Fri. Nov 2, 2018

Room1

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

[SY-C13] Symposium C-13

Chair: Jaafar A. El-Awady(Johns Hopkins University, United States of America)
9:45 AM - 11:00 AM Room1

[SY-C13] Mesoscopic studies of slip and twinning processes in hcp polycrystalline materials
○Irene Beyerlein[1], Marat Latypov[1], Jason Mayeur, Wyatt Witzen[1], Mitra Taheri[2], Tresa Pollock[1]
（1.University of California at Santa Barbara, United States of America, 2.Drexel University, United States of America）

[SY-C13] **Crystal plasticity formulation involving volume fraction-based deformation twinning model**
○Yuichi Tadano （Department of Mechanical Engineering, Saga University, Japan）

[SY-C13] **An Elastic-Viscoplastic Crystal Plasticity Modeling for Plane Strain Deformation of Pure Magnesium**
○Weidong Song, Liansong Dai （Beijing Institute of Technology, China）

[SY-C13] The Minimum Energy Pathways Identifications of Twinning Dislocation Loop Nucleation of Extension Twinning in Magnesium
○Xiao-Zhi Tang[1], Qun Zu[2], Lixin Sun[4], Yue Fan[3], Ya-Fang Guo[1] （1.Inst. of Mechanics, Beijing Jiaotong Univ., China, 2.Schl. of Mechanical Engineering, Hebei Univ. of Tech., China, 3.Dept. of Mechanical Engineering, Univ. of Michigan, United States of America, 4.Dept. of Nuclear Science and Engineering, MIT, United States of America）

Room2

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E13] Symposium E-13

Chairs: Erik Bitzek(FAU Erlangen-Nuernberg, Germany), Kisaragi Yashiro(Gifu University, Japan)
9:45 AM - 11:00 AM Room2

[SY-E13] 3D Aspects of Fracture in Crack - Obstacle Interactions and Effects of Crack Front Curvature
○Erik Bitzek[1], Polina Baranova[1], Johannes J. Möller[2]
（1.FAU Erlangen-Nuernberg, Germany, 2.Fraunhofer IWM, Germany）

[SY-E13] Vortex instabilities in the deformation of Cu|Au nanolaminates
Adrien Gola[1,2], Peter Gumbsch[2,3], ○Lars Pastewka[1,3,2]
（1.University of Freiburg, Germany, 2.Karlsruhe Institute of Technology, Germany, 3.Fraunhofer IWM, Germany）

[SY-E13] **Molecular dynamics simulation of the interaction between grain boundary and point defects**
○Liang Zhang[1], Yasushi Shibuta[1], Cheng Lu[2] （1.The University of Tokyo, Japan, 2.University of Wollongong, Australia）

[SY-E13] Deformation mode analysis by the eigenvectors of the atomic elastic stiffness
○Kisaragi Yashiro （Gifu University, Japan）

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E14] Symposium E-14

Chairs: Thierry Auger(CNRS, France), Jamila Rahmoun(LAMIH-ENSIAME, Valenciennes University, France)
11:15 AM - 12:30 PM Room2

[SY-E14] Stability Controlled Crack Evolution in Staggered Laminate Bio-material
○Yi Yan, Akihiro Nakatani （Dept. of Adaptive Machine Systems, Osaka University, Japan）

[SY-E14] A brittle to ductile transition modeling for liquid metal embrittlement
○Thierry Auger （CNRS, France）

[SY-E14] Buckling delamination of ductile thin films on rigid substrates
○Nadia Ben Dahmane, Guillaume Parry, Rafael Estevez （Univ. Grenoble Alpes, SIMAP, F-38000 Grenoble, France）

[SY-E14] An analytical model of the peeling forces at edges of multilayers subjected to temperature variations
○Chengyin Zhang[2], Neng-Hui Zhang[1,2]
（1.Department of Mechanics, College of Sciences, Shanghai University, China, 2.Shanghai Key Laboratory of Mechanics in Energy Engineering, Shanghai Institute of Applied Mathematics and Mechanics, Shanghai University, China）

[SY-E14] **Characterization and multi-scale modeling of the mechanical response of the human humerus under dynamic loading**
○Jamila Rahmoun[1], Hakim Naceur[1], Pascal Drazetic[2],

Christian Fontaine[3] （1.LAMIH-ENSIAME, Valenciennes University, France, 2.LAMIH-IUT, Valenciennes University, France, 3.Lab. d'anatomie, Lille University, France）

Room3

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

[SY-F13] Symposium F-13

Chair: Takayuki Aoki(Tokyo Institute of Technology, Japan)
9:45 AM - 11:00 AM Room3

[SY-F13] Advanced analysis tools for atomistic microstructure modeling
○Alexander Stukowski （Dept. of Materials Science, Darmstadt University of Technology, Germany）

[SY-F13] Studing thermo-oxidative degradation of polyimide in oxygen enviorment using MD simulations
○Ashwani Kumar Sengar, Sumit Basu （IIT Kanpur, India）

[SY-F13] In-plane characterization of structural and thermodynamic properties for steps at faceted chemically heterogeneous solid/liquid interfaces
○Hongtao Liang[1], Brian B. Laird[2], Mark Asta[3], Yang Yang[1] （1.Physics Department and State Key Laboratory of Precision Spectroscopy, School of Physical and Material Science, East China Normal Universit, China, 2.Department of Chemistry, University of Kansas, United States of America, 3.Department of Materials Science and Engineering, UC Berkeley, United States of America）

[SY-F13] Design of neural network for thermodynamics data of non-equilibrium multiphase field model
○Hiroshi Wakameda[1], Sukeharu Nomoto[1], Akinori Yamanaka[3], Toshiyuki Koyama[2] （1.ITOCHU Techno-Solutions Corporation, Japan, 2.Materials Design Innovation Engineering, Nagoya Univ., Japan, 3.Department of Mechanical Systems Engineering, Tokyo University of Agriculture and Technology, Japan）

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

[SY-F14] Symposium F-14

Chair: Markus Kuehbach(Max-Planck-Institut fur Eisenforschung GmbH, Germany)
11:15 AM - 12:30 PM Room3

[SY-F14] Large-scale multiphase flow simulations on a GPU supercomputer
○Takayuki Aoki （Tokyo Institute of Technology, Japan）

[SY-F14] **Transport Properties Of Fluid Mixtures In Micro- And Mesoporous Kerogen Membranes**
○Patrick Alain Bonnaud[1], Romain Vermorel[1], Julien Collell[2], Guillaume Galliéro[1] （1.University of Pau and Adour Countries, France, 2.Total E&P, France）

[SY-F14] Numerical simulation of ionic transport through deformable porous media: application to cortical bone tissue modeling
○Jana Turjanicova[1,2], Eduard Rohan[1,2], Vladimír Lukeš[2] （1.Dept. of Mechanis, Univ. of West Bohemia in Pilsen, Czech Republic, 2.NTIS - New technologies for information society, Czech Republic）

[SY-F14] Hydrogen Transport and Thermal Desorption in Multiphase Steels
○Andrej Turk[1], Pedro E.J. Rivera-Díaz-del-Castillo[2], Enrique Galindo-Nava[1] （1.University of Cambridge, UK, 2.Lancaster University, UK）

Room4

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

[SY-N7] Symposium N-7

Chair: Shotaro Hara(Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan)
9:45 AM - 11:00 AM Room4

[SY-N7] Bridging Time Scales with Variationally Enhanced Sampling
○Omar Valsson （Max Planck Institute for Polymer Research, Germany）

[SY-N7] Simulations of Branched Polyelectrolytes
○Filip Uhlik （Charles University, Czech Republic）

[SY-N7] Adaptive resolution simulations coupling molecular dynamics to dissipative particle dynamic
○Matej Praprotnik （National Institute of Chemistry, Slovenia）

[SY-N7] Using Diffusive Molecular Dynamics Simulations to Investigate Grain Boundary Segregation and Grain Boundary Structural Transformations
Louis Hebrard, ○Chad W Sinclair （Dept. of Materials Engineering, University of British Columbia, Canada）

Room8

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

[SY-D5] Symposium D-5

Chair: Jörg Neugebauer(MPIE, Germany)
9:45 AM - 11:00 AM Room8

[SY-D5] Computational exploration of strong permanent magnet compounds

○Takashi Miyake[1,2,3] (1.CD-FMat, AIST, Japan, 2.ESICMM, NIMS, Japan, 3.CMI[2], NIMS, Japan)

[SY-D5] A machine-learning approach for finding new hard-magnetic phases

Johannes J. Möller, ○Daniel F. Urban, Christian Elsässer (Fraunhofer IWM, Freiburg, Germany)

[SY-D5] High-throughput optimization of finite temperature phase stabilities of Ce-based hard magnetic materials

○Tilmann Hickel, Halil Soezen, Fritz Koermann, Joerg Neugebauer (Max Planck Institut fur Eisenforschung, Germany)

[SY-D5] Understanding pairwise magnetic interactions in Fe-based materials with machine learning techniques

○Osamu Waseda, Omkar Hegde, Tilmann Hickel, Jörg Neugebauer (MPIE, Germany)

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

[SY-D6] Symposium D-6

Chair: Daniel Urban(Fraunhofer IWM, Germany)
11:15 AM - 12:30 PM Room8

[SY-D6] Novel two-dimensional materials: Materials discovery, data provenance, and workflow reproducibility.

