Chromium Steels**

○Jacob B. J. Chapman, Pui-Wai Ma, Sergei L. Dudarev （Culham Centre for Fusion Energy (CCFE), UK）

Ferritic-martensitic (F/M) steels, with a high chromium content, are critical materials for magnetic confinement fusion technology due to high temperature stability and corrosion resistance, facilitating the thermal efficiency necessary for fusion power plant operation. To predict the evolution of the steel microstructure and mechanical properties when subjected to sustained high doses of radiation at elevated temperatures, we must understand how radiation damage affects magnetic properties of the materials, which strongly influence phase stability and chromium solubility.

We investigate the effect of neutron irradiation on the magnetic properties of F/M steel alloys, relating experimentally observed [1] concentrations, radii and number densities of Cr precipitates within a Fe-Cr matrix to the dynamics and degradation/enhancement of magnetism across a broad range of temperatures. The Curie temperature is shown to vary, strongly dependent upon microstructure, increasing significantly with Cr precipitation observed at high doses and ageing times. These large-scale non-collinear calculations are performed using a method implementing magnetic cluster expansion (MCE), parameterised using a database of DFT-generated observables [2], with spin-dynamics (SD) incorporating both transverse and longitudinal spin fluctuations [3]. SD simulations provide valuable insight into the ageing of alloys under realistic magnetic confinement conditions to inform material choices and construction strategy for fusion power plant design.

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

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[P2-14] Atomistic insights into the grain boundaries interaction with radiation-induced point defects in bcc Fe-Cr alloys

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Grain boundaries (GBs) are an immanent components of crystal structure of the structural materials, such as e.g. Fe-Cr steels. Moreover, they have considerable influence on the materials properties, especially on the mechanical one. As a consequence of that, is necessary to investigate effect of radiation-induced defects on the GBs in order to a deeper understanding of the radiation damage.

In current study, we investigated characteristics of bcc-Fe and Fe-Cr based tilt GBs interacting with point defects such as vacancy, self-interstitial (SIA, dumbbell-type), and interstitial atoms (He impurities). Several tilt GBs with the rotation axis along [100] and [110] directions were modelled with He impurities, vacancy, and SIA in Fe-Cr. Molecular dynamics (MD) simulations using the interatomic Fe-Cr-He embedded atom model potential were conducted, for twelve GBs, in order to investigate GBs energies, He segregation energies, and the weakening effect of He impurity for several Cr and He concentrations. Furthermore, spin-polarized density functional theory (DFT) calculations focused at two GBs, $\Sigma 3(111)$ and $\Sigma 5(210)$, allowed to deeper insights into GBs properties. For example, the DFT results show that the presence of He significantly influences the magnetic properties of the system in the relatively distant neighbourhood [1]. The fluctuation of magnetic moments, chemical potentials, formation and migration energies of point defects were studied as a function of distance from GB’s plane. Representative structures of GBs, with Cr content ranging 6-10%, generated using DFT-based Monte Carlo simulations [2] were used to analyse how parameters, such as alloy short-range ordering or local environment, effects on defects properties.

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[P2-15] Production and Process of Cascade Development in Irradiated Pure α-Zr from Molecular Dynamics Simulations

○Rongjian Pan[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Bang Wen[1], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3] （1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine）

The formation and development of cascade in pure α-Zr crystals at sample temperatures *T*=300K and *T* =500K, energy of 2, 6 and 10 keV and initially driving directions and of primary knock atoms (PKA) are investigated by molecular dynamics. The simulation results show that when crystals temperature is *T*=300K and 500K and initial direction of motion for PKA is the cascades volume is greater than for the initial direction at same all other parameters. The largest size of cascade is found after 0.4 ps, which regardless of crystal temperature, energy and initial direction of primary knock-on atom (PKA). The formation of crowdions is caused by channeling during cascade development.

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[P2-16] Microstructure evolution of cascade annealing in irradiated pure α-Zr from molecular dynamics simulations

○Bang Wen[1], Rongjian Pan[1], Wei Zhang[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3] （1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine）

The microstructure evolution of cascade annealing in α-Zr crystals at *T*=300K, 400K, and 500 K for energy of 2, 6 and 10 keV with initially driving directions <0001> and <01-10> of primary knocked atoms (PKA) are investigated by using molecular dynamics simulations. The results show that the relaxation time (τ_r) of cascades can play a role of an effective parameter for describing radiation damages during molecular dynamics simulations. of cascade with the larger surface area but with the same volume is much smaller, which promotes faster recombination of defects during cascade annealing. Energy is a crucial factor in the formation of cascade displacements of atoms and appearing of defects compared with temperature and direction of movement for initially knocking atoms.

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

[PO-C2] Poster Session 2

Symposium C

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[P2-18] **Prediction of Biaxial Tensile Deformation Behavior of Aluminum Alloy Sheets using Crystal Plasticity Finite Element Method and Machine Learning**

○Kota Koenuma[1], Akinori Yamanaka[1], Ikumu Watanabe[2], Toshihiko Kuwabara[1] （1.Tokyo University of Agriculture and Technology, Japan, 2.National Institute of Materials Science, Japan）

[P2-19] MobiDiC: A 3-D Dislocation Dynamics Simulation

○Ronan MADEC[1], Laurent COLOMBET[1], Ladislas KUBIN[2] （1.CEA, DAM, DIF, France, 2.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay, France）

[P2-20] Temperature dependence of fatigue crack growth in Ti-6Al-4V

○Bhargavi Rani Anne, Masaki Tanka, Tatsuya Morikawa （Dept. of Materials Science and Engineering, Kyushu University, Japan）

[P2-21] Parametric model of discrete dislocation dynamics based on mathematical theory of moving curves

○Miroslav Kolar, Jan Kratochvíl, Petr Pauš, Michal Beneš （Czech Technical University in Prague, Czech Republic）

[P2-22] On Visualization of Multiscale Information Transfer/Exchange Processes via FTMP-based Duality Diagram Representation Scheme

○Takuya Takagi, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P2-23] **Rotational Field Evolutions based on Field Theory of Multiscale Plasticity (FTMP)**

○Tadashi Hasebe[1], Yasutaka Matsubara[2] （1.Kobe Univ., Japan, 2.Graduate School of Kobe Univ., Japan）

[P2-24] **A 2D MESOSCALE STUDY OF DISLOCATIONS, CRACKS AND MARTENSITIC PHASE TRANSFORMATIONS**

○Rachel Derby, Michael Budnitzki, Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

[P2-25] Effects of Stress Distribution on the Plastic Deformation of Metallic Glasses under Different Geometries

○Chih-Jen Yeh[1], Hsuan-Teh Hu[1], Chang-Wei Huang[2], Yu-Chieh Lo[3] （1.National Cheng Kung University, Taiwan, 2.Chung Yuan Christian University, Taiwan, 3.National Chiao Tung University, Taiwan）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-18] Prediction of Biaxial Tensile Deformation Behavior of Aluminum Alloy Sheets using Crystal Plasticity Finite Element Method and Machine Learning

○Kota Koenuma[1], Akinori Yamanaka[1], Ikumu Watanabe[2], Toshihiko Kuwabara[1] （1.Tokyo University of Agriculture and Technology, Japan, 2.National Institute of Materials Science, Japan）

Aluminum alloy sheets are used for automotive body parts to reduce the weight of automotive. However, because the formability of aluminum alloy sheets is much lower than that of steel sheets, the plastic deformation behavior of aluminum alloy sheets during plastic forming processes has been predicted by sheet metal forming simulations based on the finite element method. In order to predict the plastic deformation behavior of an aluminum alloy sheet subjected to a biaxial stress state in a sheet metal forming process, we proposed the numerical biaxial tensile test (NBT) methodology using the crystal plasticity finite element method (CPFEM) and the mathematical homogenization method. The NBT method has been already applied to predict the contour of equal plastic work of a 5000-series aluminum alloy sheet. The results demonstrated that the contour of equal plastic work (the yield locus) calculated by the NBT method shows a good agreement with that measured by the experimental biaxial tensile test using a cruciform specimen. Unfortunately, because we need to perform multiple NBTs to calculate the contour of equal plastic work, the disadvantage of the NBT method is its high computational cost. In this study, in order to predict the biaxial tensile deformation behavior of aluminum alloy sheets more efficiently, we propose a new numerical material testing methodology by combining the NBT method with machine learning methods. The deformation behavior of aluminum alloy sheets predicted by the proposed method is verified by experimental multi-axitial material tests.

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[P2-19] MobiDiC: A 3-D Dislocation Dynamics Simulation

○Ronan MADEC[1], Laurent COLOMBET[1], Ladislas KUBIN[2] （1.CEA, DAM, DIF, France, 2.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay, France）

In 3D lattice-based dislocation dynamics (DD) codes, dislocation segments are discretized on an underlying lattice in which they move by discrete jumps. The first version of such codes goes by the name of microMegas and dates back to the beginning of the 1990s [1]. It makes use of a line model in which dislocations are discretized in their slip planes into a succession of straight segments with edge and screw characters. Two more sophisticated versions of the initial code are currently in use, Tridis, which retains the 'screw-edge' line model [2] and an evolved version of microMegas with two additional mixed line directions [3].

MobiDiC (for 'Mobile Dislocation Colony') derives from this last version of microMegas and is devoted to mass mesoscopic simulations involving a large number of perfect dislocations. It is designed to overcome some limitations of the parent code in order to provide an improved and efficient framework for DD simulations that can further evolve.

The specificities of this code will be presented, in particular the ability to handle complex crystallographic structures and dislocation reactions. Indeed, MobiDiC is considerably more flexible than other lattice-based

DD codes because there is no limitation to the number of vectors per slip system. In addition a semi-nodal approach is used. For instance, the movements of segments connected to a high connectivity node, like triple nodes of a junction, are coordinated to move the node with the adequate degree of freedom.

Examples of applications will be given as well as results obtained with OpenMP and hybrid parallelisms using many-core processors.

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[P2-20] Temperature dependence of fatigue crack growth in Ti-6Al-4V

○Bhargavi Rani Anne, Masaki Tanka, Tatsuya Morikawa （Dept. of Materials Science and Engineering, Kyushu University, Japan）

Fatigue properties of dual phase (α+ß and primary α) Ti-6Al-4V were studied with respect to the range of temperatures and stress intensity range. Fatigue tests were conducted with both high and low stress intensity ranges in the temperature range between room temperature and 550K. Micro crack propagation was observed. Crack growth rate (da/dN) was measured where a is a crack length and N is a number of cycles, changing temperature. It was found that da/dN was increased with temperature. It is assumed that da/dN is the Arrhenius type of equation as it shows temperature dependence. Activation energy calculations were attained from Arrhenius plot between the logarithm of da/dN and the reciprocal of temperature. The dependence of activation energy on stress intensity range was also obtained, which provides the information on the dislocation mobility controlling the fatigue crack growth. The comparison of fatigue crack growth rate with the temperature dependence of dislocation motion was also studied in detail.

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[P2-21] Parametric model of discrete dislocation dynamics based on mathematical theory of moving curves

○Miroslav Kolar, Jan Kratochvíl, Petr Pauš, Michal Beneš （Czech Technical University in Prague, Czech Republic）

In this contribution we present the comprehensive model of discrete dislocation dynamics based on the mathematical theory of moving curves. The purpose of our model is the precise and mathematically rigorous description of the dynamics of dislocations, which are represented as smooth curves evolving in their respective slip planes.

Dislocations are described by parametric curves and their motion is governed by the curvature driven flow.

The parametric model is coupled with the model of tagential velocity for increased stability, and with algorithms for topological changes which allow modeling of complex effects as merging, splitting, self-replication or interaction with obstacles.
The numerical algorithm is based on the flowing finite volume method.

We present qualitative and quantitative results of our numerical simulations. We demonstrate the capabilities of our model in the predicting of dipole formation and consequent estimation of the endurance limit, in the modeling of several interacting dislocations, and in the application of our method on complex scenarios involving moving dislocations interactiong with several obstacles.

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[P2-22] On Visualization of Multiscale Information Transfer/Exchange Processes via FTMP-based Duality Diagram Representation Scheme

○Takuya Takagi, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

It may safely be said that one of the critical issues about multiscale polycrystalline plasticity modeling are ultimately consolidated into those about “ information transfer and exchange” concurrently taking place among plural scales of spontaneously evolving kinds. In tackling these, we make an attempt here to introduce the duality diagram-based scheme of FTMP into multi-grained models under tension, where FTMP stands for Field Theory of Multiscale Plasticity. The model used is composed of systematic combinations of representative crystallographic orientations, i.e., three multi-slip [100], [110] and [111], and two single-slip [123] and [125]. Strongly orientation-dependent intragranular substructure evolutions, successfully reproduced solely via FTMP-based finite element analyses, result in distinct overall deformation/fracture modes, including, e.g., local instability-induced brittle-like fracture modes. Corresponding duality diagrams, i.e., the spatial trace of the incompatibility tensor versus fluctuation of the elastic strain energy, are drawn and are compared with their rate versions. Found first is a similarity between the two diagrams, i.e., the normal and their rate forms, when they are constructed via grain-wise net sum basis, without taking the absolute values as we have done so far. Phase space diagrams are newly introduced both for the incompatibility and strain energy fluctuation to further examine those similarities in general. Demonstrated thereby is the models yielding “ in-phase” responses roughly correspond to the cases that exhibit relatively stable and ductile deformation/fracture modes. The phase shifts, on the other hand, are shown to be closely related to instability outset, based on which the construction of a possible measure of the “ degree” of instability is also attempted.

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[P2-23] **Rotational Field Evolutions based on Field Theory of Multiscale Plasticity (FTMP)**

○Tadashi Hasebe[1], Yasutaka Matsubara[2] （1.Kobe Univ., Japan, 2.Graduate School of Kobe Univ., Japan）

FTMP-based modeling and simulations have revealed its prominent descriptive capability of deformation-induced evolving inhomogeneities, e.g., band-like dislocation substructures, which are generally accompanied by misorientation across them. Three representative cases are examined in detail, i.e., (a)spontaneously evolved dislocation substructures, (b)eigenstrain-driven misorientation development for modeling lath martensite block structures, and (c)alternative degrees of freedom-driven lattice rotations enriched by incompatibility-based modified spin. For (a), we discuss deformation-induced spontaneous evolution of misoriented dislocation substructures, comparing dislocation density contours for BCC and FCC models, while, for (b), comparison is made of the eigenstrain-driven misoriented lath block structures among three incompatibility conditions, where screw dislocation networks are commonly evolved, yielding twisted lath boundaries. For (c), we examine emerging “kink-like” patterns associated with tensile twining assisted by incompatibility-based modification of rotation, comparing component-wise contributions of incompatibility tensor on evolving rotation fields with “kink-like” morphology for Mg single crystal under c-axis tension. In addition to these, “crystallization-like” patterns evolved in single crystal sample are extensively examined, where initially-prescribed laminated misorientation distributions and/or hardening moduli are introduced to the model used in (c).

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[P2-24] A 2D MESOSCALE STUDY OF DISLOCATIONS, CRACKS AND MARTENSITIC PHASE TRANSFORMATIONS

○Rachel Derby, Michael Budnitzki, Stefan Sandfeld (TU Bergakademie Freiberg, Germany)

TRIP-Steels are of commercial interest due to their exceptional strength. This is a result of the microstructure; a matrix of both austenite and martensite that when plastically strained, exhibits strain hardening behavior. Plastic deformation arises from the presence of dislocations and the martensitic phase transformations (MT) that take place inside the metal. To understand the macroscopic properties of TRIP-Steels, it is necessary to understand the underlying dynamics occurring at the mesoscale.

Most models do not take into account the interactions between martensitic phase transformations and dislocations, and therefore are missing the impact that these two phenomena exert on each other. While MD simulations can resolve both phenomena naturally, they are prohibitively expensive for larger crystal sizes or time scales. On the contrary, continuum models cannot resolve the motion of dislocations inside the material.

We combine dislocation dynamics and martensitic phase transformations to study the interplay between the two phenomena. For the dislocation problem we use a continuum dislocation dynamics (CDD) model, allowing us to reduce computational cost and increase the system size. CDD is coupled with a Phase Field approach, which we use to model martensitic phase transformations. This allows us to study how dislocation motion can be influenced in the presence of an MT. Additionally, simple crack geometries can also be modeled as special dislocation configurations, which helps to understand how cracks and voids may trigger or inhibit MT.

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[P2-25] Effects of Stress Distribution on the Plastic Deformation of Metallic Glasses under Different Geometries

○Chih-Jen Yeh[1], Hsuan-Teh Hu[1], Chang-Wei Huang[2], Yu-Chieh Lo[3] （1.National Cheng Kung University, Taiwan, 2.Chung Yuan Christian University, Taiwan, 3.National Chiao Tung University, Taiwan）

Metallic glasses (MGs) generally have diverse mechanical properties, such as high strength and poor ductility. The deformation behaviors of MGs, to a large extent, depend on the ambient conditions. For example, the deformation of MGs is homogenous at high temperature and low stress. On the other hand, the deformation of MGs is inhomogeneous at low temperature and high stress. However, the inhomogeneous deformation further causes the shear band which is an accumulation of local plastic deformation. The formation of shear band always leads to a catastrophic failure with the increasing plastic deformation. In order to study the generation of shear band, a multiscale model which considers the microscopic shear transformation in macroscopic deformation is inevitable. In this paper, a mesoscale model combines the finite element method and the kinetic Monte Carlo method is used to investigate the properties of the metallic glasses. More mechanical properties and deformation behaviors of the MGs can be explored through the proposed model. In addition, the geometries of pores in composite MGs are investigated. Stress concentration and redistribution due to the different shapes and sizes of pores in composite MGs are discussed. These results can improve the design of the MGs and prevent MGs from catastrophic failure.

Poster Session | D. Data-Driven and Physics-Informed Materials Discovery and Design

[PO-D2] Poster Session 2

Symposium D

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-26] Generalized nano-thermodynamic model for predicting size-dependent surface segregation in multi-metal alloy nanoparticles from smaller particles

○Abhijit Chatterjee （Dept. of Chemical Engg., Indian Institute of Technology Bombay, India）

[P2-27] Development of thermodynamic database of Nd-Fe-B-based permanent magnet alloys

○Jiang Wang, Lei Xu, Kaicheng Yang, Qingrong Yao, Guanghui Rao, Huaiying Zhou （School of Material Science and Engineering, Guilin University of Electronic Technology, China）

[P2-28] Design of proteins and biopolymers: role of directional interactions and of water.

○Valentino Bianco[1], Ivan Coluzza[2] （1.University of Vienna, Austria, 2.CIC biomaGUNE, center for cooperative research in biomaterials, Spain）

[P2-29] Aquatic pollutant removal by adsorption in zeolite structures: An experimental and molecular simulation study

○Mate Erdos[1], Nan Jiang[2], Sebastian G. J. Heijman[2], Othonas A. Moultos[1] （1.Process &Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Netherlands, 2.Department of Water Management, Faculty of Civil Engineering and Geosciences, Delft University of Technology, Netherlands）

[P2-30] Optimizing elastic moduli of the silicate glasses through high-throughput atomistic modeling and machine learning techniques

Yong-Jie Hu[1], Ge Zhao[2], Tyler Del Rose[1], ○Liang Qi[1] （1.Dept. of Materials Science and Engineering, University of Michigan, United States of America, 2.Department of Statistics, Pennsylvania State University, United States of America）

[P2-31] High pressure phase transition and structural stability of transition metal compounds

○Fanyan Meng[1], Wandong Xing[1,2], Rong Yu[2] （1.Dept. of Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-32] Development of artificial neural network model for prediction of electronic density of states in atomistic systems

○Atsushi Kubo, Yoshitaka Umeno （Institute of Industrial Science, the University of Tokyo, Japan）

[P2-33] Development of First-principles Platform Technology for Energy Research

○Kanghoon Yim[1], Chan-Woo Lee[1], Jehyun Lee[1], Incheol Jeong[2], Yong Youn[3], Seungwu Han[3] （1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Dept. of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science &Technology, Korea, 3.Seoul National University, Korea）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-26] Generalized nano-thermodynamic model for predicting size-dependent surface segregation in multi-metal alloy nanoparticles from smaller particles

○Abhijit Chatterjee （Dept. of Chemical Engg., Indian Institute of Technology Bombay, India）

Multi-metal alloy nanoparticles (NPs) offer new avenues for exploration and design of nanoscale-properties, e.g., catalytic, electronic and optical, by virtue of their tunable composition. Unfortunately, a method that can aid such exploration by accurately predicting the size-, shape- and composition-dependent elemental distribution associated with nanomaterials is crucially missing. A nano-thermodynamic model based on distribution coefficients Δ is introduced to fill this gap. Δ is employed to predict surface segregation in NPs as a function of the NP size and composition. Interestingly, we find Δ to be independent of size for NPs beyond 2 nm. This key finding motivates the construction of thermodynamic tables for distribution coefficients using segregation observed with one or more NP sizes. The tables can enable accurate prediction of phase diagrams for nanomaterials across a wide-range of sizes. Key concepts of this new theory are demonstrated with Au-Pt-Pd, Ag-Au-Pd and Ni-Pt-Pd, which are found to exhibit complex size-dependent segregation behavior for 2-6 nm NPs and relatively weaker size-dependence beyond 6 nm. Numerically well-converged values of Δ are calculated for small NPs using Monte Carlo simulations in the canonical ensemble. Simulations are based on an embedded atom method (EAM) potential for metal alloys.
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[P2-27] Development of thermodynamic database of Nd-Fe-B-based permanent magnet alloys

○Jiang Wang, Lei Xu, Kaicheng Yang, Qingrong Yao, Guanghui Rao, Huaiying Zhou （School of Material Science and Engineering, Guilin University of Electronic Technology, China）

Nd-Fe-B permanent magnets with excellent magnetic properties have been used in the industrial applications including medical apparatus and instruments, electrical machinery, aerospace, permanent magnet motor and wind power. In order to fully balance the application of rare-earth resource in magnetic materials and reduce the costs, it is a promise way to introduce high abundant rare earth (RE) metals (e.g. La, Ce, Y) into Nd-Fe-B permanent magnets [1-3]. Phase diagrams and thermodynamic information of the RE-Fe-B alloys are necessary to understand the effect of the abundant rare earth metals on phase formation, microstructure and magnetic properties of Nd-Fe-B permanent magnets.

In this work, the RE-Fe, RE-B and Fe-B sub-binary systems were reviewed firstly in the published literature. After that, the RE-Fe-B (RE=La, Ce, Pr, Nd) ternary systems were assessed using CALPHAD method on the basis of thermodynamic data and phase equilibria data, which is fundamental to obtain the thermodynamic database of multi-component RE-Fe-B alloy systems. The calculated results including liquid projects, isothermal sections and vertical sections as well as the solidification path of some alloys were compared with the experimental results using the thermodynamic database obtained. The thermodynamic database of the Nd-Fe-B-based permanent magnet alloy systems with high abundant rare earth elements is developed finally, which is necessary to design alloy composition and heat treatments of novel Nd-Fe-B permanent magnets

with good magnetic properties and low costs.

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Acknowledgements

This work was supported financially by National Key Research and Development Program of China (2016YFB0700901), National Basic Foundation of China (2014CB643703), National Natural Science Foundation of China (51761008, 51461013), Guangxi Natural Science Foundation (2016GXNSFDA380015, 2016GXNSFGA380001) and Guangxi Project of Science and Technology (2017AD23031).

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-28] Design of proteins and biopolymers: role of directional interactions and of water.

○Valentino Bianco[1], Ivan Coluzza[2] （1.University of Vienna, Austria, 2.CIC biomaGUNE, center for cooperative research in biomaterials, Spain）

The design of a (bio-)polymer is a rational scheme allowing to transfer the one-dimensional information contained in the polymer sequence into the three-dimensional information contained in the polymer folded conformation.

Proteins are an example of designable heteropolymers able to fold in unique target structures. The stability of the native conformation depends on the protein sequence and on the thermodynamic conditions of temperature and pressure.

In our work we use a multiscale approach to investigate how the geometry of the polymer backbone and the properties of the surrounding water affect the selection and the stability of proteins and, more in general, of artificial heteropolymers.

We find that the key actors are: i) the directional interactions along the backbone and ii) the hydrophilic/hydrophobic composition of the surface and core of the folded structure.

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(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-29] Aquatic pollutant removal by adsorption in zeolite structures: An experimental and molecular simulation study

○Mate Erdos[1], Nan Jiang[2], Sebastian G. J. Heijman[2], Othonas A. Moultos[1] （1.Process &Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Netherlands, 2.Department of Water Management, Faculty of Civil Engineering and Geosciences, Delft University of Technology, Netherlands）

Water contamination with micropollutants poses a serious threat to public health and the ecosystem. Technologies based on adsorption are widely used to remove micropollutants (inorganic and organic) from wastewater. Zeolites show a promising potential as adsorbents in these applications. Zeolites are crystalline, microporous aluminosilicates with well-defined 3-dimensional structure, composed of tetrahedral SiO_4 and AlO_4 clusters connected to each other by shared oxygen atoms. To compensate the charge imbalance caused by the aluminum content of the framework, exchangeable cations (usually alkali and alkaline earth cations) are located in the cavities of the structure. By removing the aluminum content of the framework the hydrophobicity of the zeolite can be increased, providing favorable adsorption characteristic to organic molecules. In this study, the effect of aluminium content of zeolite structures for aquatic pollutant removal are investigated. To that end, molecular simulations using Monte Carlo method are performed. In comparison with experimental methods, these simulation techniques can provide fundamental understanding of the nano scale behavior of the system which is crucial for designing new materials.