○Nicola Marzari (EPFL, Switzerland)

[SY-D6] In silico screening of Metal-Organic Frameworks for adsorption driven heat pumps and chillers

○Mate Erdos[1], Martijn F. de Lange[1], Freek Kapteijn[2], Othonas A. Moultos[1], Thijs J. H. Vlugt[1] (1.Engineering Thermodynamics, Process &Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Netherlands, 2.Catalysis Engineering, Chemical Engineering Department, Delft University of Technology, Netherlands)

[SY-D6] Machine learning assisted by first-principles calculations for designing intermetallic-typed metallic glasses

○Tokuteru Uesugi, Manami Sakai, Yorinobu Takigawa, Kenji Higashi (Dep. of Materials Science, Osaka Prefecture Univ., Japan)

Room9

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

[SY-H11] Symposium H-11

Chair: Erik Van der Giessen(University of Groningen, Netherlands)
9:45 AM - 11:00 AM Room9

[SY-H11] A Hierarchical Multiscale Simulations Approach for Modeling Failure in Polymer Matrix Composites

Xiawa Wu[1], Amin Aramoon[1], Christopher Woodward[2], ○Jaafar A. El-Awady[1] (1.Johns Hopkins University, United States of America, 2.Air Force Research Laboratory, United States of America)

[SY-H11] Some Positive Aspect of Structural Defects in Graphene/Polymer Nanocomposites Studied by Abinitio,Molecular Dynamics, and Continuum Approaches

○Seunghwa Yang[1], Janghyuk Moon[1], Maenghyo Cho[2] (1.School of Energy Systems Engineering, Chung-Ang University, Korea, 2.School of Mechanical and Aerospace Engineering, Seoul National University, Korea)

[SY-H11] Linear and non-linear viscoelastic properties of model fractal-like aggregates polymer nanocomposites

○Samy MERABIA[1], Yang WANG[1], François DETCHEVERRY[1], Marc COUTY[2], Gaëtan MAUREL[2] (1.CNRS and Universite Lyon 1, France, 2.MFP Michelin, Clermont-Ferrand , France)

[SY-H11] **Topological defect structure in the self-assembly of semiflexible polymers under spherical confinement**

○Mihir Khadilkar, Arash Nikoubashman (Johannes GutenBerg University Mainz, Germany, Germany)

[SY-H11] Molecular dynamics simulation of the detachment force between graphene and epoxy resin

○Kazuki Mori[1], Makoto Yabe[2], Yuji Kohno[2], Jun Koyanagi[3] (1.ITOCHU Techno-Solutions Corporation, Japan, 2.Yokohama National University, Japan,

3.Tokyo University of Science, Japan）

[SY-H11] Relation between deformation and electrical conductivity for electroconductive polymer nanocomposites with highly segregated structure

○Oleg V. Lebedev[1], Sergey Abaimov[1], Alexander Ozerin[2], Anton Trofimov[1], Iskander Akhatov[1]
（1.Center for Design, Manufacturing and Materials, Skolkovo Institute of Science and Technology, Russia, 2.Laboratory of the Structure of Polymer Materials, N.S. Enikolopov Institute of Synthetic Polymer Materials of RAS, Russia）

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

[SY-H12] Symposium H-12

11:15 AM - 12:00 PM Room9

Room10

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

[SY-B9] Symposium B-9

Chair: Michael Tonks(University of Florida, United States of America)
9:45 AM - 11:00 AM Room10

[SY-B9] Ab Initio Modeling of Self-Interstitial and Vacancy Migration in Zirconium

○Emmanuel Clouet[1], Céline Varvenne[2] （1.CEA Saclay, France, 2.CNRS - Aix-Marseille University, France）

[SY-B9] Atomistic modelling of point defect clusters in zirconium and impact on the microstructure evolution and crystal growth under irradiation

Benjamin CHRISTIAEN[3], Christophe DOMAIN[3,2], ○Ludovic THUINET[1,2], Antoine AMBARD[3,2], Alexandre LEGRIS[1,2] （1.UMET, UMR CNRS 8207, Lille university, F-59655 Villeneuve d’Ascq, France, 2.EM2VM, EDF-CNRS, France, 3.EDF R&D, MMC, Les Renardieres, F-77810 Moret-sur-Loing, France）

[SY-B9] Modeling of dislocation climb assisted glide in crystal plasticity models

○Alankar Alankar, Vikram Phalke, Ritesh Dadhich, Ashish Mishra （IIT Bombay, India）

[SY-B9] The role of oxide grain boundaries in the oxidation of zirconium alloy fuel cladding

○Maria S Yankova[1], Felicity Baxter[1,2], Alistair Garner[1], Philipp Frankel[1], Christopher P Race[1] （1.Materials Performance Centre, School of Materials, University of Manchester, UK, 2.Corrosion and Materials Science, Wood. PLC, UK）

[SY-B9] Advances in X-ray Diffraction Line Profile Analysis of Dislocation Loops in Zr - Insights from Atomistic Modelling.

○Chris P Race, Rory Hulse, Tamas Ungar （University of Manchester, UK）

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

[SY-B10] Symposium B-10

Chair: Frederic Soisson(CEA Saclay, France)
11:15 AM - 12:15 PM Room10

[SY-B10] Sink strengths of point defects near tilt grain boundaries: A phase field model

○Pengchuang Liu[1], Songlin Zheng[2], Pengcheng Zhang[1], Sanqiang Shi[3], Kaiguo Chen[2] （1.Institute of Materials, China academy of engineering physics, China, 2.Institute of Fluid Physics, China academy of engineering physics, China, 3.Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hong Kong）

[SY-B10] Modelling swelling and growth under irradiation using the phase field method

○Daniel Schwen, Andea M. Jokisaari （Dept. of Fuels Modeling and Simulation, Idaho National Laboratory, United States of America）

[SY-B10] Phase-field modelling of dislocation loop evolution under irradiation : application to radiation induced segregation prediction near the dislocation cores

○Gabriel Franck BOUOBDA MOLADJE[1], Ludovic THUINET[1], Alexandre LEGRIS[1], Charlotte BECQUART[1], Maylise NASTAR[2], Frédéric SOISSON[2] （1.CNRS, université de Lille, France, 2.CEA, Université Paris-Saclay, France）

[SY-B10] **Theoretical derivation of the ABVI model from cluster expansion Hamiltonian**

○Antonio Fernandez Caballero[1,2], Jan Wrobel[3], Paul Mummery[1], Duc Nguyen-Manh[2] （1.School of Mechanical, Aerospace and Civil Engineering, University of Manchester, UK, 2.Department of Materials Science and Scientific Computing, CCFE, United Kingdom Atomic Energy Authority, Abingdon OX14 3DB, UK, UK, 3.Faculty of Materials Science and Engineering, Warsaw University of Technology, UI.

Wołoska 141, 02-507 Warsaw, Poland, Poland）

Room11

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K4] Symposium K-4

Chairs: Tetsuo Mohri(IMR, Tohoku University, Japan), Akihiro Nakatani(Dept. of Adaptive Machine Systems, Osaka Univ., Japan)
9:45 AM - 11:00 AM Room11

[SY-K4] Disclination dipole model of kink deformation in layered solid

○Akihiro Nakatani[1], Xiao-Wen Lei[2] （1.Dept. of Adaptive Machine Systems, Osaka Univ., Japan, 2.Dept. of Mechanical Engineering, Univ. of Fukui, Japan）

[SY-K4] Large-scale coarse-grained molecular dynamics simulations on fracture processes of lamellar structure in crystalline polymers

○Yuji Higuchi （The University of Tokyo , Japan）

[SY-K4] Grain boundary sliding within the entropy production rate theory

○Tetsuo Mohri （IMR, Tohoku University, Japan）

[SY-K4] Molecular Dynamics Simulation on Intergranular Cracking Mechanism of Iron Material in High Temperature Pressurized Water Environment

○Qian Chen, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Materials Research, Tohoku University, Japan）

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K5] Symposium K-5

Chairs: Masanori Kohyama(AIST, Japan), Masatake Yamaguchi(Japan Atomic Energy Agency, Japan)
11:15 AM - 12:15 PM Room11

[SY-K5] Effects of a bulk-region size in the first-principles tensile test of a grain boundary

○Masanori Kohyama[1], Hao Wang[2], Shingo Tanaka[1] （1.AIST, Japan, 2.Shanghai Univ., China）

[SY-K5] Combined analysis of first-principles calculations and fracture mechanics experiments on intergranular embrittlement of an alloy steel

○Masatake Yamaguchi （Center for Computational Science and e-Systems, Japan Atomic Energy Agency, Japan）

[SY-K5] First-principles local energy analysis of grain boundary segregation of sp-elements on bcc Fe

○Kazuma Ito[1,2], Somesh Kr. Bhattacharya[3], Shingo Tanaka[3], Masanori Kohyama[3], Hideaki Sawada[2], Shigenobu Ogata[1] （1.Osaka University, Japan, 2.Nippon Steel &Sumitomo Metal Corporation, Japan, 3.National Institute of Advanced Industrial Science and Technology, Japan）

[SY-K5] Fast and scalable prediction of local energy at grain boundaries: Machine-learning based modeling of first-principles calculations

○Tomoyuki Tamura[1,2], Masayuki Karasuyama[1,2,3], Ryo Kobayashi[1,2], Ryuichi Arakawa[1], Yoshinori Shiihara[4], Ichiro Takeuchi[1,2,5] （1.Nagoya Institute of Technology, Japan, 2.Center for Materials Research by Information Integration (CMI2), Research and Services Division of Materials Data and Integrated System (MaDIS), National Institute for Materials Science (NIMS), Japan, 3.PRESTO, JST, Japan, 4.Toyota Technological Institute, Japan, 5.RIKEN Center for Advanced Intelligence Project, Japan）

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

[SY-C13] Symposium C-13

Chair: Jaafar A. El-Awady(Johns Hopkins University, United States of America)

Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room1

[SY-C13] Mesoscopic studies of slip and twinning processes in hcp polycrystalline materials

○Irene Beyerlein[1], Marat Latypov[1], Jason Mayeur, Wyatt Witzen[1], Mitra Taheri[2], Tresa Pollock[1] （1.University of California at Santa Barbara, United States of America, 2.Drexel University, United States of America）

[SY-C13] Crystal plasticity formulation involving volume fraction-based deformation twinning model

○Yuichi Tadano （Department of Mechanical Engineering, Saga University, Japan）

[SY-C13] An Elastic-Viscoplastic Crystal Plasticity Modeling for Plane Strain Deformation of Pure Magnesium

○Weidong Song, Liansong Dai （Beijing Institute of Technology, China）

[SY-C13] The Minimum Energy Pathways Identifications of Twinning Dislocation Loop Nucleation of Extension Twinning in Magnesium

○Xiao-Zhi Tang[1], Qun Zu[2], Lixin Sun[4], Yue Fan[3], Ya-Fang Guo[1] （1.Inst. of Mechanics, Beijing Jiaotong Univ., China, 2.Schl. of Mechanical Engineering, Hebei Univ. of Tech., China, 3.Dept. of Mechanical Engineering, Univ. of Michigan, United States of America, 4.Dept. of Nuclear Science and Engineering, MIT, United States of America）

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room1)

[SY-C13] Mesoscopic studies of slip and twinning processes in hcp polycrystalline materials

Invited

○Irene Beyerlein[1], Marat Latypov[1], Jason Mayeur, Wyatt Witzen[1], Mitra Taheri[2], Tresa Pollock[1] （1.University of California at Santa Barbara, United States of America, 2.Drexel University, United States of America）

Under deformation, strain and lattice orientation gradients can develop near crystalline heterogeneities, such as grain boundaries, deformation twins, and voids. These important effects have been studied intensely most often in materials that deform by a single slip mode. In this presentation, we discuss multiscale crystal plasticity modeling efforts to understand the development of lattice orientation gradients induced near and at the boundaries of microstructural defects within crystals of materials with either a BCC or HCP crystal structure. These two material classes commonly deform by multiple slip modes and this distinction is taken into account in the modeling. The results presented in this talk will highlight the effects of microscopic differences in the strengths of these slip modes on the evolution of dislocation density.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room1)

[SY-C13] Crystal plasticity formulation involving volume fraction-based deformation twinning model

○Yuichi Tadano （Department of Mechanical Engineering, Saga University, Japan）

Deformation twinning is an important deformation mechanism of metallic materials as well as slip deformation, especially in hexagonal closed-packed (HCP) metals such as magnesium and titanium. Therefore, understanding twinning behavior is essential to improve mechanical properties of HCP metals. HCP metals generally have a strong anisotropy in crystalline scale. For example, in case of magnesium, plastic deformation due to slip along the c-axis is hard to occur because of much higher critical resolved shear stress of pyramidal slip system, and deformation twinning occur to enhance plastic deformation along the c-axis. The most dominant twinning in magnesium is {10-12}<11-20> tensile twinning system, the number of which is six. As several experimental results showed that untwinned and twinned regions can simultaneously exist in a grain, the author proposed a crystal plasticity model considering the volume fraction of deformation twinning. In the practical problems, multiple twinning systems may be simultaneously activated in a grain because of inhomogeneity of deformation. Therefore, the deformation twinning model has been extended to incorporate the volume fraction of multiple twinning systems. To represent the polycrystalline behaviors of materials, the homogenization-based finite element method is adopted, so that the mechanical behaviors of polycrystalline magnesium can appropriately be reproduced. Numerical investigation using the proposed model is performed, and the adequacy of the model is validated.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room1)

[SY-C13] An Elastic-Viscoplastic Crystal Plasticity Modeling for Plane Strain Deformation of Pure Magnesium

○Weidong Song, Liansong Dai （Beijing Institute of Technology, China）

A rate-dependent elastic-viscoplastic constitutive model is proposed. The model of plane deformation of single crystal magnesium is established by considering seven orientations with different loading directions. The basal, prismatic and pyramidal slip systems in the parent grain, compressive twinning (CT) and tensile twinning (TT) are incorporated in the model. The constitutive descriptions of CT and TT are distinguished to better characterize their effects on the overall hardening of magnesium. The contributions of different deformation modes to the macroscopic plastic deformation of magnesium single crystals in the seven cases are presented. These computational predictions are compared with their corresponding macroscopic experimental observations (stress-strain responses) and other numerical results. These results prove that it is necessary to distinguish different twinning systems and their associated hardening laws for the plastic deformation of magnesium and its alloy.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room1)

[SY-C13] The Minimum Energy Pathways Identifications of Twinning Dislocation Loop Nucleation of Extension Twinning in Magnesium

○Xiao-Zhi Tang[1], Qun Zu[2], Lixin Sun[4], Yue Fan[3], Ya-Fang Guo[1] （1.Inst. of Mechanics, Beijing Jiaotong Univ., China, 2.Schl. of Mechanical Engineering, Hebei Univ. of Tech., China, 3.Dept. of Mechanical Engineering, Univ. of Michigan, United States of America, 4.Dept. of Nuclear Science and Engineering, MIT, United States of America）

The twinning dislocation loop nucleation on the coherent twin boundary in magnesium is investigated by potential energy approaches, and also the dynamic simulations at various temperatures and strain rates.

Based on our numerical results of extension twinning, the single lattice transformation within the coherent twin boundary migration is identified to be the elementary migration process, and its stress-free potential energy barrier is lower than the thermal energy at room temperature. The migration can be triggered thermally once the shear stress makes the transformed lattice at a low energy state. Both the nucleation energy and the critical radius of a twinning dislocation loop are calculated. We believe our discoveries pursue a better understanding of the plasticity of hexagonal close-packed metals.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E13] Symposium E-13

Chairs: Erik Bitzek(FAU Erlangen-Nuernberg, Germany), Kisaragi Yashiro(Gifu University, Japan)

Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room2

[SY-E13] 3D Aspects of Fracture in Crack - Obstacle Interactions and Effects of Crack Front Curvature

○Erik Bitzek[1], Polina Baranova[1], Johannes J. Möller[2] （1.FAU Erlangen-Nuernberg, Germany, 2.Fraunhofer IWM, Germany）

[SY-E13] Vortex instabilities in the deformation of Cu|Au nanolaminates

Adrien Gola[1,2], Peter Gumbsch[2,3], ○Lars Pastewka[1,3,2] （1.University of Freiburg, Germany, 2.Karlsruhe Institute of Technology, Germany, 3.Fraunhofer IWM, Germany）

[SY-E13] Molecular dynamics simulation of the interaction between grain boundary and point defects

○Liang Zhang[1], Yasushi Shibuta[1], Cheng Lu[2] （1.The University of Tokyo, Japan, 2.University of Wollongong, Australia）

[SY-E13] Deformation mode analysis by the eigenvectors of the atomic elastic stiffness

○Kisaragi Yashiro （Gifu University, Japan）

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room2)

[SY-E13] 3D Aspects of Fracture in Crack - Obstacle Interactions and Effects of Crack Front Curvature

Invited

○Erik Bitzek[1], Polina Baranova[1], Johannes J. Möller[2] (1.FAU Erlangen-Nuernberg, Germany, 2.Fraunhofer IWM, Germany)

Traditionally, fracture mechanics mainly considers 2D problems in which the crack front is approximated by a straight line. At the nanoscale, cracks can, however, be strongly curved, e.g., in the case of crack nuclei or as a result of the interaction of a propagating crack with obstacles. Nanoscale crack front curvature can significantly influence the fracture behavior of semi-brittle materials that show a brittle-to-ductile transition with increasing temperature, like refractory metals, intermetallics or semiconductors. Their fracture behavior is ultimately determined by the competition between the dynamics of the atomic bond-breaking processes and dislocation activity in the direct vicinity of the crack. The relative orientation of the local crack front to possible dislocation slip systems can therefore have a major impact on crack tip processes.

Here we present the results of our atomistic simulations of straight cracks in W, Fe and NiAl interacting with various obstacles. Cracks interacting with individual pre-existing lattice dislocations showed stimulated dislocation nucleation and new crack tip blunting mechanisms. Voids were shown to efficiently stop propagating cracks by impeding the re-nucleation of a sharp crack and by facilitating dislocation emission. Fully-3D simulations of penny-shaped cracks revealed an increased tendency for crack tip plasticity compared to straight cracks due to the availability of more slip systems and the resulting dislocation - crack interactions. The results are discussed in the context of the development of predictive multiscale models for fracture toughness.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room2)

[SY-E13] Vortex instabilities in the deformation of Cu|Au nanolaminates

Adrien Gola[1,2], Peter Gumbsch[2,3], ○Lars Pastewka[1,3,2] (1.University of Freiburg, Germany, 2.Karlsruhe Institute of Technology, Germany, 3.Fraunhofer IWM, Germany)

Vortex-instabilities are typically associated with fluid-type flow patterns, such as the well-known Kelvin-Helmholtz instability that can be directly observed in cloud patterns. Recently, Vortex-type instabilities have been observed during the deformation of multilayered materials, both with nano- [1] and micrometer-sized [2] layers. We here use molecular dynamics simulation to investigate Vortex formation in Cu|Au nanolaminates. Our simulations reveal an instability that leads to corotation of neighboring regions of the nanolaminate, giving rise to deformation pattern reminiscent of Kelvin-Helmholtz instabilities. Contrary to the latter instabilities, the plastic Vortex formation occurs at strains below 2 which appears compatible with strains experienced during frictional loading [1]. We compare our molecular dynamics results with deformation patterns generated through ideal plastic and fluid mechanical models.