In this study, two types of zeolites (FAU, BEA) with different aquatic pollutants (2,4,6-trichlorophenol, triclosan) are investigated experimentally and with simulations. The simulated and experimentally measured results show qualitative agreement. To obtain insights into the adsorption mechanisms, radial distribution functions, and the distribution of adsorbates are calculated for each structure. The preferred adsorption sites and configuration of adsorbates (e.g., pi-pi stacking, H-bonding) are identified for each adsorbates and structures. Based on the simulation and experimental results the relationship of aluminium content and adsorption affinity can be determined and the performance of the different zeolites can be evaluated.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-30] Optimizing elastic moduli of the silicate glasses through high-throughput atomistic modeling and machine learning techniques

Yong-Jie Hu[1], Ge Zhao[2], Tyler Del Rose[1], ○Liang Qi[1] （1.Dept. of Materials Science and Engineering, University of Michigan, United States of America, 2.Department of Statistics, Pennsylvania State University, United States of America）

Chemical design of the silicate glass with high elastic moduli is of great interest. However, it is difficult to find a universal expression to predict the elastic moduli according to the glass composition before synthesis since the elastic moduli are a complex function of several material properties at different length scales. This work presents a computational framework to efficiently predict the elastic moduli of the silicate glass across a multicomponent compositional design space, including 11 types of additive oxides, by integrations of high-throughput molecular dynamic (MD) calculations and machine learning (ML) techniques. Our newly developed ML model can predict the elastic moduli for k-nary silicate glass systems, using the learning datasets generated from MD calculations for only binary and ternary systems. The usefulness of our model is

illustrated by identifying the most relevant materials descriptors that determine the elastic moduli and screening for the silicate glasses with high stiffness.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-31] High pressure phase transition and structural stability of transition metal compounds

○Fanyan Meng[1], Wandong Xing[1,2], Rong Yu[2] （1.Dept. of Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

The lattice, charge, spin and other degrees of freedom in transition metal compounds couple to one another, giving these materials rich physics and properties. The extreme conditions of high pressure and high temperature provide a new way to create new structures that do not exist at ambient pressure, which has become an important way for the discovery of novel transition metal compounds. In recent years, important progress has been made in the theoretical prediction and high pressure synthesis of new structures. First, this work suggests a lot of new materials to be investigated by changing stoichiometry in phase diagrams. Taking the V-C binary system as an example, here we report the first-principles prediction of a new type of vanadium carbide, V_5C_3, which has an unprecedented stoichiometry in the V-C system. It is demonstrated that the new phase is mechanically stable, and is energetically favorable than known phases under high pressures. We believe that this work opens a door to materials design by changing stoichiometry. And the relationship between the crystal structure, electronic structure and physical properties are discussed. Secondly, the phase transition under high pressure will be analyzed to understand the structural stability of materials at high temperatures and high pressures, providing important theoretical basis for optimizing high-pressure synthesis conditions.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-32] Development of artificial neural network model for prediction of electronic density of states in atomistic systems

○Atsushi Kubo, Yoshitaka Umeno （Institute of Industrial Science, the University of Tokyo, Japan）

Recently, the artificial neural network (ANN) model has been intensively applied to interatomic potentials for atomistic simulations. ANN-based potential functions possess basic characteristics; i.e., (1) they do not have any physical background besides the least geometrical conditions, e.g., physical quantity conservation against any coordinate transformation; (2) theoretically they can mimic any continuous functions. These features make ANN potentials applicable to complex atomistic systems, where various crystal structures and phases are relevant.

Since an ANN potential can be simply regarded as a mapping from atomistic structure to a real number, it is found that the application of ANNs does not have to be limited only for prediction of potential energy; i.e., ANNs are applicable to prediction of other physical quantities or material properties of the atomistic systems, e.g., electronic density of states (DoS), magnetic moment, etc. However, to the best of our knowledge, there has been no attempt to apply ANNs to prediction of physical quantities beside potential energy in atomistic systems. It will be of great impact if we can evaluate physical quantities such as electric or magnetic properties in huge atomistic structures using ANNs with the accuracy of the first-principles calculation.

In this study, we developed an ANN model to predict the DoS, as an exemplified case of prediction of general physical quantities in atomistic systems with ANNs. The ANN was optimized to reproduce the DoS in various crystal structures of silicon-carbon system that was obtained by first-principles calculations based on the density functional theory.

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[P2-33] Development of First-principles Platform Technology for Energy Research

○Kanghoon Yim[1], Chan-Woo Lee[1], Jehyun Lee[1], Incheol Jeong[2], Yong Youn[3], Seungwu Han[3] （1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Dept. of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science &Technology, Korea, 3.Seoul National University, Korea）

As future energy technologies such as high-capacity energy storage and renewable energy applications require exceptional functionalities of host materials, the importance of employing a novel material is getting bigger and bigger. However, discovering a new superior material is very hard to success though it requires large costs and manpower. Recently, many researchers attempt to use an informatics technology such as machine learning in materials screening to overcome the realistic limitations of conventional trial and error method. The key to successive research using informatics technology largely depends on the quantity and quality of the considered database rather than technical details of informatics model. Since property data from experiments are usually sparse or biased to favorable materials in industry, it is hard to obtain a practical database for the informatics research. In that point of view, first-principles calculation is an excellent tool for generating systematic and reliable data of materials properties. However, first-principles calculation itself also requires considerable computational resources and many practical properties are hard to obtain by simple calculations. Therefore, a decent automation of first-principles calculation can do a significant role to establish a successive database. In this talk, I’ll introduce the first-principles platform of Korea Institute of Energy Research aiming at providing a practical computing platform for various researchers with different backgrounds. After introducing the importance of well-defined automation procedure in former materials design studies such finding novel high-k dielectrics and p-type transparent oxides, I'll introduce the automated platform technology for surface-adsorption reactions which have great importance in most energy applications.

Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E2] Poster Session 2

Symposium E

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-34] Dynamics of a solidification front made by invasion of fluid with a different temperature

○So Kitsunezaki, Chika Yamanaka （Nara Women's Univ., Japan）

[P2-35] Strengthening through solid solution in $W_{1-x}Ta_xB$ system

○lijuan liu[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-36] Desiccation crack patterns based on phase-field modeling and their statistical properties

○Shin-ichi Ito[1], Satoshi Yukawa[2] （1.The Univ. of Tokyo, Japan, 2.Osaka Univ., Japan）

[P2-37] Ce-terminated (111) surface of CeO_2

○YaNan Zhao[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-39] **Numerical analysis of elasto-plastic behavior of metallic architectured materials**

○Filip Siska[1], Ivo Dlouhy[1], Jan Cizek[2], Hanus Seiner[3] （1.Institute of Physics of Materials, Czech Academy of Sciences, Czech Republic, 2.Institute of Materials Science and Engineering, Brno University of Technology, Czech Republic, 3.Institute of Thermomechanics, Czech Academy of Sciences, Czech Republic）

[P2-40] Automatic analysis and numerical prediction of flow stress curves for aluminium alloys

○Evgeniya Kabliman, Johannes Kronsteiner, Ana-Helena Kolody （Light Metals Technologies Ranshofen, Center fo Low-Emission Transport, Austrian Institute of Technology, Austria）

[P2-41] Comparison of different alkali activated mortars with hemp fibres response during fracture test by acoustic emission method

Libor Topolar[1], ○Hana Simonova[1], Barbara Kucharczykova[1], Zbynek Kersner[1], Jelena Dragas[2], Ivan Ignjatovic[2], Miroslav Komljenovic[3], Violeta Nikolic[3] （1.Brno University of Technology, Faculty of Civil Engineering, Czech Republic, 2.University of Belgrade, Faculty of Civil Engineering, Serbia, 3.University of Belgrade, Institute for Multidisciplinary Research, Serbia）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-34] Dynamics of a solidification front made by invasion of fluid with a different temperature

○So Kitsunezaki, Chika Yamanaka （Nara Women's Univ., Japan）

When fluid flows into another hotter or colder fluid, solidification often occurs in narrow regions at the vicinity of the interface. Such interfaces exhibit peculiar patterns in the growth process because of accompanying solidification fronts. Similar phenomena are observed in soft membranes created by chemical reactions of two fluid, as reported by H.~Wagatsuma et al.(Physical Review E, 2017). In geological scales, we could also see examples of such phenomena in pillow lava and growth of a volcanic island.
We carried out experiments by pouring ice-cold water into paraffin melt in a Hele-Shaw cell and found that solidification of paraffin causes fingering patterns with large meandering. The melting temperature of paraffin we used is about 56-58 degrees C, but the rheological measurements indicated that paraffin behaves as a soft viscoelastic material under the temperature. We infer that precipitous increase of the viscosity of paraffin is mainly responsible for large meandering of fingering growth.
A simple two-dimensional mathematical model is considered to find an interface dynamics in such phenomena theoretically. Although a standard method of the center-manifold reduction can not be used for solidification fronts growing in time, we develop a similar systematic method to derive the equations of interface motion.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-35] Strengthening through solid solution in $W_{1-x}Ta_xB$ system

○lijuan liu[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

The elastic properties, electronic structures and the energy barriers in slip processes of $W_{1-x}Ta_xB$ system have been studied using first-principles calculations. It was found that the (110) plane is the easiest slip plane in tungsten monoboride. By substituting tungsten with tantalum, slipping on the (110) plane can be hindered through dislocation pinning, resulting in the increase of overall hardness of tungsten monoboride Strengthening of the easiest planes is an effective approach to creating new hard materials in more metallic materials.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-36] Desiccation crack patterns based on phase-field modeling and their statistical properties

○Shin-ichi Ito[1], Satoshi Yukawa[2] （1.The Univ. of Tokyo, Japan, 2.Osaka Univ., Japan）

We investigate morphological properties on desiccation crack patterns through numerical simulations of a phase-field (PF) model. Since our PF model does not require any assumptions related to crack nucleations and numerical lattice configurations, we can investigate the pattern formations that purely depend on material/external parameters. Our PF model showed us various pattern formations depending on a drying speed and material constants. We discovered, in particular, the difference of the drying speed provides a significantly qualitative difference in the pattern formations. Cellular patterns resulting from sequential fragmentations of straight cracks can be observed when using a slow drying speed, while random network patterns resulting from connections of micro cracks that appear simultaneously can be observed when using a rapid drying speed. We quantify the difference of the pattern formations statistically, and explain the origin of the difference on the basis of a simple continuum theory of a thin layer of viscoelastic material.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-37] Ce-terminated (111) surface of CeO_2

○YaNan Zhao[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

Surface structure and properties of ceria are closely related to the applications of ceria in catalysis. Here, the atomic structures of the (111) surface of CeO_2 nanoparticles have been studied combining aberration-corrected transmission electron microscopy and first-principles calculations. Besides the oxygen termination that have reported extensively previously, the cerium termination has also been revealed by direct atomic imaging, which can be viewed as the simultaneous loss of surface and subsurface oxygen. The stabilization mechanism, electronic structure and magnetism of the surface, and the behavior of oxygen vacancies have been discussed.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-39] Numerical analysis of elasto-plastic behavior of metallic architectured materials

○Filip Siska[1], Ivo Dlouhy[1], Jan Cizek[2], Hanus Seiner[3] （1.Institute of Physics of Materials, Czech Academy of Sciences, Czech Republic, 2.Institute of Materials Science and Engineering, Brno University of Technology, Czech Republic, 3.Institute of Thermomechanics, Czech Academy of Sciences, Czech Republic）

Architectured materials is a class of materials that is characteristic by the ordering of constituents in specific geometrical manner. Such geometry provides an extra degree of freedom which allows reaching combinations of properties that cannot be obtained by standard materials. Metallic architectured materials are especially attractive because metals are important structural materials and adding internal architecture can enhance their performance in particular applications.

Our study is focused on a numerical investigation of an elasto-plastic response of different planar architectured patterns under the basic types of loading (tension-compression, bending). These patterns are made by different combinations of basic metals (for example: Al, Fe, Ti). The objective is to find the relation between the geometry and the resulting properties like stiffness, strength, hardening, ductility, buckling resistance. These relations will help to find optimal internal structure geometries for given materials combinations and loadings. The results from FE simulations will be further used for the production of the real structures using cold spray technology which is very well suited for a fabrication of structures and materials made of metals with different mechanical and physical properties.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-40] Automatic analysis and numerical prediction of flow stress curves for aluminium alloys

○Evgeniya Kabliman, Johannes Kronsteiner, Ana-Helena Kolody （Light Metals Technologies Ranshofen, Center fo Low-Emission Transport, Austrian Institute of Technology, Austria）

In present work, we develop a toolkit for automatic analysis of experimental flow stress curves as well for their numerical prediction by a combined approach of physics based and data driven modelling. By using a single environment it is possible to filter measured raw data, account for temperature increase during a deformation process, extract the mechanical properties such as yield and ultimate strength, obtain the processing maps for the optimization of deformation conditions, as well as to predict the flow stress curves by using a dislocation density based model in combination with algorithms of machine learning. It is possible to account for processes such as work hardening and recovery due to spontaneous annihilation of dislocations and their climb. For testing purposes we choose a conventional AA6082 alloy and perform a series of hot compression tests by using a deformation and quenching dilatometer DIL805A/D of TA Instruments. In order to choose the most suitable algorithm of machine learning, different approaches found in literature for the prediction of flow stress curves are compared. A modified version of a flow stress model is formulated and implemented into a finite element framework, as a result.