[1] Luo, Z.-P., Zhang, G.-P. &Schwaiger, R. Microstructural vortex formation during cyclic sliding of Cu/Au multilayers. *Scr. Mater.* **107,** 67-70 (2015).
[2] Pouryazdan, M., Kaus, B. J. P., Rack, A., Ershov, A. &Hahn, H. Mixing instabilities during shearing of metals. *Nat. Commun.* **8,** 1611 (2017).

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room2)

[SY-E13] Molecular dynamics simulation of the interaction between grain boundary and point defects

○Liang Zhang[1], Yasushi Shibuta[1], Cheng Lu[2] (1.The University of Tokyo, Japan, 2.University of Wollongong, Australia)

Molecular dynamics simulations were carried out to investigate the dynamic interaction between different grain boundaries (GBs) and two types of point defects, namely the stacking fault tetrahedron (SFT) and the void. The GB can migrate itself under the shear strain and can serve as a sink to remove SFT and void. The sink efficiency of GBs is sensitive to their structural characteristics, the size of point defects, and temperature. The high-angle GBs can show a great ability to remove the point defects even at a low temperature, while the increase of temperature can facilitate the annihilation of the point defects at the low-angle GBs. The simulation reveals a new possible GB-mediated damage healing mechanism of irradiated materials. In particular, the nanotwinned metals are generally anticipated to be less effective in the alleviation of radiation damage because they contain mostly coherent twin boundaries, which are low-energy boundaries and are inefficient defect sinks in irradiated metallic materials. However, recent *in situ* studies have indicated that some nanotwinned metals exhibit unprecedented radiation tolerance, and the unexpected self-healing of twin boundaries in response to radiation was observed. In this work, we proposed two possible self-healing mechanisms of twin boundaries by considering the defective coherent twin boundary structures which contained incoherent twin segments or self-interstitial atoms. The mechanisms were confirmed and atomistic evidence was provided by carrying out the long-time molecular dynamics simulations.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room2)

[SY-E13] Deformation mode analysis by the eigenvectors of the atomic elastic stiffness

○Kisaragi Yashiro (Gifu University, Japan)

Inspired by the Wang's stability criteria based on the "elastic stiffness" coefficients, we have proposed to evaluate the local stability by the atomic elastic stiffness matrix and discuss the onset of local deformation such as dislocation nucleation, crack propagation, etc, with the positive definiteness of the matrix. The 6x6 matrix of the elastic stiffness correlates the stress and strain in the 6 dimensional strain space; thus the loss of the positiveness means the emergence of the unstable deformation path. The stiffness matrix is *not* identical to the "elastic coefficients" or usually named as "elastic constants" except in the no-load equilibrium or in the linear elasticity. In the thermodynamics of crystal lattices, the stress and the elastic coefficients are defined as the 1st and 2nd order derivatives of the internal energy per unit volume, respectively, and the stiffness in the nonlinear region is expressed with the elastic coefficients *plus* the stress contribution. In the atomic simulations based on the interatomic potential function, the internal energy is the sum of each atom contribution so that we can define the atomic stress and atomic elastic coefficients, then evaluate 6x6 stiffness matrix and its eigenvalue for each atom. The negative eigenvalue can be found on the surface and various lattice defects as already reported, then we advanced our instability analysis with the corresponding eigenvector of the atoms with negative eigenvalue. That is, the principal strain axes of the 3x3

strain tensor are evaluated as unstable deformation path for the atoms with negative eigenvalue and corresponding eigenvector of 6 strain components. In the case of crack initiation from the surface at the equator line of circular hole in the bcc-Fe under [110] tension, the deformation mode at the crack tip is normal to the (010) cleavage plane although the resulting crack opening occurs in the (110) planes. Another example is the dislocation emission from same circular hole under [111] tension, the deformation modes at the dislocation core are not only parallel to the [112] slip plane but also large normal mode corresponding to the Peierls barriers. In the presentation, we demonstrate various application of our deformation analysis to bcc-Fe, hcp-Mg, and 3C-SiC etc.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E14] Symposium E-14

Chairs: Thierry Auger(CNRS, France), Jamila Rahmoun(LAMIH-ENSIAME, Valenciennes University, France)

Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room2

[SY-E14] Stability Controlled Crack Evolution in Staggered Laminate Bio-material

○Yi Yan, Akihiro Nakatani （Dept. of Adaptive Machine Systems, Osaka University, Japan）

[SY-E14] A brittle to ductile transition modeling for liquid metal embrittlement

○Thierry Auger （CNRS, France）

[SY-E14] Buckling delamination of ductile thin films on rigid substrates

○Nadia Ben Dahmane, Guillaume Parry, Rafael Estevez （Univ. Grenoble Alpes, SIMAP, F-38000 Grenoble, France）

[SY-E14] An analytical model of the peeling forces at edges of multilayers subjected to temperature variations

○Chengyin Zhang[2], Neng-Hui Zhang[1,2] （1.Department of Mechanics, College of Sciences, Shanghai University, China, 2.Shanghai Key Laboratory of Mechanics in Energy Engineering, Shanghai Institute of Applied Mathematics and Mechanics, Shanghai University, China）

[SY-E14] **Characterization and multi-scale modeling of the mechanical response of the human humerus under dynamic loading**

○Jamila Rahmoun[1], Hakim Naceur[1], Pascal Drazetic[2], Christian Fontaine[3] （1.LAMIH-ENSIAME, Valenciennes University, France, 2.LAMIH-IUT, Valenciennes University, France, 3.Lab. d'anatomie, Lille University, France）

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room2)

[SY-E14] Stability Controlled Crack Evolution in Staggered Laminate Bio-material

○Yi Yan, Akihiro Nakatani （Dept. of Adaptive Machine Systems, Osaka University, Japan）

Nacre that is a bio-material with a staggered laminate micro-structure of hard and soft constituents shows a good performance of strength, stiffness, and toughness. The toughness of nacre with 95% hard and brittle phase and less than 5% soft collagen phase remarkably increases with cracking. Recent research shows that cracking in the bio-material is a stable process in macroscopic point of view, in which the fracture process zone widely spreads and in space, rather than the unstable process in many brittle/quasi-brittle materials, and that the high performance of the material is achieved by a shear ligament toughening mechanism. In this study, we solve a problem on cracking process under tensile test of model specimen with staggered micro-structure by using FEM and a simplified model, and discuss the relationship between the macroscopic behaviour and the fundamental properties of micro-structure. We find that the crack initiation in such staggered micro-structure originates from the loss of macroscopic stability and the following strain concentration. Coupling the normal debonding and shear sliding at interface of hard phases, a stable behaviour is achieved globally before a globally unstable point in stress-strain space, in which locally unstable domains do not contribute to the macroscopic instability. This mechanism can be considered as a stability enhancement, i.e. a kind of toughening. The cracking behaviour of our model shows size effect. The macroscopic stable stage is significantly affected by both the model and grain size of hard phase. Our research offers a different angle of view in exploring the microscopic mechanism of cracking process of staggered laminate bio-material.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room2)

[SY-E14] A brittle to ductile transition modeling for liquid metal embrittlement

○Thierry Auger （CNRS, France）

Liquid metal embrittlement is a surface adsorption induced fracture phenomenon that is currently not easily amenable to modeling. A strategy framed in terms of a competition between dislocation emission and Griffith fracture at the crack tip will be presented within the standard brittle to ductile transition realm. The goal is to be able to qualitatively predict the sensitivity to LME by coupling atomic scale modeling with a semi-continuous approach. The brittle to ductile transition description of an elastically loaded crack tip has been adapted to LME that relies on solid-liquid surface energy modeling at the atomic scale by AbInitio molecular dynamics and generalized stacking faults modeled at the atomic scale within the Peirls-Nabarro framework. We will present preliminary results on a model system for LME and a comparison with experimental results in terms of sensitivity.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room2)

[SY-E14] Buckling delamination of ductile thin films on rigid substrates

○Nadia Ben Dahmane, Guillaume Parry, Rafael Estevez （Univ. Grenoble Alpes, SIMAP, F-38000 Grenoble, France）

Thin film coatings submitted to high compressive stresses may experience a simultaneous buckling and delamination phenomenon called "blistering". The mechanism of formation and propagation of blisters in the form of straight wrinkles and circular blisters has been extensively studied in the literature considering a linear elastic behaviour of the film [1,2] *. The recent developments in numerical calculations allowed a better understanding of the mechanism of formation and propagation of complex buckling geometries including wavy buckles. In particular, the relationship between the mode mixity dependent interfacial toughness and the morphology of the wavy buckles has been elucidated* [3].

However, up-to-date, the response of ductile thin films deposited on rigid substrates remains an open issue. For instance, it has been evidenced experimentally [4] *that circular blisters in ductile thin films exhibit larger folding angles at their base compared to the elastic model predictions. In addition, recent experimental observations of 400nm gold films deposited on silicon wafers showed straight buckles with higher deflections compared to the elastic model. These differences in morphology are thought to originate from the elastic-plastic response of the film but the governing features need to be clarified.*

In this work, we are interested in the observation and characterization of buckling structures observed on gold films deposited on silicon substrates. In this context, we carried out a Finite Elements simulations with a model that accounts for isotropic yielding and the non-linearity of the film. A mode mixity dependent cohesive zone model is used to describe the thin film/substrate interface. This model allowed us to highlight the effect of plasticity on the equilibrium profiles resulting from elastic-plastic blistering, for both straight and circular blisters morphologies. In particular, a stabilizing effect of the circular blister form, which has been observed experimentally, has been demonstrated through calculation.