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[P2-41] Comparison of different alkali activated mortars with hemp fibres response during fracture test by acoustic emission method

Libor Topolar[1], ○Hana Simonova[1], Barbara Kucharczykova[1], Zbynek Kersner[1], Jelena Dragas[2], Ivan Ignjatovic[2], Miroslav Komljenovic[3], Violeta Nikolic[3] （1.Brno University of Technology, Faculty of Civil Engineering, Czech Republic, 2.University of Belgrade, Faculty of Civil Engineering, Serbia, 3.University of Belgrade, Institute for Multidisciplinary Research, Serbia）

In last decades, natural fibres are increasingly used as reinforcements for the production of low-cost composites in civil engineering. The benefits of natural fibers include non-abrasive nature, high specific properties, and biodegradability. However, their disadvantages are the bad moisture absorption, poor wettability and large scattering in mechanical properties. The aim of this paper is contribute to the better understanding of mechanical behaviour and failure modes of alkali activated materials reinforced by hemp fibers. Two different mortars based on alkali activated fly ash and slag were investigated. The paper includes the results of acoustic emission measurement captured during the three-point bending fracture test of specimens made of mentioned composites. Acoustic emission method is proving useful for the capability of real-time monitoring of materials over the whole volume and with high sensitivity to any processes generating stress waves. The effect of different mix composition and amount of hemp fibers on the acoustic signal features such as the energy, counting and amplitude is including in this research. The obtained acoustic emission results together with mechanical fracture parameters can serve as input values of material models used for modelling of structure response.

This outcome has been achieved with the financial support of the Czech Science Foundation, project No. 18-12289Y and the results obtained within the project DS-2016-0060, which belongs to Multilateral Scientific and Technological Cooperation Project in Danube Region between Technische Universität Wien, Brno

University of Technology and University of Belgrade, are presented in this paper.

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

[PO-F2] Poster Session 2

Symposium F

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-43] Design of spontaneous formation-based 3D plasmonic optical structure, using multyphysics modeling

○Jihwan Song[1], Inhee Choi[2], Yonghee Shin[3], SoonGweon Hong[5], Younggeun Park[5], Dongchoul Kim[4], Taewook Kang[3], Luke Lee[5] (1.Dept. of Mechanical Engineering, Hanbat National University, Korea, 2.Dept. of Life Science, University of Seoul, Korea, 3.Dept. of Chemical and Biomolecular Engineering, Sogang University, Korea, 4.Dept. of Mechanical Engineering, Sogang University, Korea, 5.Dept. of Bioengineering and Berkeley Sensor and Actuator Center, University of California, Berkeley, United States of America)

[P2-44] **Characterization of $K_xNa_{1-x}NbO_3$ powders and ceramics prepared by hydrothermal synthesis**

○Jing Yang, Aifen Tian, Xuan Xi, Huiling Du (Dept. of Materials Science and Engineering, Xi An Univ. of Science and Technology, China)

[P2-45] Numerical and experimental investigation of liquid metal dealloying of Cu-Ni alloy in liquid silver.

○Pierre-Antoine Geslin[1,2,3], Takumi Suga[2], Takeshi Wada[2], Hidemi Kato[2] (1.INSA Lyon/CNRS, France, 2.Institute for Materials Research, Tohoku University, Japan, 3.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan)

[P2-46] **Application of DLVO theory to predict dispersion stability of ZrO_2 submicron particles in electrolyte solutions**

○Ming-Hong Chiueh, Tien-Jung Huang (Industrial Technology Research Institute, Taiwan)

[P2-47] Multi-GPU large-scale phase-field lattice Boltzmann simulation of dendrite growth with thermal-solutal convection

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

[P2-48] Stress analysis of 4H-SiC power devices via FEM and Raman spectroscopy

○Hiroki Sakakima[1], Asuka Hatano[1], Akihiro Goryu[2], Kenji Hirohata[2], Satoshi Izumi[1] (1.The Univ. of Tokyo, Japan, 2.Toshiba, Japan)

[P2-49] A Functionally Graded Multi-Phase Micromechanical Model for Carbon Nanotube - Polymer Composites

○Vahidullah Tac[1,2], Ercan Gurses[1] (1.Middle East Technical University, Turkey, 2.Turkish Aerospace Industries, Turkey)

[P2-50] **Atomic surface treatment of copper nanowires by electron beam irradiation simulated by first principle calculation**

○Shih Kuang Lee (National Chiao Tung University, Taiwan)

[P2-51] Molecular-Dynamic Simulation of Rapid Solidification of Dipolar Molecular Crystal from Its Melt

○Xianqi Xu, Yang Yang (East China Normal University, China)

[P2-52] Intrinsic Analysis of Structural Order Parameter at Equilibrium Crystal-Melt Interfaces

○Wenliang Lu, Hongtao Liang, Yang Yang （EAST CHINA NORMAL UNIVERSITY, China）

[P2-53] Multiscale Modelling of Indirect-to-Direct Band Gap Transition in Silicon Nanosheets

○Byung-Hyun Kim[1], Chan-Woo Lee[1], Mina Park[2], Gyubong Kim[2], Kersti Hermansson[3], Peter Broqvist[3], Heon-Jin Choi[4], Kwang-Ryeol Lee[2] （1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Computational Science Research Center, Korea Institute of Science and Technology, Korea, 3.Dept. of Chemistry-Ångström Laboratory, Uppsala University, Sweden, 4.Dept. of Materials Science and Engineering, Yonsei University, Korea）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-43] Design of spontaneous formation-based 3D plasmonic optical structure, using multyphysics modeling

○Jihwan Song[1], Inhee Choi[2], Yonghee Shin[3], SoonGweon Hong[5], Younggeun Park[5], Dongchoul Kim[4], Taewook Kang[3], Luke Lee[5] （1.Dept. of Mechanical Engineering, Hanbat National University, Korea, 2.Dept. of Life Science, University of Seoul, Korea, 3.Dept. of Chemical and Biomolecular Engineering, Sogang University, Korea, 4.Dept. of Mechanical Engineering, Sogang University, Korea, 5.Dept. of Bioengineering and Berkeley Sensor and Actuator Center, University of California, Berkeley, United States of America）

Oil droplets in water or water droplets in oil have been generated fascinating science and utilized in enormous applications from medicine to energy harvesting. However, the creation of integrated three-dimensional architectures by liquid droplet and immiscible liquid interface is relatively less investigated. Here we report interfacial energy-driven and spontaneous formation of plasmonic cavity at room temperature without an external force. With the multiphysics approach considering the densities and interfacial energies of two different liquids, we simulated the spontaneous formation of cavity when a liquid water droplet meets immiscible liquid interface. At the interface, the metal ions in the liquid droplet are automatically reduced and they form the interfacial plasmonic layer onto the cavity surface. Due to the both optical cavity and integrated plasmonic structure, the significantly enhanced fluorescence is obtained by 1000 times. We believe our findings could offer a new avenue and advance in a variety of photonic and plasmonic materials and devices.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-44] **Characterization of $K_xNa_{1-x}NbO_3$ powders and ceramics prepared by hydrothermal synthesis**

○Jing Yang, Aifen Tian, Xuan Xi, Huiling Du （Dept. of Materials Science and Engineering, Xi An Univ. of Science and Technology, China）

There is an increasing demand to replace $Pb(Zr,Ti)O_3$-based piezoelectric materials with lead-free alternatives, because of the toxicity of lead oxide which is largely used during the production process. $K_xNa_{1-x}NbO_3$ (KNN) is considered as one of the most promising candidates for lead free piezoelectric ceramics due to its high Curie temperature and good electrical properties.

$K_xNa_{1-x}NbO_3$ ceramics can be used for several applications such as high frequency transducers, ultra-sonic diagnostics and tunable micro-wave components. However, it is well known that dense and well-sintered $K_{0.5}Na_{0.5}NbO_3$ ceramics are very difficult to obtain by the ordinary sintering process owing to the high volatility of alkali elements at high temperatures. The major strategy to overcome this problem is simply to synthetized KNN powders at low temperature. One method of making dense $(K_xNa_{1-x})NbO_3$ ceramics is to use refined powder with improved sintering activity, prepared in the molten salt process, sol-gel routine or hydrothermal process. In this work, $(K_xNa_{1-x})NbO_3$ powders and ceramics were prepared by hydrothermal synthesis. X-ray diffraction and scanning electron microscope were performed to investigate the structure and surface morphology of the $(K_xNa_{1-x})NbO_3$ powders and ceramics. The results showed that all the KNN powders possessed the pervoskite structure and a handful of second phases. The $K_{0.7}Na_{0.3}NbO_3$ ceramic prepared by the powders exhibits relatively good properties (relative dielectric constant $\varepsilon = 416$ and piezoelectric coefficient d_{33}=40 pC/N).

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-45] Numerical and experimental investigation of liquid metal dealloying of Cu-Ni alloy in liquid silver.

○Pierre-Antoine Geslin[1,2,3], Takumi Suga[2], Takeshi Wada[2], Hidemi Kato[2] （1.INSA Lyon/CNRS, France, 2.Institute for Materials Research, Tohoku University, Japan, 3.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan）

Liquid metal dealloying has emerged as a promising technique to produce finely porous structures of various nature (non-noble metals, refractory metals or semi-conductors) presenting a high surface area, valuable in a numerous applications (catalysis, battery materials, sensors,...). This process consists in emerging a binary precursor alloy (i.e. Cu-Ni) in a liquid metal (Ag) chosen such that only one element of the precursor alloy (Cu) dissolves into the metallic melt while the other element (Ni) reorganizes into a porous structure. We investigated the formation of this microstructure based on the ternary phase diagram of the Ni-Cu-Ag system. First, we developed a quantitative phase-field model to investigate the initiation of this dealloying process. The phase-field method is particularly adapted to investigate this kind of free-boundary problem and the complex morphogenesis of the structures, but is enable to reach the experimental time and size-scales. In a multi-scale approach, we use phase-field results and experimental observations to develop a macroscopic diffusion model able to reproduce the kinetics and the composition profiles obtained experimentally. Also, based on this work on the Cu-Ni-Ag model system, we were able to generalize our findings to other systems and assess the potential of other systems to form finely porous microstructures upon dealloying.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-46] **Application of DLVO theory to predict dispersion stability of ZrO_2 submicron particles in electrolyte solutions**

○Ming-Hong Chiueh, Tien-Jung Huang （Industrial Technology Research Institute, Taiwan）

In the manufacturing process of multi-layer ceramic capacitors (MLCC), electronic components often used in modern mobile phones, dispersion stability of ZrO_2 submicron particles can be improved by altering the pH of electrolyte solution. In this study we used the DLVO theory to predict the energy barriers of interaction forces between two ZrO_2 particles in various electrolyte solutions at different pH. The electrolyte solutions may be strong basic, weakly acidic, or strong acidic. The distance-dependent potentials of van der Walls force and electrical double layer force were calculated. The calculation results show that weakly acidic solution induces larger energy barrier between ZrO_2 particles, because of stronger electrical double layer force. This larger energy barrier can prevent aggregation of ZrO_2 particles and lead to dispersion stability.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-47] Multi-GPU large-scale phase-field lattice Boltzmann simulation of dendrite growth with thermal-solutal convection

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

Thermal-solutal convection, that inevitably occurs during terrestrial solidification of an alloy, drastically changes the dendrite morphology and microsegregation. Although phase-field method is the most powerful computational tool for predicting the dendrite morphology and microsegregation, we need many computational costs in the phase-field simulation taking the thermal-solutal convection into account. In this study, we enable a large-scale simulation for phase-field lattice Boltzmann model, which can express the dendrite growth with the transport of solute and heat and the fluid flow. Here, to reduce the computational cost, we employ a multi-level mesh and multi-level time step when solving phase-field equation, advection-diffusion equations for heat and solute, and lattice Boltzmann equation for computing the fluid flow. In addition, to accelerate the large-scale simulation, we implement the parallel computation using multiple graphics processing units (GPU). By employing the developed scheme, we perform the dendrite growth simulation during directional solidification of a binary alloy with thermal-solutal convection and investigate the effects of thermal-solutal convection on the dendrite morphology.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-48] Stress analysis of 4H-SiC power devices via FEM and Raman spectroscopy

○Hiroki Sakakima[1], Asuka Hatano[1], Akihiro Goryu[2], Kenji Hirohata[2], Satoshi Izumi[1] （1.The Univ. of Tokyo, Japan, 2.Toshiba, Japan）

We developed a scheme to analyze the stress distribution of 4H-SiC power devices by FEM and Raman spectroscopy. Raman spectroscopy is widely applied as a method for evaluating stress distribution of semiconductor devices. However, the relationship between phonon frequency, which is measured by Raman spectroscopy, and stress tensor is not clarified for 4H-SiC. In addition, it is impossible to evaluate the distribution of the stress tensor having six components only by Raman spectroscopy since the phonon frequency is a scalar quantity. To solve these problems, we detected phonon deformation potentials, which are the relationships between phonon frequency and stress tensor, and developed the analysis method combining FEM and Raman spectroscopy. Firstly, phonon deformation potentials were detected by first principle calculation. The phonon frequency of the strained crystal is calculated. All components of the phonon deformation potential constants were obtained from the relationship between the magnitude of stress and the phonon frequency shift. The calculated deformation potential constants were validated by previous experimental results. Secondly, multi-step thermal-stress FEM analysis which reproduces actual fabrication process was conducted for a pin diode. Young's modulus, linear expansion coefficient and intrinsic stress of thin films formed on SiC substrates were measured. The obtained stress distribution was converted into the distribution of the phonon frequency shift and validated through comparison with the result of the micro Raman spectroscopy. The obtained stress distribution and its origin will be presented. This work was supported by Council for Science, Technology and Innovation(CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), “Next-generation power electronics/Consistent R&D of next-generation SiC power electronics” (funding agency: NEDO)

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-49] A Functionally Graded Multi-Phase Micromechanical Model for Carbon Nanotube - Polymer Composites

○Vahidullah Tac[1,2], Ercan Gurses[1] （1.Middle East Technical University, Turkey, 2.Turkish Aerospace Industries, Turkey）

Carbon nanotubes (CNT) are widely known for their superior stiffness as well as strength since their discovery in 1991. While our current level of understanding of carbon nanotubes prevent us from using them in structural parts per se, embedding them in polymers for strengthening and stiffening purposes shows a great potential. However practical efforts towards designing, manufacturing and employing such nanocomposite materials have not yet fully culminated largely due to a lack of understanding of the bonding between the nanotube and the polymer.

Latest experimental and molecular mechanical observations of the region around a carbon nanotube embedded inside a polymer indicate the presence of at least four distinct “phases” in nanocomposites; the CNT, the thin interfacial gap between the CNT and the polymer, a large portion of polymer around the CNT with linearly varying properties, and the bulk polymer phase.

Hence, to accurately model nanocomposite material the varying nature of polymer in the proximity of the CNT has to be taken into account, among other things.

We adopt a multi-phase micromechanical model that allows gradual degradation/upgradation of the constituent phases to study the mechanical properties of CNT-Polymer composites. Using this model the mechanical properties of the polymer is gradually enhanced in the vicinity of the CNT. We also study the effect of the gap between the CNT and the polymer and the role it plays in such nanocomposites. The results of our analyses are then compared to experimental data and discussed in detail.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-50] **Atomic surface treatment of copper nanowires by electron beam irradiation simulated by first principle calculation**

○Shih Kuang Lee （National Chiao Tung University, Taiwan）

Atomic surface treatment of copper nanowires by electron beam irradiation simulated by first principle calculation

Alex Lee [a],Ting-Yi Lin [a], Yu-Chieh Lo [a], and Wen-Wei Wu [a]

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Recently, the techniques of atomic surface treatment by electron beam etching has developed vigorously. However, the improvement and more details should be understood specially in atomic scale. In the experiment when we applied the electron beam on copper nanowires with copper oxide (111) surface without heating, it was found the reduction reaction and the following Cu clusters slip on Cu (111) surface. For further complete the mechanism, we provide the Vienna ab initio simulation package (vasp) to perform the GGA calculation with PAW pseudopotentials. For reduction reaction, we compare the energy between the theoretical structure of Cu with oxide surface and Cu (111) surface to predict the binding energy of oxygen. For the slip of Cu clusters, we calculate the energy mapping of slip path on Cu (111) surface to find the most probable routine of slip. The calculation data should help us control the intensity of electron beam radiation when we do the surface treatment of material and be the complement of slip observation.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-51] Molecular-Dynamic Simulation of Rapid Solidification of Dipolar Molecular Crystal from Its Melt

○Xianqi Xu, Yang Yang （East China Normal University, China）

We present results of molecular dynamics (MD) simulations of crystal growth from the melt. The work focuses on a face-centered-cubic molecular crystal consist with molecules modeled by an extended point dipole model. We will present results of non-equilibrium MD growth simulations as a function of temperature and molecular dipole moment. An analysis of the interfacial position as the function of simulation time was employed to extract the steady-state, and the data of the kinetic coefficients vs. molecular dipole moments and their anisotropies were calculated and will be presented. Values of the kinetic coefficient for the (100), (110) interfaces are compared quantitatively to the prediction of Mikheev-Chernov (MC) theory. Our study suggest that incorporating a second relaxation time due to the dipolar fluctuation beside the relaxation time of density waves, is necessary for extending MC theory to be applicable for molecular crystals.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-52] Intrinsic Analysis of Structural Order Parameter at Equilibrium Crystal-Melt Interfaces

○Wenliang Lu, Hongtao Liang, Yang Yang （EAST CHINA NORMAL UNIVERSITY, China）

We present atomistic simulations of precisely equilibrated crystal-melt interface under ambient pressure, for pure Ni and Fe. We demonstrate the capillary waves roughen the surface, but the intrinsic interfaces can be sharply defined. We use different types of local structural order-parameter together with a reference lattice to characterize the intrinsic interface. The statistical analysis on the structural order-parameters for the interfacial solid and interfacial liquid atoms represents universal scaling behavior, nearly independent of the order parameter type, crystal structure and interface orientations. We will discuss the potential application of such intrinsic analysis to the investigations of crystal nucleation and steady-state crystallization from melt.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-53] Multiscale Modelling of Indirect-to-Direct Band Gap Transition in Silicon Nanosheets

○Byung-Hyun Kim[1], Chan-Woo Lee[1], Mina Park[2], Gyubong Kim[2], Kersti Hermansson[3], Peter Broqvist[3], Heon-Jin Choi[4], Kwang-Ryeol Lee[2] （1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Computational Science Research Center, Korea Institute of Science and Technology, Korea, 3.Dept. of Chemistry-Ångström Laboratory, Uppsala University, Sweden, 4.Dept. of Materials Science and Engineering, Yonsei University, Korea）

Two-dimensional (2D) nanomaterials such as graphene, boron nitride (BN), and MoS_2 have attracted great attention owing to their exceptional and tuneable properties, which are distinguishable from those of their bulk phases. Recently, Si nanosheets (Si NSs) have been synthesized by various experimental techniques. Compared to other materials, Si-based nanostructures have great advantages when it comes to commercialization, as Si is compatible with the conventional device manufacturing processes in the microelectronics industry.

In experiments, (111) Si NSs showed thickness-dependent light emissions in the visible wavelength regime, originating from quantum confinement effects. This observation indicates that thin (111) Si NSs have a direct band gap, whereas bulk Si normally has an indirect band gap. However, the question of the physical origin behind this nano-effect of Si left unanswered.

The effect of biaxial strain on the band structure of 2D Si NSs with (111), (110), and (001) exposed surfaces was investigated by means of a multiscale modelling approach combining molecular dynamics simulations with a reactie force field and the density functional theory. For all the considered Si NSs, an indirect-to-direct band gap transition occurs as the lateral dimensions of Si NSs increase, i.e. increasing lateral biaxial strain from compressive to tensile always enhances the direct band gap characteristics. Further analysis revealed the mechanism of the transition which is caused by preferential shifts of the conduction band edge at a specific *k*-point due to their bond characteristics. Our results explain a photoluminescence result of the (111) Si NSs [U. Kim *et al.*, *ACS Nano* **2011**, *5*, 2176-2181] in terms of the plausible tensile strain imposed in the unoxidized inner layer by the surface oxidation.

Poster Session | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[PO-G2] Poster Session 2

Symposium G

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-54] **Component-wise Effect of Incompatibility Tensor on Misorientation Development in Lath Block Structure Model based on FTMP**

○Yuta Amano, Tadashi Hasebe, Yasutaka Matsubara （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P2-55] Construction of virtual ITZ specimens using extended stochastic optimization and evaluation of their permeability

○Se-Yun Kim, Tong-Seok Han （Dept. of Civil and Environmental Engineering, Yonsei Univ., Korea）

[P2-56] Estimation for probabilistic distribution of material response according to microstructural characteristics

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

[P2-57] **Hypervelocity impact and shock behavior of pillared graphene foams**

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

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-54] **Component-wise Effect of Incompatibility Tensor on Misorientation Development in Lath Block Structure Model based on FTMP**

○Yuta Amano, Tadashi Hasebe, Yasutaka Matsubara （Dept. of Mechanical Engineering, Kobe Univ., Japan）

Modeling complex microstructures, e.g., those like lath martensite structures in high Cr ferritic heat resistant steels, are one of the critical issues in multiscale modeling of materials, although neither conventional schemes exist nor effective methodologies have been developed to date. In the present study, FTMP (Field Theory of Multiscale Plasticity)-based Di-CAP (Deformation-induced Context-dependent Autonomic Pluripotency) concept is applied to computationally fabricate complex microstructured samples to be further utilized in various deformation analyses based on, e.g., FEM. Here, we focus on the process of modeling single lath-block structures, which can be obtained in preliminary bi-axial compression analyses, provided the corresponding eigenstrain distributions based on the Bain lattice correspondence is initially introduced. One of the keys for the lath-block modeling is the development of misorientation across the lath boundaries, roughly satisfying K-S variant, together with the attendant internal stress fields. FTMP-based approach exhibits spontaneous evolution of such misorientation when substantial contribution of the incompatibility tensor is introduced in the hardening law. Here we decompose the incompatibility tensor into (a)pure deformation and pure rotation, (b)edge and screw, and (c)spherical (isotropic) and deviatoric components, respectively, to examine the mechanisms for the misorientation developments. Analyses are conducted using two basic models for a single lath block structure, i.e., vertical and horizontal models, where lath sub-blocks are aligned vertically and horizontally to the [111] axis, respectively. Demonstrated for (a) is that the pure deformation part shows relatively larger contributions to the misorientation developments, while, for (b), dominant contributions of the screw component are confirmed. For (c), on the other hand, the weighted spherical part is shown to have weak but basically the same contribution.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-55] Construction of virtual ITZ specimens using extended stochastic optimization and evaluation of their permeability

○Se-Yun Kim, Tong-Seok Han （Dept. of Civil and Environmental Engineering, Yonsei Univ., Korea）

The external substance penetrates into an interfacial transition zone (ITZ) that is located between an aggregate and bulk cement paste and has a relatively high porosity than the bulk cement paste. However, it is difficult to confirm the 3-D microstructure of the ITZ with the functionally graded void distribution to evaluate its permeability. In this study, 3-D microstructures of bulk cement pastes with three kinds of porosities and the void gradient of the ITZ obtained from 2-D SEM image are used to construct the virtual 3-D microstructures of the ITZ. Based on the two information, the phase distribution characteristics of the ITZ are generated, and they are used for constructing the virtual ITZ specimen using a stochastic optimization. The stochastic optimization is an appropriate method to construct a random heterogeneous material [1], but the ITZ has the functionally graded void distribution, which depends on the distance from the aggregate. To construct the functionally graded microstructure, an extended stochastic optimization is proposed. In addition, an efficient iteration method for stochastic optimization is proposed and utilized for construction of the virtual ITZ specimens, which improved the computational cost. The permeability of the virtual ITZ

specimens are evaluated by a finite element method. The effect of the ITZ from the penetration of the external substances is confirmed by the permeability analysis using the virtual ITZ specimen. This study shows that the proposed extended stochastic optimization process is effective for constructing functionally graded phase distribution, while the real 3-D microstructure is difficult to obtain from experimental techniques. This study also confirms that the virtual experiment procedure can be synergistically used with the real experimental approaches.

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(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-56] Estimation for probabilistic distribution of material response according to microstructural characteristics

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

There is a strong correlation between the material microstructure and its response [1]. It is expected that the statistical distribution of material response has a relation with that of the microstructure characteristics, so that the effect of the microstructure to the response can be investigated. In this study, the sensitivity of the material responses due to microstructural characteristics is investigated using a first-order second moment (FOSM) method [2]. The FOSM method is a probabilistic method, which determines the mean and deviation of a function of responses with random input variables. For applying the FOSM method, specimens with certain microstructure characteristics might have to be reconstructed. For this reason, the reconstruction process [3] to generate the target specimens are needed. The area of lineal-path function and porosity of cement paste specimens are selected as random input variables, and the stiffness and strength evaluated by phase field fracture model are selected as output variables. The result of sensitivity analysis from the FOSM method is compared to the simulation results using whole specimens. From this result, the sensitivity of material response to microstructure is estimated using two reconstructed specimens, and the FOSM method is confirmed to reduce the time and cost for evaluating the probabilistic distribution of properties.

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(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-57] Hypervelocity impact and shock behavior of pillared graphene foams

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

The effectiveness of graphene as material for impact protection has been confirmed both by atomistic simulations [1] and microscale experiment [2] obtaining unprecedented impact toughness up to ~50 MJ/kg at the nanoscale [1]. However, specific energy absorption could be, in principle, further increased by tailoring inter-layer interaction [3] via interface structuring or functionalization. In this study we present a modified graphene nanoarmor concept obtained by the introduction of pillar structures in the form of carbon nanotubes [4] of variable spatial density, aspect ratio, and size which allow the realization of stable graphene multilayers with variable spacing. Impact strength and shock behavior of such structures are investigated via molecular dynamics (MD) simulations and the effect of foam geometry on the specific energy absorption capability is evaluated across different size-scales.