[1] Hutchinson et al., Adv. in Appl. Mech. 29 (1992) 63.
[2] Hutchinson et al. Acta Metallurgica Materialia, 40 (1992) 295
[3] Faou et al., J. Mech. Phys. Sol., 75 (2015) 93.
[4] Coupeau et al., Thin Solid Films 469 (2004) 221.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room2)

[SY-E14] An analytical model of the peeling forces at edges of multilayers subjected to temperature variations

○Chengyin Zhang[2], Neng-Hui Zhang[1,2] （1.Department of Mechanics, College of Sciences, Shanghai University, China, 2.Shanghai Key Laboratory of Mechanics in Energy Engineering, Shanghai Institute of Applied Mathematics and Mechanics, Shanghai University, China）

Due to different mechanical properties of various materials in a multilayered beam or plate, there is a thermal mismatch between layers when the structural temperature changes. The interfacial peeling stresses and interfacial shear stresses caused by the thermal mismatch can result in a delamination between layers, especially in the edge regions, and this can lead to the damage of a layered structures. Because of the complexity of the boundary stresses, it is difficult to obtain exact a closed-form solution for these interfacial thermal stresses in the edge regions. Therefore, instead of the precise stress field, we divert to the interfacial

peeling moment integrated by the localized interfacial normal stress and the interfacial shear force integrated by the localized interfacial shear stresses. The in-plane stresses in terms of Zhang’ s two-variables are integrated across the cross section in the far-field region in order to formulate the interfacial peeling moment and interfacial shear force in the edge regions for the multilayered beam system. To verify the applicability of the analytical model of the peeling forces (including interfacial peeling moment and shear force), an aluminum-silicon bimaterial beam in electronic devices is taken as a calculating sample. The influence of the thickness and Young’ s modulus of the film on the peeling forces are discussed. And the analytical predictions have a good agreement with the results from a finite-element analysis.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room2)

[SY-E14] Characterization and multi-scale modeling of the mechanical response of the human humerus under dynamic loading

○Jamila Rahmoun[1], Hakim Naceur[1], Pascal Drazetic[2], Christian Fontaine[3] (1.LAMIH-ENSIAME, Valenciennes University, France, 2.LAMIH-IUT, Valenciennes University, France, 3.Lab. d'anatomie, Lille University, France)

The relevance and biofidelity level of the human numerical models are key issues in car accidents related trauma research. To limit the risk of injuries of upper extremities and plan the preventive intervention, the humerus biomechanical properties must be correctly assessed. However, the constitutive laws used are largely derived from experimental characterizations carried out at the macroscopic scale without taking into account the bone architecture. A multi-scale approach coupled with nanoindentation experiments revealed to be more appropriate when the robustness of computation and accuracy of results are of interest.

In this study, we propose a multi-scale approach for the accurate characterization and modeling of the mechanical behavior of the human humerus under dynamic loading. The present model is based on the coupling between the Mori-Tanaka homogenization scheme, and an isotropic elastic damage model in the thermodynamic framework. In order to consider the strain rate effect on the humerus behavior, the standard model of Johnson-Cook is adopted. The obtained model is implemented using a User Material routine within the code LS-DYNA. The validity of the resulting FE model has been validated by comparing numerical predictions with experimental observations from characterization tests at different length-scales. To this end, a first experimental campaign was undertaken by means of nanoindentation tests on prismatic samples extracted directly from the same humerus diaphysis in order to determine its microscopic elastic properties. Then, local measurements of the damage effects were performed using several tension/compression and bending tests on small humerus specimens. Once the humerus material parameters were determined, a set of global validation bending impact tests composed of nine humeri were carried out using a drop tower for the determination of the mechanical response and the damage growth until complete humerus fracture.

The outcome of the proposed multi-scale model appears to correctly predict the general trends observed experimentally via the good estimation of the humerus ultimate impact load. The fracture patterns predicted by the proposed damage model are consistent with the physical humerus rupture even if this model is limited only to the estimation of the failure initiation.

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

[SY-F13] Symposium F-13

Chair: Takayuki Aoki(Tokyo Institute of Technology, Japan)

Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room3

[SY-F13] Advanced analysis tools for atomistic microstructure modeling

○Alexander Stukowski （Dept. of Materials Science, Darmstadt University of Technology, Germany）

[SY-F13] Studing thermo-oxidative degradation of polyimide in oxygen enviorment using MD simulations

○Ashwani Kumar Sengar, Sumit Basu （IIT Kanpur, India）

[SY-F13] In-plane characterization of structural and thermodynamic properties for steps at faceted chemically heterogeneous solid/liquid interfaces

○Hongtao Liang[1], Brian B. Laird[2], Mark Asta[3], Yang Yang[1] （1.Physics Department and State Key Laboratory of Precision Spectroscopy, School of Physical and Material Science, East China Normal Universit, China, 2.Department of Chemistry, University of Kansas, United States of America, 3.Department of Materials Science and Engineering, UC Berkeley, United States of America）

[SY-F13] Design of neural network for thermodynamics data of non-equilibrium multiphase field model

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

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room3)

[SY-F13] Advanced analysis tools for atomistic microstructure modeling

Invited

○Alexander Stukowski （Dept. of Materials Science, Darmstadt University of Technology, Germany）

Direct molecular dynamics (MD) simulations of materials microstructures become feasible thanks to fast growing computing capacities and can deliver a wealth of important observations on fundamental mechanisms. Such simulations are cross-scale rather than multi-scale, i.e. simultaneously large enough to represent meso- and macroscopic structures and processes and yet fully resolved, tracing every "jiggle" of atomic motion. Our recent MD simulations of dislocation-based crystal plasticity will be presented as an example [Nature 550, 492-495 (2017)].

To deal with the overwhelming complexity of processes on these scales, we develop advanced computational methods and tools to recast the massive transient trajectory data generated in large-scale MD simulations into a human comprehensible and analyzable form using methods of "in-situ computational microscopy". These algorithms automatically identify grain boundaries, surfaces and interfaces, dislocations, other defects, structural phases and deformation fields and can track their evolution. The data reduction and transformation of the underlying MD model into high-level microstructure representations make insightful visualization, quantitative analyses and linking with higher-scale materials models possible.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room3)

[SY-F13] Studing thermo-oxidative degradation of polyimide in oxygen enviorment using MD simulations

○Ashwani Kumar Sengar, Sumit Basu （IIT Kanpur, India）

Polyimides are important class of high-temperature polymers. These polyimides finds applications in diverse fields such as aerospace, electronics and automobiles. PMR-15 is one these polyimide which is extensively used as matrices for composite in the aerospace industry due to its high glass transition temperature, mechanical strength with high modulus of elasticity. However diffusion of oxygen in polymer and subsequent reaction with polymer leads to formation of oxidized layer. This layer drastically changes the mechanical properties of the polymer. Since these polyimide’ s founds application in aircraft design, so thermo-oxidative degradation of polymer may prove fatal and catastrophic in oxygen rich environment. Crack initiation and damage growth also follows due to thermo-oxidative degradation. We will be studying thermo oxidative degradation of PMR-15 polymer through molecular dynamics(MD) simulation. Molecular simulations has been become quite popular tool to predict macroscopic properties of polymer through statistical study at atomistic level. However getting correct force field parameter to simulate an exact material is challenging and of utmost importance. We attempt to study PMR-15 polymer with its full atomistic details intact and predicting it micromechanical properties through MD simulation. Due to some computational and forcefield limitations, coarse grained model of polyimide had been previously studied. In our analysis, we don’ t make any pre-assumption of course graining during sample preparation. We prepare our sample of PMR-15 with correct cross linking strategy such that we get density close to experimental value of 1.324. We will quantifies mechanical properties such as elastic constant and phenomenogical quantities such as diffusion constant and tries to predict the life of polymer due to thermo-oxidative degradation. We want challenge the time and scale limitations of MD simulation by attempting to simulate full scale atomistic model of the polymer PMR-

15. This study will give more insight about capabilities of MD simulations and also provides reasons where it fails to give us valid results. This study will provide an alternative path to study the systems where experimental analysis is difficult to setup or too expensive and cumbersome.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room3)

[SY-F13] In-plane characterization of structural and thermodynamic properties for steps at faceted chemically heterogeneous solid/liquid interfaces

○Hongtao Liang[1], Brian B. Laird[2], Mark Asta[3], Yang Yang[1] (1.Physics Department and State Key Laboratory of Precision Spectroscopy, School of Physical and Material Science, East China Normal Universit, China, 2.Department of Chemistry, University of Kansas, United States of America, 3.Department of Materials Science and Engineering, UC Berkeley, United States of America)

We present a methodology for studying steps at faceted chemically heterogeneous solid/liquid interfaces based on molecular-dynamics simulations. The methodology is applied to a faceted Al(111)/Pb(liquid) interface yielding a direct calculation of step free energy and extensive atomic-scale characterization for the interfacial layer containing the step. We characterized the step by calculating the in-plane density, potential energy, pressure components and stresses profiles. Main findings include: i) Calculated step free energy is in good agreement with TEM experimental measurement. ii) The step is connecting the interface liquid under tension and the interface solid under compression. iii) Fundamental properties of interface solid and interface liquid show orders of magnitudes difference in comparing with those predicted from the bulk Al-Pb alloy phase diagram. It is hoped that the methodology is extendable to the exploration of complexion equilibria/transitions at grain boundaries.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room3)

[SY-F13] Design of neural network for thermodynamics data of non-equilibrium multiphase field model

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

We construct neural network which estimates Gibbs free energy and chemical potential from temperature and composition of system for non-equilibrium multiphase field model. The mini-batch gradient descent method is selected for training of which data is led from calculation of non-equilibrium multiphase field model using Thermo-Calc thermodynamic database. We achieve highly precision neural network enough to use in non-equilibrium multiphase field model by introducing minimum and maximum data to the mini-batch method.