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

[PO-H2] Poster Session 2

Symposium H

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-58] Studying the kinetics of a self-propelled cruiser in 2D granular media under gravity

○Guo-jie Jason Gao (Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan)

[P2-59] A Discrete Tetris model showing two flow regimes for hard particles exiting a hopper with an adjustable obstacle

○Tomoya Yasuno[1,2], Guo-jie Jason Gao[1] (1.Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan, 2.Dept. of Complex Systems Science, Nagoya Univ., Japan)

[P2-60] Effect of water molecules on polymer chain motion in dense chain ensembles of nafion membrane

○Isamu Riku, Ryoma Oka, Koji Mimura (Osaka Prefecture Univ., Japan)

[P2-61] A Coarse-Grained Model for Competitive Adsorption on the Surface of Inorganic Nanomaterials

○Stefano Poggio[1], Hender Lopez[2], David Power[1], Vladimir Lobaskin[1] (1.School of Physics, University College Dublin, Ireland, 2.Institute Laue-Langevin, Grenoble, France)

[P2-62] Molecular Dynamics of Inorganic and Organic Interfaces with Force-Field Parameters Based on DFT Simulations

○Kosuke Ohata, Hiroya Nitta, Kenta Chaki, Taku Ozawa (JSOL Corporation, Japan)

[P2-63] **Molecular dynamics screening for developing compounds of electrolytes with high performance in lithium ion batteries**

○Yoshihiro Takai[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] (1.Graduate school of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan)

[P2-64] Molecular dynamics study on transmission mechanism of torsional deformation in cellulose nanofibers with hierarchical structure

○Kentaro Takada[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] (1.Graduate School of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan)

[P2-65] Bubble dynamics of foam flow around an obstacle

○Antti Puisto, Juha Koivisto, Leevi Viitanen, Mikko J Alava (Aalto University, Department of Applied Physics, Finland)

[P2-66] Shape Deformation and Mechanical Relationship of Ionic Droplet Under An Electric Field

Bo-Yu Shih[1], ○Wei-Chun Lin[1], Alice Hu[2], Hsuan-Teh Hu[1], Yu-Chieh Lo[3] (1.Department of Civil Engineering,National Cheng Kung University, Taiwan, 2.Department of Mechanical and Biomedical Engineering, City University of Hong Kong, Hong Kong, 3.Department of Materials Science and Engineering, National Chiao Tung University, Taiwan)

[P2-67] Multiscale modeling of surface functionalized graphene/polymer nanocomposites: insight into the effect of covalent grafting

○Jeong-ha Lee[1], Seunghwa Yang[2] (1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea)

[P2-68] Durability analysis on the environmental aging of epoxybased nanocomposite

○Sunyong Kwon[1], Man Young Lee[2], Seunghwa Yang[3] （1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Agency for Defense Development, Korea, 3.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-58] Studying the kinetics of a self-propelled cruiser in 2D granular media under gravity

○Guo-jie Jason Gao （Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan）

Experimentally and numerically, it has been shown that placing an obstacle near the orifice of a hopper can locally enhance the flow rate for hard discs leaving the hopper under gravity. Besides, the enhanced flow rate happens regardless the interparticle friction, the obstacle geometry, or particle dispersity. In this study, we propose a Tetris model to further clarify the physics behind this phenomenon. The model sequentially moves one particle at a time towards the hopper orifice, governed by Gaussian displacement functions. A particle can move as long as the movement creates no overlap between the particle and the others, the obstacle, or the boundaries of the hopper. Our model reduces the dynamics in the system to its minimal and allows no interparticle collaborative motion due to Newtonian dynamics. Using this model, we successfully reproduce the locally enhanced flow rate, which can be explained by a flow rate difference between its value near the obstacle and its maximal value without an obstacle. Our results show that the flow rate difference is the fundamental reason causing this phenomenon - universal with minimal dynamics involved.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-59] A Discrete Tetris model showing two flow regimes for hard particles exiting a hopper with an adjustable obstacle

○Tomoya Yasuno[1,2], Guo-jie Jason Gao[1] （1.Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan, 2.Dept. of Complex Systems Science, Nagoya Univ., Japan）

Placing an obstacle near the orifice of a hopper has been shown experimentally and numerically to locally enhance the flow rate for hard particles leaving the hopper under gravity. A flow rate difference between its value near the obstacle and its maximal value without an obstacle can explain this phenomenon with minimal dynamics involved. When the obstacle sits close to the hopper orifice, the flow rate near the obstacle is smaller than the maximal value, which corresponds to a fluidized flow regime. On the other hand, when the obstacle is placed further from the orifice, the flow rate near the obstacle becomes larger than the maximal value and a clogging flow regime appears. In this study, we employ a Tetris model in 2D discretized space and successfully demonstrate the two flow regimes. Without creating overlap between any objects in the system, our model sequentially relocates one particle at a time into its von Neumann or Moore neighborhood closer to the hopper orifice. Our results show that in the fluidized regime, where flow rate is low, the Moore protocol, which allows higher freedom to move particles, gives higher flow rate than the von Neumann protocol. The trend reverses in the clogging regime, where higher freedom to move particles renders lower flow rate.

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[P2-60] Effect of water molecules on polymer chain motion in dense chain ensembles of nafion membrane

○Isamu Riku, Ryoma Oka, Koji Mimura （Osaka Prefecture Univ., Japan）

Because of the high power density, high efficiency, fast start-up, and zero emission at the point of use, proton exchange membrane fuel cells (PEMFCs) are the most promising candidates for replacing internal combustion engines in automobiles, and are also being developed for portable and distributed stationary power generation applications.
However, the life of PEMFCs is currently limited by the mechanical endurance of polymer electrolyte membranes (PEMs). The failure of PEM is believed to be the result of a combined chemical and mechanical effect acting together. Recently, it is found that cyclic hydration of the membrane during the operation cycles (start/shut down) of the fuel cell may cause mechanical degradation of the membrane.
Therefore, in this paper, to investigate such mechanical degradation of the membrane subjected to fuel cell cycles, we perform a series of molecular dynamic simulations for the membrane made from the sulfonated tetrafluoroethylene copolymer with the trade name Nafion. The effect of the water molecules on the polymer chain motion in dense chain ensembles of nafion membrane is to be clarified.

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[P2-61] A Coarse-Grained Model for Competitive Adsorption on the Surface of Inorganic Nanomaterials

○Stefano Poggio[1], Hender Lopez[2], David Power[1], Vladimir Lobaskin[1] （1.School of Physics, University College Dublin, Ireland, 2.Institute Laue-Langevin, Grenoble, France）

The increased use of nanoparticles (NP) and nanomaterials is pushing scientific research into trying to understand the mechanisms governing interactions between biomolecules and inorganic materials. It is known that, once a NP is in contact with a biological medium, a protein corona forms on its surface, and that the nature of the corona is what regulates the interaction between the NP and the other biomolecules.
In this work we propose a method to coarse grain the interactions of inorganic nanomaterials in contact with biological fluids of arbitrary composition. Biomolecules (lipids, proteins and carbohydrates) are coarse grained by mapping their main chemical fragments onto single beads, and their interaction with the NP surface is described a potential of mean force from atomistic simulations [2]. The NP is represented by a two-layer model where the surface interacts with the molecule beads by using the beads PMF with a slab of the material, corrected by a geometric factor, while the core interacts with via van der Waals forces calculated using Lifshitz theory. This model can describe the kinetics of competitive adsorption of biomolecules on the surface of a NP.
We have studied the kinetics of adsorption and the corona composition of Au NPs in a biological environment with the typical composition of lung lining fluid and blood plasma. This methodology can then be combined with adverse outcome pathway analysis to build mechanism-based predictive schemes for toxicity assessments.

Funding: H2020 grant SmartNanotox, contract No. 686098

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(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-62] Molecular Dynamics of Inorganic and Organic Interfaces with Force-Field Parameters Based on DFT Simulations

○Kosuke Ohata, Hiroya Nitta, Kenta Chaki, Taku Ozawa　(JSOL Corporation, Japan)

Nanocomposites are important in the engineering field. However, the controlling of the properties of interfaces between inorganic solid fillers and organic molecules is one of the key issues. We have investigated the interaction between solids and polymers with a combination of Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations. DFT is a reliable method for calculating potential energy surface (PES). The force field parameters for MD simulations were determined by using our scheme for interfacial systems based on the DFT simulation. Then the scheme was applied to a solid-polymer interface. Utilizing the determined coarse-grained and full-atomistic force field parameters, the MD simulations were conducted. In this study, we utilized SIESTA for the QM simulation and J-OCTA for the system modeling and the MD simulation.

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[P2-63] **Molecular dynamics screening for developing compounds of electrolytes with high performance in lithium ion batteries**

○Yoshihiro Takai[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2]　(1.Graduate school of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan)

Recently, there is great interest in development of electric vehicles, so it demands improvement in performance of Lithium-ion Battery (LIB). For higher performance, it is important to develop new substances used for electrolyte or electrode. In particular, electrolyte is an important chemical factor for moving lithium ions between positive and negative electrodes in the battery. When the amount of ions moving is enhanced, the performance of the battery will be effectively improved. But there are hundreds of thousands of compounds as candidates for electrolytes, so we need to screen and choose ones from these many compounds. In this research, we perform atomistic evaluation about various characteristics of possible compounds of electrolyte (such as viscosity, ionic conductivity, degree of dissociation and diffusion coefficient) by mainly using molecular dynamics (MD) simulations. In evaluating at a molecular level, we can understand how the molecular level structure and properties affect the behavior of electrolyte. Molecule models we are using are ethylene carbonate (EC), fluoro ethylene carbonate (FEC), propylene carbonate (PC), butylene carbonate (BC), γ-butyrolactone (GBL), γ-valerolactone (GVL), dimethyl carbonate (DMC), ethyl-methyl carbonate (EMC), diethyl carbonate (DEC), and lithium hexafluorophosphate ($LiPF_6$). An electrolytes system in which 1 mol of $LiPF_6$ is mixed per 1 L of single solvent (solvent + 1M-$LiPF_6$) is simulated. The results suggest that we can determine a criterion for the screening of superior compounds based on information about molecular structures and properties of electrolyte. It is found that the smaller solvent molecules that easily diffuse contribute to the higher ionic conductivity of electrolytes. This is because diffusion coefficient of Li cation is greatly affected by that of solvent molecules. It is also found that solvation structure and size around Li cation take large effect on its diffusivity.

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[P2-64] Molecular dynamics study on transmission mechanism of torsional deformation in cellulose nanofibers with hierarchical structure

○Kentaro Takada[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] （1.Graduate School of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan）

Cellulose nanofiber (CNF) has high strength comparable to steel, and it shows low environmental load during a cycle of production and disposal. Beside it has many excellent properties and functions such as high rigidity, light-weight, flexibility and shape memory effect, so it is expected as a next-generation new material. CNF is a fibrous and nano-sized substance produced by decomposition of bulk-type cellulose which is a main component of plants. Usually it is constituted by many cellulose micro fibrils (CMFs) in which molecular chains of cellulose are aggregated in a crystal structure. It is also possible to make composite material of CNF together with other components, and then a new material with lightweight as well as high strength and high toughness will be realized. In such case, knowledge of mechanical properties for each CMF units is important. Since actual fibrils are complicatedly intertwined, it is also crucial to elucidate the transmission mechanism of force and deformation not only in one fibril but also in between fibrils. Indeed, how the dynamic and hierarchical structure composed of CMFs responds to bending or torsion, which includes gradient of stress and strain, is an interesting issue. However, little is known on torsional characteristics (shear modulus, torsional rigidity, etc.) concerning CMF. In general, in a wire-like structure, it is difficult to enhance torsional rigidity and strength, compared with tensile ones. Therefore, in this study, we try to build a hierarchical model of CNF by multiplying CMF fibers and to conduct molecular dynamics simulation for torsional deformation, by using a hybrid modeling between all-atoms and united-atoms models. First, shear modulus was estimated for one CMF fibril and it showed a value close to the experimental values. In addition, it is revealed that intermolecular hydrogen bonds (HBs) are dynamically changed and the HB mechanism is likely to work as strong resistance in torsional deformation.

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[P2-65] Bubble dynamics of foam flow around an obstacle

○Antti Puisto, Juha Koivisto, Leevi Viitanen, Mikko J Alava （Aalto University, Department of Applied Physics, Finland）

Foams are one of the rare examples of simple yield stress fluids. Formed of bubbles embedded in liquid they are often studied in the context of jamming [1]. Foam flow is interesting not only because the start-up requires a dynamical unjamming transition (yielding), but also due to novel technological applications related to forming technologies [2].

Here, we study a foam flow through a 2D Hele-Shaw shell with an obstacle, forming a constriction. For this purpose, we use bubble scale dynamics model (the Durian bubble model), which we extend with the appropriate descriptions for the boundary effects coming from the walls and the top and bottom plates. We

observe a negative wake behind the obstacle, analogous to the one observed in gas bubble motion in a viscoelastic medium. There, the medium is succesfully described by an Oldroyd-B model. This suggests that in the present conditions, the foam acts as a typical viscoelastic fluid, rather than the expected elastoviscoplasticity [3]. We compare the simulations data against experiments, foam intruder experiments, where we find a similar flow pattern. We find a reasonable agreement in the flow dynamics and the overshoots between the experimental data and the bubble model. Finally, we identify a viscoelastic timescale, which determines the magnitude of the velocity overshoot.

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(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-66] Shape Deformation and Mechanical Relationship of Ionic Droplet Under An Electric Field

Bo-Yu Shih[1], ○Wei-Chun Lin[1], Alice Hu[2], Hsuan-Teh Hu[1], Yu-Chieh Lo[3] （1.Department of Civil Engineering,National Cheng Kung University, Taiwan, 2.Department of Mechanical and Biomedical Engineering, City University of Hong Kong, Hong Kong, 3.Department of Materials Science and Engineering, National Chiao Tung University, Taiwan）

Nano-sized symmetric double Taylor cone forms a capillary liquid bridge while electric field applied on Ionic liquids (2-dimethyl-3-propylimidazolium- bis(trifluoromethylsulphonyl)imide). This ionic liquid bridge size is around 20 nm. We attempt to understand the critical dimensions and stability criteria for nano-bridge forming mechanism. Therefore, we conduct molecular dynamics simulation under electric field to investigate ionic droplets electrohydrodynamic behavior with different structures and potential functions. Factors that affect liquid bridge size through extensive parameter are studied thoroughly in this work. We also investigate the influence of changing velocity field and shape deformation under different electric field conditions. The mechanical relationship between electric stress, Coulomb electrostatic force and the intermolecular interactions are analyzed. Through this complete studies, surface tension coefficient and ionic liquid viscosity are obtained. Results show that shape deformation and size of liquid bridge are mainly controlled by surface tension coefficient and viscosity.

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[P2-67] Multiscale modeling of surface functionalized graphene/polymer nanocomposites: insight into the effect of covalent grafting

○Jeong-ha Lee[1], Seunghwa Yang[2] （1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea）

Polymer nanocomposites is applied in various industries to improve their mechanical, electrical, thermal properties instead of using pure polymer. In view of improving mechanical properties of polymer nanocomposites, graphene nanosheets is typical reinforcement due to its excellent properties. However, agglomeration of graphene nanosheets in polymer reduces their mechanical and thermal properties. Besides,

weak cohesive energy between graphene and polymer by poor van der waals interaction causes slip condition in their interfacial region. To improve their intrinsic weak interfacial strength and dispersion properties between graphene and polymer nanocomposites, surface treatment of graphene such as covalent grafting or functionalization on graphene nanosheets have been generally used in graphene/polymer nanocomposites.

In this study, multiscale modeling approach for pristine and covalently functionalized graphene included polypropylene nanocomposites is implemented. Representative unit cell consists single-layered graphene and polypropylene matrix is modeled with three-dimensional periodic boundary conditions. Different number of covalent grafting on graphene is considered to investigate effect of grafting density. In molecular dynamics simulations, reactive forcefield for hydrocarbon structure is used to describe carbon-carbon bond breakage in graphene. Through statistical ensemble simulations, thermoelastic behavior of graphene/polypropylene nanocomposites are determined with grafting density differences at single-layered graphene interface. For equivalent continuum modeling to account for covalent grafting, the mean field micromechanics model is supplemented to characterize interfacial and interphase properties of nanocomposites in accordance with number of covalent grafting. In heat of vaporization perspective, correlation of covalent grafting and dispersion inside the polymer matrix is examined.

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[P2-68] Durability analysis on the environmental aging of epoxybased nanocomposite

○Sunyong Kwon[1], Man Young Lee[2], Seunghwa Yang[3] （1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Agency for Defense Development, Korea, 3.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea）

Aging is a slow and steady process which occurs by various environmental factors including moisture, uv light, changes in temperature and pressure. Hygroscopic aging of polymer nanocomposite occurs by consistent exposure to moisture in service condition. As bounded water in the material causes microscopic changes in chemical and physical structure of the composite material, it eventually leads to swelling, plasticization, degradation of mechanical and interfacial properties. Thus, to properly examine the long-time process of aging, correlation between aging time-structure-corresponding properties should be developed. Therefore, in this study, multiscale bridging method incorporating atomistic approach of molecular dynamics (MD) simulation and continuum modeling is presented.

To define the relationship between aged structure and corresponding properties, MD simulation is firstly adopted. Different crosslinking ratio of 30% to 70% is established by crosslinking reaction between bisphenol F type epoxy (EPON862®) resin and triethylenetetramine (TETA) curing agent. A single layered defect-free graphene is added as fiber reinforcement in the nanocomposite structure. Also, to observe the hygroelastic behavior of nanocomposite, weight fraction of 0, 2, 4wt% water is included in the nanocomposite unit cell. After isobaric-isothermal (NPT) ensemble simulation, diffusion coefficient of water, coefficient of moisture expansion (CME), elastic modulus and cohesive zone law of epoxy/graphene nanocomposite models are predicted. Based on the results of MD simulation, equilibrium hygroelastic constitutive models incorporating interfacial properties between epoxy and graphene are used to accurately measure the nanoscale effect observed in MD simulations with moisture.

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

[PO-I2] Poster Session 2

Symposium I

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-69] **Topological evolution of the microstructures of thin films during grain growth**

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

[P2-70] Molecular dynamics simulations of phase transformations in nanocrystalline NiTi shape-memory alloys

○Won-Seok Ko （University of Ulsan, 93 Daehak-ro, Nam-gu, Ulsan, 44610, Korea）

[P2-71] An attempt to connect migration of grain boundaries to their atomic structures with help of Molecular Dynamics

Zakaria El Omari, ○Sylvain Queyreau, Charlie Kahloun, Brigitte Bacroix （Universite Paris XIII, Sorbonne Paris Cite, Laboratoire des Sciences des Procedes et des Materiaux, LSPM UPR 3407, France）

[P2-72] Disconnection interaction in Cu grain boundaries

○Christian Brandl （Karlsruhe Institute of Technology, Germany）

[P2-73] Phase-field Approach to Thermo-mechanical Behavior of Through-silicon Vias

Wooju Lee, ○jaekeun yoon, Dongchoul Kim （Sogang Univ., Korea）

[P2-74] **Grain-Growth in Nanocrystalline Metals under Ion Irradiation: A Thermal Spike Model**

○Djamel Kaoumi[1], Robert Birtcher[2], Arthur Motta[3] （1.North Carolina State University, United States of America, 2.Argonne National Laboratory, United States of America, 3.Penn State University, United States of America）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-69] Topological evolution of the microstructures of thin films during grain growth

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Historically, metallography has been the two-dimensional characterization of materials microstructures by optical microscopy. Consequential problems have long been known: A two-dimensional section through a three-dimensional object gives us only a very poor idea about size and form of the object. The same holds for the complex grain boundary networks of various kinds of polycrystalline materials. Therefore, many attempts have been made to gain three-dimensional information experimentally. Nevertheless, in simulations and analytical theories thin films are commonly still treated as two-dimensional objects making comparisons with three-dimensional experimental data rather hard.

In the present work, based on experimental measurements, grain growth in metallic thin films is investigated in detail by three-dimensional Monte Carlo Potts model simulations focusing particularly on the transition from bulk-like growth to columnar microstructures. Changes not only in average growth behaviour from a linear increase of the average grain area with annealing time to near-stagnation, but particularly temporal changes in local topology and individual growth kinetics, e.g., in terms of the Lewis-law as well as of the von Neumann-Mullins-law are discussed.

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[P2-70] Molecular dynamics simulations of phase transformations in nanocrystalline NiTi shape-memory alloys

○Won-Seok Ko （University of Ulsan, 93 Daehak-ro, Nam-gu, Ulsan, 44610, Korea）

Molecular dynamics simulations are performed to investigate temperature- and stress-induced phase transformations in nanocrystalline nickel-titanium shape-memory alloys. Our results provide detailed insights into the origins of the experimentally reported characteristics of phase transformations at the nanoscale, such as the decrease of the transformation temperature with grain size and the disappearance of the plateau in the stress-strain response. The relevant atomic scale processes, such as nucleation, growth, and twinning are analyzed and explained. We suggest that a single, unified mechanism--dominated by the contribution of a local transformation strain--explains the characteristics of both temperature- and stress-induced phase transformations in nanocrystalline nickel-titanium.

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[P2-71] An attempt to connect migration of grain boundaries to their atomic structures with help of Molecular Dynamics

Zakaria El Omari, ○Sylvain Queyreau, Charlie Kahloun, Brigitte Bacroix （Universite Paris XIII, Sorbonne Paris Cite, Laboratoire des Sciences des Procedes et des Materiaux, LSPM UPR 3407, France）

Grain Boundary (GB) migration is at the origin of microstructure evolutions in a large variety of crystalline materials. One of the many challenges to fully understand GB motion has to do with the GB vast panel of atomic configurations and existence of several motive forces or impacting parameters. In this context, atomistic simulations have proven to be particularly useful since GB migration can be investigated under well defined conditions, and large scale systematic investigations are now possible (i.g. [1]).

In this work we report a Molecular Dynamics investigation of the migration of a large panel of CSL GB in fcc Ni. In order to construct lesser known GB with mixed tilt+twist or asymmetric character, we orient and constrain the simulation domain to the CSL lattice defined by the two crystal orientations, in a fashion very similar to the approach proposed in [2]. GB motion may be initiated by a synthetic driving force as defined in [3]. As a result, very different temperature behaviour are observed ranging from athermal, to thermally activated and non monotonous thermal behaviour. Different behaviours are sometimes observed for very similar GBs, confirming the important of the GB atomic structure over the macroscopic geometrical parameters describing GB.

In an attempt to rationalise these results we developed an automated post-processing of the atomic configurations into a discrete modelling of GB in terms of intrinsic dislocations and disconnections when present. This analysing tool is applied to a dozen of simple GB and a correlation is made when possible between elementary migration mechanisms -atomic shuffling or disconnection motion- and discrete structure of GB.

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(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-72] Disconnection interaction in Cu grain boundaries

○Christian Brandl （Karlsruhe Institute of Technology, Germany）

Recent molecular dynamics (MD) simulations and transmission electron microscopy indicate that the grain boundary (GB) migration in asymmetric GB plane orientation is mediated by the nucleation and migration of disconnections in the GB plane. The collective motion and reaction of disconnections also initiates the formation of facets as the agglomeration of disconnections into a disconnection arrays.

In MD simulations we address the interaction of disconnection and disconnection dipoles at zero stress in S3 and S7 GBs. The diffusive rearrangement at finite temperate is analyzed in terms of one-dimensional random walks and the drift signatures are used to deduce the interaction strength and the disconnection core interaction. The implications of the disconnection-interaction on the collective migration of asymmetrical GBs is discussed in context of grain coarsening in fcc metals at elevated temperatures and the transition to stress-driven grain coarsening in nanocrystalline metals.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-73] Phase-field Approach to Thermo-mechanical Behavior of Through-silicon Vias

Wooju Lee, ○jaekeun yoon, Dongchoul Kim (Sogang Univ., Korea)

Three-dimensional stacking of silicon chips via *Through-silicon vias (TSVs)* is an innovative technique for electronic devices due to the drastically shortened electrical path which leads to the faster operation. When TSVs are exposed to high temperature, the higher coefficient of thermal expansion (CTE) of Cu generate the out-of-plane extrusion of Cu from TSV, so-called Cu pumping, which may damage the above lying silicon chip. Furthermore, the thermal expansion is irreversible because the Cu grains are coarsened during the annealing. The comprehensive understanding of Cu pumping mechanism according to the geometry of TSV and annealing conditions is indispensably required to ensure the reliability of electronic devices. A finite element analysis has been used to predict the Cu pumping. However, the finite element method does not incorporate the grain coarsening mechanisms that reduce the elastic energy generated by the thermal expansion. Here, we propose a phase field model that is modified to consider the thermal expansion of Cu polycrystalline during annealing process. The phase field model is the most suitable method to model the evolution of microstructures, since it has benefits for incorporating multiple mechanisms simultaneously. In this study, the significant mechanisms of Cu pumping, including grain boundary migration, thermal expansion, and interfacial characteristics, are considered into the free energy functional of the phase field model

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(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-74] **Grain-Growth in Nanocrystalline Metals under Ion Irradiation: A Thermal Spike Model**

○Djamel Kaoumi[1], Robert Birtcher[2], Arthur Motta[3] (1.North Carolina State University, United States of America, 2.Argonne National Laboratory, United States of America, 3.Penn State University, United States of America)

Grain growth was observed in nanocrystalline metallic foils in situ in a transmission electron microscope in a wide range of irradiation doses, temperature (from 20K to 773K) for four different pure metals (Zr, Pt, Cu and Au). The average grain size increased monotonically with ion fluence and similarly to thermal grain growth, the ion-irradiation induced grain growth curves could be best fitted with curves of the type:. With respect to temperature, the experimental results showed the existence of a low-temperature regime (below about 0.15-0.22Tm), where grain growth is independent of the irradiation temperature, and a thermally assisted regime where grain growth is enhanced with increasing irradiation temperature. A model is proposed to describe grain growth under irradiation in the temperature-independent regime, based on the direct impact of the thermal spikes on grain boundaries. In the model, grain-boundary migration occurs by atomic jumps, within the thermal spikes, biased by the local grain-boundary curvature driving. The experimental results will be presented as well as the model proposed to describe grain-growth kinetics in the low-temperature regime (cryogenic temperatures).