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

[SY-F14] Symposium F-14

Chair: Markus Kuehbach(Max-Planck-Institut fur Eisenforschung GmbH, Germany)

Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room3

[SY-F14] Large-scale multiphase flow simulations on a GPU supercomputer

○Takayuki Aoki （Tokyo Institute of Technology, Japan）

[SY-F14] **Transport Properties Of Fluid Mixtures In Micro- And Mesoporous Kerogen Membranes**

○Patrick Alain Bonnaud[1], Romain Vermorel[1], Julien Collell[2], Guillaume Galliéro[1] （1.University of Pau and Adour Countries, France, 2.Total E&P, France）

[SY-F14] Numerical simulation of ionic transport through deformable porous media: application to cortical bone tissue modeling

○Jana Turjanicova[1,2], Eduard Rohan[1,2], Vladimír Lukeš[2] （1.Dept. of Mechanis, Univ. of West Bohemia in Pilsen, Czech Republic, 2.NTIS - New technologies for information society, Czech Republic）

[SY-F14] Hydrogen Transport and Thermal Desorption in Multiphase Steels

○Andrej Turk[1], Pedro E.J. Rivera-Díaz-del-Castillo[2], Enrique Galindo-Nava[1] （1.University of Cambridge, UK, 2.Lancaster University, UK）

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room3)

[SY-F14] Large-scale multiphase flow simulations on a GPU supercomputer

Invited

○Takayuki Aoki （Tokyo Institute of Technology, Japan）

GPU (Graphics Processing Unit) was originally designed for graphics rendering and has been widely used for supercomputers in the world, since it has high computational performance and wide memory bandwidth and suitable for scientific computing. We have developed stencil codes written in CUDA and executed them on a GPU supercomputer TSUBAME. Several simulations of gas-liquid and gas-solid two-phase flows are demonstrated with the numerical methods and the algorithms such as AMR (Adaptive Mesh Refinement) and dynamic load balance for efficient large-scale simulations.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room3)

[SY-F14] Transport Properties Of Fluid Mixtures In Micro- And Mesoporous Kerogen Membranes

○Patrick Alain Bonnaud[1], Romain Vermorel[1], Julien Collell[2], Guillaume Galliéro[1] （1.University of Pau and Adour Countries, France, 2.Total E&P, France）

With the exhaustion of conventional resources, the production of gas from organic-rich shales has encountered a rising interest over the last 15 years. In such resources, gas is trapped in nodules of organic matter scattered in an inorganic matrix mostly constituted of quartz, clays, and calcite. Nodules represent only few percentages of the total volume of shales and result from a maturation process during the burial stage. These nodules of organic matter contain mostly kerogen that acts as a source, but also as a container of hydrocarbons. Various forms were reported differentiating to each other by their origin, their maturity, and sediment history, which affects, for example, their chemical composition, their density, and the porosity. A common feature of kerogens is their multi-scale porous network with pore sizes ranging from micropores (<2 nm) to macropores (>50 nm). Structure and connectivity of pores greatly affect the materials permeability. In porous structures where the flow is limited by micropores (e.g., pore throats), very low permeabilities are observed.

Despite the important development of shales, fluid flow mechanisms within kerogen matrix remains poorly understood. While experimental characterization remains difficult, molecular dynamics simulations were proven very useful to characterize transport mechanisms within kerogen membranes. The aforementioned studies staid limited to microporous systems, while mass transfer originating from small pores and transiting to larger pores, fractures, and production wells is a multi-scale mechanism. In this work, we designed and developed molecular simulation tools to capture both microporosity and mesoporosity of kerogen through the aggregation and the spatial arrangement of smaller basic units in order to generate representative molecular structures. From those models, we investigated by molecular dynamics simulations how the nature (i.e., maturity and sediment origin) and the chemical composition influence both the porous network and the related physical and transport properties of fluid mixtures (e.g., selectivity, phase coexistence, diffusivity) in kerogen.

This method and findings underscore the importance of accounting for both micro- and mesoporosity to

accurately model fluid transport in kerogen.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room3)

[SY-F14] Numerical simulation of ionic transport through deformable porous media: application to cortical bone tissue modeling

○Jana Turjanicova[1,2], Eduard Rohan[1,2], Vladimír Lukeš[2] （1.Dept. of Mechanis, Univ. of West Bohemia in Pilsen, Czech Republic, 2.NTIS - New technologies for information society, Czech Republic）

Cortical bone tissue is known to have a strictly hierarchical porous structure on multiple scales. On the canalicular-lacunar scale, it consist of two phases: deformable collagen-apatite matrix charged by a small electric charge and bone fluid filling the pore space created by network of small interconnected channels. Bone fluid is considered an electrolyte solution of two species of charged monovalent ions of opposite polarizations. Due to the potential differences, the electrical double layer occurs in the proximity of the solid-fluid interface. Considering its effect, the transport of such electrolyte through a network of small channels with charged surface is controlled by coupling between the electric field , Stokes flow, the migration-diffusion process and deformation of solid matrix.
In order to describe cortical bone effective properties on the macroscopic scale, the unfolding homogenization method is applied on the model of ionic transport through deformable porous media. The microstructure on canalicular-lacunar scale is simplified by assumption of its periodicity and is represented by so-called representative periodic cell. The characteristic responses on this cell are used to compute the effective coefficients describing cortical bone behavior on the macroscopic scale (scale of one osteon). Macroscopic model behavior was tested on the simple boundary value problem. Implementation of upscaling process as well as numerical simulation on the macroscopic model was made in in-house developed python based FEM software SfePy.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room3)

[SY-F14] Hydrogen Transport and Thermal Desorption in Multiphase Steels

○Andrej Turk[1], Pedro E.J. Rivera-Díaz-del-Castillo[2], Enrique Galindo-Nava[1] （1.University of Cambridge, UK, 2.Lancaster University, UK）

Hydrogen diffusion is modelled using a 2D multi-trap diffusion model. It takes into account trapping on crystal defects (dislocations, carbides and grain boundaries), as well as the presence of secondary phases with different hydrogen diffusivity and solubility. Secondary phases introduce local discontinuities in the hydrogen concentration field and this problem has not been modelled systematically in multiphase steels. The first studied case is a 2D simulation of thermal desorption in high-strength bainitic steels with varying fractions of retained austenite where the effects of austenite morphology are highlighted. The second case is a different thermal desorption problem in a high-temperature iron-nickel FCC alloy in which grain boundaries are known to be fast diffusion pathways. As the boundaries require a prohibitively fine discretisation in 2D, the microstructure is parameterised and reduced to 1D. The effects of grain boundary properties on hydrogen diffusion are studied. Lastly, we explore the application of the model to other interstitial elements and metallic systems, where the morphology and spatial arrangement of the microstructure strongly affects

elemental diffusion.

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

[SY-N7] Symposium N-7

Chair: Shotaro Hara(Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan)
Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room4

[SY-N7] Bridging Time Scales with Variationally Enhanced Sampling

○Omar Valsson （Max Planck Institute for Polymer Research, Germany）

[SY-N7] Simulations of Branched Polyelectrolytes

○Filip Uhlik （Charles University, Czech Republic）

[SY-N7] Adaptive resolution simulations coupling molecular dynamics to dissipative particle dynamic

○Matej Praprotnik （National Institute of Chemistry, Slovenia）

[SY-N7] Using Diffusive Molecular Dynamics Simulations to Investigate Grain Boundary Segregation and Grain Boundary Structural Transformations

Louis Hebrard, ○Chad W Sinclair （Dept. of Materials Engineering, University of British Columbia, Canada）

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room4)

[SY-N7] Bridging Time Scales with Variationally Enhanced Sampling

Invited

○Omar Valsson （Max Planck Institute for Polymer Research, Germany）

The usefulness of atomistic simulations is generally hampered by the presence of several metastable states separated by high barriers leading to kinetic bottlenecks. Transitions between metastable states thus occur on much longer time scales than one can simulate. Numerous enhanced sampling methods have been introduced to alleviate this time scale problem, including methods based on identifying a few crucial order parameters and enhancing their sampling through the introduction of an external biasing potential.

Here will we discuss Variationally Enhanced Sampling (Valsson and Parrinello, PRL 113 090601, 2014), a generally applicable enhanced sampling method where an external bias potential is constructed by minimizing a convex functional. We present numerous examples from physics and chemistry which show the flexibility and practicality of the method. We will furthermore show how the variational property of the method can be used to extend the method in various innovative ways, e.g.: to obtain kinetic information from atomistic simulation; to accelerate nucleation events by employing models from classial nucleation theory; and to incorporate experimental information into molecular simulations.

We will also introduce the VES code (http://www.ves-code.org), an open-source library for the PLUMED 2 plugin that implements methods based on Variationally Enhanced Sampling

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room4)

[SY-N7] Simulations of Branched Polyelectrolytes

○Filip Uhlik （Charles University, Czech Republic）

Polyelectrolytes (PEs) are polymers with ionizable groups. Under suitable conditions, PEs are soluble in aqueous media. This property makes them attractive for biological, medicinal and environment-friendly applications that require organization of matter at nanoscale. The applications of PEs range from drug carriers, water pollutants removal, oil recovery to sea water desalination. In some of them, *e.g.* as thickening agents or super-absorbents in diapers, they have already reached mass production.