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

[PO-N2] Poster Session 2

Symposium N
Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-75] **Why the structure-property relationship in metallic glasses should be established beyond short-range order: Insight from potential energy landscape**

○Dan Wei[1,2], Yunjiang Wang[1,2], Lanhong Dai[1,2] （1.University of Chinese Academy of Sciences, China, 2.Institute of Mechanics, Chinese Academy of Sciences, China）

[P2-76] Vacancy segregation analysis near grain boundaries in metallic systems by long-time atomistic simulations

○Shotaro Hara （Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan）

[P2-77] **EXPERIMENTAL AND DENSITY FUNCTIONAL THEORY STUDIES OF PRECIPITATE INTERFACES IN ALUMINIUM ALLOYS, WITH FOCUS ON β" & β**

○Haris Rudianto, Deni Hariadi, Andriansyah Andriansyah （Gunadarma University, Indonesia）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-75] **Why the structure-property relationship in metallic glasses should be established beyond short-range order: Insight from potential energy landscape**

○Dan Wei[1,2], Yunjiang Wang[1,2], Lanhong Dai[1,2] （1.University of Chinese Academy of Sciences, China, 2.Institute of Mechanics, Chinese Academy of Sciences, China）

For crystals, structures provide all information needed for predicting material properties. However, what determines non-crystalline solids properties remains elusive for many years. Extensive work has been performed to identify structures playing an important role in glass, but a key question arises that what is the hidden rule of structural feature that can predict properties. Here we calculate an atom’ s activation energy (the system’ s long-time property) for thermally activated relaxation with the Activation-Relaxation Technique (ART) and correlate the searched local potential energy landscape with several of the successful structural predictors. We find a common nature in the successful structural predictors that spatial correlation of structural information matters a lot once they tend to determine an atom’ s properties. There exists a critical correlation length of about sub-nanometer which is corresponding to the second shell of the pair correlation function of glassy structures. We further demonstrate this concept by manipulating the cutoff distance of local structural entropy - one of the successful structural feature - that only if this local structure is defined beyond the short-range order it can predict activation of local atom rearrangement in the model metallic glass. In this way, we question the prevailing approach of materials science aimed at identifying simple structural motifs responsible for metallic glass properties.

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[P2-76] Vacancy segregation analysis near grain boundaries in metallic systems by long-time atomistic simulations

○Shotaro Hara （Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan）

Long-term degradation phenomena in metallic systems under a high temperature, such as creep voiding, are governed by the vacancy diffusion, accumulation and growth processes at an atomistic scale around the material heterogeneities like grain boundaries. However, the basic properties such as the equilibrium vacancy concentrations and the kinetics near grain boundaries are not still understood because a molecular dynamics simulation often suffers from tracking thermally-activated processes due to its limited time scale. In this study, the vacancy segregation behavior at grain boundary has been analyzed using diffusive molecular dynamics simulations, which is a novel approach for exploring the atomic level mass action along the chemical potential gradient at diffusive time scale. The equilibrium vacancy concentrations and the chemical potential distributions at grain boundaries are computed for the different grain boundary character. The correlation between the grain boundary energies and their concentrations have also been considered. Furthermore, the kinetic nature of grain boundary sliding was investigated using this new scheme and the effect of stress on the sliding was discussed.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-77] EXPERIMENTAL AND DENSITY FUNCTIONAL THEORY STUDIES OF PRECIPITATE INTERFACES IN ALUMINIUM ALLOYS, WITH FOCUS ON β" & β

○Haris Rudianto, Deni Hariadi, Andriansyah Andriansyah （Gunadarma University, Indonesia）

Aluminium is the third most abundant element in the Earth’ s crust, after oxygen and silicon. Before the start of the last century, aluminium started to come into wide use as a structural material. Since then, it has reached the position of being the second most used metal in the world, with only steel beating it to the throne. One important structural limitation of aluminium is their fatigue strength. Precipitation hardening is utilized to strengthen a wide variety of alloy systems especially for Aluminum Alloys. An example is the class of commercially important Al-Mg-Si based alloys which are strengthened by a number of metastable precipitate phases, where the needle-shaped β’ ’ -Mg5Si6 precipitates are often the main contributor to hardening. Beginning with the supersaturated solid solution (SSS), the generic precipitation sequence in Al-Mg-Si alloys is generally believed to be :

SSS -> Mg/Si clusters -> Guinier-Preston zones -> β’’ -> β’ -> β

In practice, the sequence can be even more complex and a number of other metastable phases, depending on alloy composition and the heat treatment time and temperature. In this research, interface energy was calculated by Quantum Espresso with super cells designed on VESTA. For comparison, in this research, experimental was also carried out to determine effects of strengthening precipitates on mechanical properties. T6 heat treatment was done starting from solid solution treatment, quenching and finished my artificial aging. Hardness was done to determine mechanical properties and SEM-EDS and XRD were done to characterize the materials.

Keywords; Aluminum Alloys, DFT, Strengthening Precipitates, Heat Treatment

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

[PO-O2] Poster Session 2

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[P2-78] Adsorption of Volatile Organic Compounds (VOCs) on Silicene by Density Functional Theory Calculations

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

[P2-79] Atomistic insights into defect formation mechanism in single crystal SiC based on molecular dynamics simulation

○Kenji Nishimura[1], Koji Miyake[1], Ken-ichi Saitoh[2] （1.AIST, Japan, 2.Kansai Univ., Japan）

[P2-80] **Potential cathode material Na_xVOPO_4 for rechargeable Sodium - ion batteries: DFT investigation**

○Duc Huu Luong[1], An Van Dinh[1,2], Yoshitada Morikawa[3], Yoji Shibutani[2,1] （1.Nano Technology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan, 3.Department of Precision Science and Technology, Graduate School of Engineering, Osaka University, Japan）

[P2-81] **Two-dimensional Na_xSiS as a promising anode material for rechargeable Sodium-based batteries: Ab initio material design.**

Thi Dung Pham[1], ○Van An Dinh[1,2], Kazunori Sato[3], Yoji Shibutani[1,2] （1.Nanotechnology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan, 3.Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, Japan）

[P2-82] Modelling and analysis of SiO2 interfaces of non-firing solids

○Tomohiro Sato[1], Ken-ichi Saitoh[1], Masayoshi Fuji[2], Chika Yamashita Takai[2], Hadi Razavi[2], Masanori Takuma[1], Yoshimasa Takahashi[1] （1.Dept. of Mechanical Engineering, Kansai Univ., Japan, 2.Advanced Ceramics Reserch Center, Nagoya Institute of Technology, Japan）

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Cancer can be regarded as a rising threat towards modern societies. Detecting cancer at an early stage significantly improves the curability of the disease [1]; unfortunately, currently available methods for early diagnosis of cancer are scarce and inefficient. In fact, the concentration of VOCs in cancer patients in the breath is different from that in normal people [2]. Therefore, development of new sensors that can detect VOCs at low concentrations, corresponding to the early stage of cancer, is desirable. 2D materials are expected as attractive materials for these sensors due to their large surface area to volume ratio. In this work, we investigated the adsorption mechanism of some small-to-medium VOCs on the surface of silicene by the quantum simulation method. The images of the potential energy surfaces for different positions of the adsorbate on the silicene surface were explored by *Computational DFT-based Nanoscope* [3] for determination of the most stable configurations and diffusion possibilities. The adsorption energy profiles were calculated by three approximations of van der Waals interation: revPBE-vdW, optPBE-vdW, and DFT-D2. It is found that the adsorption energies of the VOCs in question vary in the range of 0.6-1.0 eV, which indicates that silicene is considerably sensitive with these VOCs. The charge transfer between the substrate and VOCs and the effect of an electric field on the adsorption configurations, energies, and band structures were also addressed.

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[P2-79] Atomistic insights into defect formation mechanism in single crystal SiC based on molecular dynamics simulation

○Kenji Nishimura[1], Koji Miyake[1], Ken-ichi Saitoh[2] （1.AIST, Japan, 2.Kansai Univ., Japan）

Silicon carbide (SiC) is a promising next-generation semiconductor for high-power, high-temperature, and high-voltage devices because of its wide bandgap, high breakdown field, and high thermal conductivity. However, the efficient and smooth machining of SiC is technically difficult due to its intrinsic nature of high hardness and brittleness as well as strong anisotropy. It is still a great challenge to understand machining

processes in which damage layers caused by stress-induced phenomena such as plastic deformation and fracture are introduced beneath grinding surface. In this study, we perform one million-atom molecular dynamics simulations of nanoindentation tests on cubic SiC single crystal using a nano-sized spherical indenter to clarify the plastic deformation mechanism and defect formation criteria in SiC. An analytical bond-order Tersoff-type interatomic potential for SiC developed by Erhart *et al.*, which reproduces the elastic, defect, and thermal properties, is adopted. The load-displacement curves of the nanoindentation tests obtained by our simulations demonstrate transition from elastic deformation to plastic deformation so-called "pop-in" event. Our results also predict the decrease of the CRSS (critical resolved shear stress) of single crystal SiC with increasing temperature from 300 K to 2000 K for both (001) and (111) indent, which means less energy is required to activate slip systems at higher temperature. These results are similar to the feature of ductile materials such as metals, although SiC is known as brittle materials. In addition, we identify crystalline slips and defects generated beneath the indenter after the pop-in event by means of a novel type of structural analysis method using sub-lattice of Si or C which is based on common neighbor analysis. The structural analysis we propose reveals that dislocation loops in {111} planes which correspond to the slip plane of SiC are developed with increasing indenter depth. Furthermore, we find that for lower temperature perfect dislocations are dominantly formed, while for higher temperature partial dislocations together with stacking faults are superior to the perfect dislocations, resulting in the dramatic increase of the partial dislocations.

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Using the density functional calculations, we investigated the crystal and electronic structures, electrochemical properties and ion diffusion mechanism of Sodium - polaron complex in Sodium Vanadyl phosphate $NaVPO_5$. A calculated voltage of 3.77 V (GGA+U) and 3.58 V (HSE06) corresponding to a redox reaction of potential couple $V^{4+/}V^{5+}$ were in good agreement with experimental result [1]. The diffusion mechanism of charge carriers was explored using GGA+U. In the charge process, a Sodium ion is removed from the crystal structure so that the Sodium vacancy appears and a positive small polaron forms at one the two first nearest VO_6 octahedron. The diffusion of Na+ ion which is accompanied by a positive small polaron is described by three elementary diffusion processes, including single, crossing and parallel diffusions [2]. With the smallest activation energy of 395 meV, the pathway of Sodium diffusion along the [010] direction is the most favorable diffusion pathway and it is significantly higher than previous calculation which did not mention the small polaron formation. In the discharge process, Sodium ion is intercalated to structure of β-$VOPO_4$, then the negative small polaron forms at one of the nearest neighbour VO_6 octahedron. In addition, the elementary diffusion process of sodium ion is more favorable in the [010] direction. However, because of about 10% smaller volume, the diffusion activation energy (627 meV) is significantly higher than those required in the charge process. Compared with the other materials, it is obviously that this material would perform as well as some common materials for cathode such as Olivine.

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The rapidly rising demand of energy storage system for electronic devices presents an imperative need to develop sodium-ion batteries with high energy density, high conductivity, and low barrier energy. In this work, we present the density functional study on properties of the two-dimensional (2D) Na_xSiS as a promising anode material for rechargeable sodium ion batteries (SIBs). Energetically stable structures of Na-adsorbed *Silicene sulfide* Na_xSiS were explored. It is found that *silicene sulfide* has an adsorption energy to sodium atom about of -0.4 eV, which is large enough to ensure a good stability for sodium inserting into SiS during sodiate process. The electronic structure and capacity of Na_xSiS were calculated. The electronic structure of pristine SiS monolayer and Na adsorbed layer shows the distinction of a semiconductor material. The fully sodiated phase of SiS is $Na_{0.5}SiS$ corresponding to a highest theoretical capacity of 187.2 mAh/g per one side layer. The diffusion mechanism of Na ions was also investigated by using NEB method. Two possible elementary processes are explored: one is along *a*-and the other is along *b*-direction. Most importantly, *Silicene sulfide* shows a good sodium mobility with an energy barrier along two dimension is only 183 meV, which is much smaller than that in Li_xSiS (430meV), 2D TiS_2 (220meV), and 2D MoS_2 (280-680 meV). Our investigations also reveal that SiS exhibits the better electrochemical performance as an anode in the SIBs than in the LIBs. All these characteristics suggest that 2D SiS can expected to be a promising anode material for sodium batteries.

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[P2-82] Modelling and analysis of SiO2 interfaces of non-firing solids

○Tomohiro Sato[1], Ken-ichi Saitoh[1], Masayoshi Fuji[2], Chika Yamashita Takai[2], Hadi Razavi[2], Masanori Takuma[1], Yoshimasa Takahashi[1] （1.Dept. of Mechanical Engineering, Kansai Univ., Japan, 2.Advanced Ceramics Reserch Center, Nagoya Institute of Technology, Japan）

Generally, ceramics are manufactured by using sintering process. However, this process needs high temperature and loss a lot of fuels. CO2 emission in the process is also need to improve. So, non-fire process is focused to make ceramics products.

For non-fire process, surfaces of SiO2 particles are polished and put hydrogen on the activate surfaces. These SiO2 particles are compressed and put into water that is non-fire process of ceramics. In this study, SiO2 interface models were constructed for molecular dynamics simulation. Interactions between SiO2 and H2O were presented by using ReaxFF potential. At first, SiO2 interfaces model without OH as end groups were conducted. By put water molecules between SiO2 interfaces, some atoms were changed their combinations. Some of them achieved lower potential energy through the simulation. It is seemed that a part

of non-fire process was reproduced. For example, hydrogen atom connected the oxygen atom of SiO2. However, connection of SiO2 did not observed over SiO2 interfaces.

Then, SiO2 interfaces model with OH as end groups were conducted. At relaxation of the models, SiOH exists in the model. After relaxation, water molecules were put into the surfaces. However, changes of connection between SiO2 and H2O or SiO2 interfaces did not observed. Energetic or structural stability of SiOH surfaces were seemed to effect the result.

Distance of interfaces, conducting compressed SiO2 including OH as end groups models might be key to improve the ability of reaction between atoms.