In this contribution a general and efficient simulation technique based on hybrid Monte Carlo (HMC) method will be described. HMC uses dynamics for evolution, but dynamics of a long polymer with N beads is itself slow (Rouse time $\propto N^2$). For this reason we use a faster *unphysical* evolution with a modified Hamiltonian while still efficiently Monte Carlo sampling the Boltzmann distribution with the original one. The resulting simulation is much faster than molecular dynamics and other methods. It is
also well suited for simulations of coarse-grained models of PEs and allows for using reaction and other ensemble [F. Uhlik *et al.* Macromolecules 47 (2014) 4004].

Results for several types of branched PEs (*e.g.*, stars and combs) for different conditions of solvent quality, Bjerrum and Debye lengths will be given. While strong PEs remain fully ionized, the degree of ionization of weak PEs can be influenced by both changing pH and ionic strength. This results in a responsiveness to external stimuli needed in many applications. The conformations of weak PEs are coupled with charge redistribution and this can lead to unexpectedly complex behavior. For example, strong PE stars in marginally

poor solvents form bundles while weak PE stars redistribute charge and form core-shell structures with some arms uncharged and collapsed and others charged and extended. Behavior of other branching types as well as formation of inter-polyelectrolyte complexes will be also discussed.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room4)

[SY-N7] Adaptive resolution simulations coupling molecular dynamics to dissipative particle dynamic

○Matej Praprotnik （National Institute of Chemistry, Slovenia）

We present the hybrid coupling of the molecular dynamics (MD) and dissipative particle dynamics (DPD) methods, bridging the micro- and mesoscopic levels of detail. The coupling is achieved using the adaptive resolution scheme (AdResS), which is a linear momentum conserving multiscale method. Our methodology is thus suitable for simulations of liquids on the micro/mesoscopic scale, where hydrodynamics is crucial. The presented approach is showcased for water at ambient conditions. The supramolecular coupling is carried out by our clustering algorithm SWINGER that assembles, disassembles, and reassembles water clusters on demand during the course of the simulation. This allows for a seamless coupling between standard atomistic MD and DPD models.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room4)

[SY-N7] Using Diffusive Molecular Dynamics Simulations to Investigate Grain Boundary Segregation and Grain Boundary Structural Transformations

Louis Hebrard, ○Chad W Sinclair （Dept. of Materials Engineering, University of British Columbia, Canada）

We have investigated the time evolution of segregation on both grain boundary structural and chemical transitions in Al-Mg alloys by means of alloy diffusive molecular dynamics (a-DMD) calculations. The predictions with regard to segregation are compared with classic continuum approaches including the calculation of grain boundary free energy curves. The role that chemical segregation plays in grain boundary structural transitions (complexions) is studied and used to construct temperature-pressure-composition stability plots for one particular grain boundary.

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

[SY-D5] Symposium D-5

Chair: Jörg Neugebauer(MPIE, Germany)

Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room8

[SY-D5] Computational exploration of strong permanent magnet compounds

○Takashi Miyake[1,2,3] （1.CD-FMat, AIST, Japan, 2.ESICMM, NIMS, Japan, 3.CMI[2], NIMS, Japan）

[SY-D5] A machine-learning approach for finding new hard-magnetic phases

Johannes J. Möller, ○Daniel F. Urban, Christian Elsässer （Fraunhofer IWM, Freiburg, Germany）

[SY-D5] High-throughput optimization of finite temperature phase stabilities of Ce-based hard magnetic materials

○Tilmann Hickel, Halil Soezen, Fritz Koermann, Joerg Neugebauer （Max Planck Institut fur Eisenforschung, Germany）

[SY-D5] Understanding pairwise magnetic interactions in Fe-based materials with machine learning techniques

○Osamu Waseda, Omkar Hegde, Tilmann Hickel, Jörg Neugebauer （MPIE, Germany）

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room8)

[SY-D5] Computational exploration of strong permanent magnet compounds

Invited

○Takashi Miyake[1,2,3] (1.CD-FMat, AIST, Japan, 2.ESICMM, NIMS, Japan, 3.CMI[2], NIMS, Japan)

Modern strong magnets are rare-earth magnets in which high saturation magnetization and high Curie temperature come from transition-metal 3d electrons, and strong magnetorcystalline anisotropy originates from rare-earth 4f electrons [1]. There are various types of crystal structures and chemical composition, and exploration of a new magnet compound is a hot topic. Among them, RFe$_{12}$-type compounds with the ThMn$_{12}$ structure are attracting renewed interest because of their high iron content. Recently synthesized NdFe$_{12}$N$_x$ film has higher saturation magnetization and anisotropy field than Nd$_2$Fe$_{14}$B, although its bulk phase is thermodynamically unstable. I will present a first-principles study on the effect of element substitution on magnetism and structural stability. I will also discuss how machine learning accelerates magnetic-materials discovery. Application to the Curie temperature of RFe$_{12}$-type compounds shows that Bayesian optimization offers an efficient way to optimize chemical composition of magnet compounds. Kernel ridge regression using orbital-field matrix as a descriptor reproduces the magnetic moment and formation energy of thousands of transition-metal compounds in reasonable accuracy [2], which can be utilized for virtual screening of new magnetic compounds. Bayesian optimization approach to crystal structure prediction is also presented [3].

[1] Takashi Miyake and Hisazumi Akai, J. Phys. Soc. Jpn. **87**, 041009 (2018).
[2] T.L. Pham et al., Sci. Tech. Adv. Mater. **18**, 756 (2017).
[3] T. Yamashita et al., Phys. Rev. Mater. **2**, 013803 (2018).

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room8)

[SY-D5] A machine-learning approach for finding new hard-magnetic phases

Johannes J. Möller, ○Daniel F. Urban, Christian Elsässer (Fraunhofer IWM, Freiburg, Germany)

Data-mining and machine-learning (ML) techniques play an increasingly important role in the discovery and development of new materials. In this contribution, we use kernel-based learning methods to predict optimal chemical compositions for new permanent magnets, which are key components in many green-energy technologies. The magnetic-property data used for training and testing the ML models were obtained by a combinatorial high-throughput screening (HTS) using density-functional theory calculations. For encoding the structural and chemical information of the HTS data in a machine-readable format, we use several existing and newly developed material descriptors and assess the predictive power of the ML models built with them. The accuracy of the ML models with an optimal choice of descriptor and model parameters enables the prediction of promising structurecomposition combinations for substitutes of state-of-the-art magnetic materials like Nd2Fe14B - with similar intrinsic hard-magnetic properties but no or less amounts of critical rare-earth elements.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room8)

[SY-D5] High-throughput optimization of finite temperature phase stabilities of Ce-based hard magnetic materials

○Tilmann Hickel, Halil Soezen, Fritz Koermann, Joerg Neugebauer （Max Planck Institut fur Eisenforschung, Germany）

While the present search for novel materials concepts to improve hard magnetic applications is concentrated on the magnetic properties of individual phases, their finite temperature phase stabilities are largely unknown. In the Ce-Fe-Ti ternary system, for example, the promising phase $CeFe_{11}Ti$ is competing with various Laves phases as demonstrated by energy-dispersive X-ray spectroscopy (EDS) measurements. We therefore use concepts of ab initio thermodynamics capturing vibrational, electronic and magnetic entropy contributions in order to determine the Helmholtz free energy of all relevant phases. Several additional elements have been considered within this formalism, to investigate their partitioning and impact on the relative phase stabilities. The insights obtained demonstrate how the screening of a complete set of transition metals in quarternary hard magnetic materials can be performed most efficiently and which alloying elements improve the stability of promising phases such as $CeFe_{11}Ti$ most substantially.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room8)

[SY-D5] Understanding pairwise magnetic interactions in Fe-based materials with machine learning techniques

○Osamu Waseda, Omkar Hegde, Tilmann Hickel, Jörg Neugebauer （MPIE, Germany）

Magnetic interactions are crucial to the stability of structural phases as well as for various thermophysical effects such as magnetocalorics. Despite their importance, there is no experimental procedure which allows for the understanding of magnetic interactions at the atomic level, and there is no exact theoretical model capable of describing them precisely except for expensive ab initio methods. It has been recently suggested that the Heisenberg Landau model has sufficient versatility to map the contribution of complex magnetic interactions of Fe-based materials to the free energy. Its original form, however, contains a high number of parameters which make it prone to overfitting. In this study, we mapped the magnetic interactions created from spin-polarised DFT calculations to extended Heisenberg-Landau models via various machine learning regression techniques. The free energy contribution of the magnetic interactions is then determined through Monte Carlo simulations for millions of atoms which would otherwise not be achievable with ab initio methods. The results enable us to understand the overall effects of impurities contained within microstructures on the magnetism in iron based materials.

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

[SY-D6] Symposium D-6

Chair: Daniel Urban(Fraunhofer IWM, Germany)

Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room8

[SY-D6] Novel two-dimensional materials: Materials discovery, data provenance, and workflow reproducibility.

○Nicola Marzari （EPFL, Switzerland）

[SY-D6] In silico screening of Metal-Organic Frameworks for adsorption driven heat pumps and chillers

○Mate Erdos[1], Martijn F. de Lange[1], Freek Kapteijn[2], Othonas A. Moultos[1], Thijs J. H. Vlugt[1]
（1.Engineering Thermodynamics, Process &Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Netherlands, 2.Catalysis Engineering, Chemical Engineering Department, Delft University of Technology, Netherlands）

[SY-D6] Machine learning assisted by first-principles calculations for designing intermetallic-typed metallic glasses

○Tokuteru Uesugi, Manami Sakai, Yorinobu Takigawa, Kenji Higashi （Dep. of Materials Science, Osaka Prefecture Univ., Japan）

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room8)

[SY-D6] Novel two-dimensional materials: Materials discovery, data provenance, and workflow reproducibility.

Invited

○Nicola Marzari （EPFL, Switzerland）

Two-dimensional materials have seen in the past decade very dedicated experimental and theoretical efforts in the quest for novel physics and functionalities. Here, we systematically explore with first-principles calculations known inorganic materials, to identify those that could be exfoliated into two-dimensional layers. We start by curating experimental materials databases, collecting reliable data for 110,000 unique compounds. Then, we identify those that appear layered according to simple geometric and bonding criteria, and launch high-throughput calculations - based on van-der-Waals density-functional theory and 2D density-functional perturbation theory - to characterize binding energies, stability, and properties. Remarkably, we find close to 2000 inorganic compounds that could be exfoliated into novel two-dimensional materials, and recover in the process the known ones - from graphene to transition-metal dichalcogenides to boron nitride and black phosphorus. I’ll provide a perspective on the promising properties we are uncovering - topological, electrical, magnetic, chemical - while highlighting the need for scalable approaches to data and calculations, able to persist and query the full provenance of the data and ensure reproducibility of the calculations’ workflows.

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room8)

[SY-D6] In silico screening of Metal-Organic Frameworks for adsorption driven heat pumps and chillers

○Mate Erdos[1], Martijn F. de Lange[1], Freek Kapteijn[2], Othonas A. Moultos[1], Thijs J. H. Vlugt[1] （1.Engineering Thermodynamics, Process &Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Netherlands, 2.Catalysis Engineering, Chemical Engineering Department, Delft University of Technology, Netherlands）

20% of the total energy demand is attributed to hot water production and space heating/cooling of buildings. Although, it is intended to produce more and more energy from clean low carbon sources for heating/cooling, 75% of it is still acquired by using fossil fuels. To ameliorate the dependence on fossil fuels and increase energy efficiency, several technologies have emerged recently, utilizing renewable energy sources for heating/cooling applications. Among these, adsorption driven heat pumps and coolers (AHP/ACs) are promising candidates because these devices can utilize thermal energy instead of electricity. However, a drawback of AHP/ACs systems is the lower performance compared to heat pumps based on absorption or chemical reactions. One possible way to improve the energy efficiency of AHP/ACs is by finding adsorbents with enhanced adsorption and thermophysical properties. Metal-Organic Frameworks in conjunction with alcohols (methanol, ethanol) are promising working pairs for this application.
A computational screening of MOFs is carried out to find the best performing structures for AC applications with methanol and ethanol as working fluids. Molecular simulations using Monte Carlo method are conducted to investigate 2930 structures. An efficient screening methodology is devised with 4 subsequent screening steps. The commensurate adsorption behavior of the adsorbates is exploited to reduce computational effort. In the last screening step, the 6 best performing MOFs with high deliverable working capacities (~0.6 ml working fluid in 1 ml structure) and diverse adsorption step locations are selected from

the original 2930 structures for each adsorbate. The finally selected structures show higher deliverable working capacities than the reported highest values (~0.45 ml working fluid in 1 ml structure).

(Fri. Nov 2, 2018 11:15 AM - 12:30 PM Room8)

[SY-D6] Machine learning assisted by first-principles calculations for designing intermetallic-typed metallic glasses

○Tokuteru Uesugi, Manami Sakai, Yorinobu Takigawa, Kenji Higashi （Dep. of Materials Science, Osaka Prefecture Univ., Japan）

Metallic glasses have interesting properties such as low Young’s moduli, high corrosion resistance and high wear resistance and are considered new materials in many fields. The factors that contribute to the glass-forming ability (GFA) are an important consideration in the design of new metallic glasses. Ternary metallic glasses are classified into three types on the basis of their atomic size distribution. The factors that affect the GFAs of the metallic glasses are presumed to vary among the three types. However, metallic glasses with two alloying elements exhibit irregular composition ratios or atomic radii; thus, in these cases, the contributing factor is unclear. The binary metallic glasses usually crystallize only intermetallic crystalline phase after heating. For example, Ti-Cu and Ti-Ni binary metallic glasses crystallized as only TiCu and Ti_2Ni intermetallic compounds. Therefore, these metallic glasses such as Ti-Cu and Ti-Ni are able to be called as intermetallic-typed metallic glasses (IMG). In this work, we aimed to elucidate the design criteria of IMG and design new metallic glasses based on the machine learning assisted by the first-principles calculations. First, the first-principles calculations were performed on intermetallic compounds and then, explanatory variables were calculated. Second, a regression systems of GFA was constructed using artificial neural networks (ANN) and logistic regression analysis (LRA). The results of ANN validation showed very high accuracy than the results of LRA validation. The partial regression coefficients of LRA indicated the design criteria of intermetallic-typed metallic glasses. The obtained regression systems were applied to intermetallic compounds whose GFA are unknown, and the alloy systems of a novel metallic glass were predicted.

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

[SY-H11] Symposium H-11

Chair: Erik Van der Giessen(University of Groningen, Netherlands)

Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room9

[SY-H11] A Hierarchical Multiscale Simulations Approach for Modeling Failure in Polymer Matrix Composites

Xiawa Wu[1], Amin Aramoon[1], Christopher Woodward[2], ○Jaafar A. El-Awady[1] （1.Johns Hopkins University, United States of America, 2.Air Force Research Laboratory, United States of America）

[SY-H11] Some Positive Aspect of Structural Defects in Graphene/Polymer Nanocomposites Studied by Abinitio,Molecular Dynamics, and Continuum Approaches

○Seunghwa Yang[1], Janghyuk Moon[1], Maenghyo Cho[2] （1.School of Energy Systems Engineering, Chung-Ang University, Korea, 2.School of Mechanical and Aerospace Engineering, Seoul National University, Korea）

[SY-H11] Linear and non-linear viscoelastic properties of model fractal-like aggregates polymer nanocomposites

○Samy MERABIA[1], Yang WANG[1], François DETCHEVERRY[1], Marc COUTY[2], Gaëtan MAUREL[2] （1.CNRS and Universite Lyon 1, France, 2.MFP Michelin, Clermont-Ferrand , France）

[SY-H11] Topological defect structure in the self-assembly of semiflexible polymers under spherical confinement

○Mihir Khadilkar, Arash Nikoubashman （Johannes GutenBerg University Mainz, Germany, Germany）

[SY-H11] Molecular dynamics simulation of the detachment force between graphene and epoxy resin

○Kazuki Mori[1], Makoto Yabe[2], Yuji Kohno[2], Jun Koyanagi[3] （1.ITOCHU Techno-Solutions Corporation, Japan, 2.Yokohama National University, Japan, 3.Tokyo University of Science, Japan）

[SY-H11] Relation between deformation and electrical conductivity for electroconductive polymer nanocomposites with highly segregated structure

○Oleg V. Lebedev[1], Sergey Abaimov[1], Alexander Ozerin[2], Anton Trofimov[1], Iskander Akhatov[1] （1.Center for Design, Manufacturing and Materials, Skolkovo Institute of Science and Technology, Russia, 2.Laboratory of the Structure of Polymer Materials, N.S. Enikolopov Institute of Synthetic Polymer Materials of RAS, Russia）

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room9)

[SY-H11] A Hierarchical Multiscale Simulations Approach for Modeling Failure in Polymer Matrix Composites

Xiawa Wu[1], Amin Aramoon[1], Christopher Woodward[2], ○Jaafar A. El-Awady[1] (1.Johns Hopkins University, United States of America, 2.Air Force Research Laboratory, United States of America)

Polymer matrix composites (PMCs) are widely used in many automotive, marine, and aerospace applications. Predicting the damage and failure of such systems is of crucial interest for their reliable performance. In this work, a coarse-grained MD model has been developed to characterize the evolution of free volume density (voids) in DGEBA polymers under loading and its subsequently plastic deformation (e.g. hardening and failure). A detailed atomic monomer is coarsened to create the tailored plastic behavior. Cross-linked polymer networks are created under different curing conditions, including temperature, and cross-linker functionality using a dynamic cross-linking algorithm. The effect of chain size, and degree of cross-linking are also investigated. The free volumes are measured as a function of strain by fitting the largest ellipsoids between neighboring chains in the network. From these simulations we develop a direct correlation between the evolution of plastic deformation and the free volume density. The results of these simulations are then upscaled into a finite element simulations to model the damage and failure of PMCs.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room9)

[SY-H11] Some Positive Aspect of Structural Defects in Graphene/Polymer Nanocomposites Studied by Abinitio,Molecular Dynamics, and Continuum Approaches

○Seunghwa Yang[1], Janghyuk Moon[1], Maenghyo Cho[2] (1.School of Energy Systems Engineering, Chung-Ang University, Korea, 2.School of Mechanical and Aerospace Engineering, Seoul National University, Korea)

In this study, we reveal some positive aspect of the intrinsic defect commonly observed in two dimensional nanocarbon structure of graphene as a multifunctional reinforcement. Among the intrinsic defects commonly observed in graphene, we focus on the crystallographic defect of the Thrower-Tone-Wales (TSW) defect. Since the formation of the TSW defects in graphene involves 90 degree of rotation of the two covalently bonded neighboring carbon atoms and the resultant change in electron density, we firstly adopt the density functional theory to investigate the adhesion characteristics of the carbon atoms in TSW defect to the to the polypropylene (PP) monomers. In order to observe the effect of the arbitrarily generated TSW defect on representative volume element level mechanical properties, we modeled transversely isotropic molecular unit cell model of single layer graphene reinforced PP nanocomposites. The stress-strain curves in tension and shear are predicted from a constant strain rate ensemble simulation at below the glass transition temperature of the PP matrix and at the atmospheric pressure. At the same time, the mechanical properties of single layer graphene embedding the TSW defect is studied using the same ensemble simulations. To correlate the locally rippled configuration of the TSW defected sites to the macroscopic stress-strain relation, we analyzed the surface roughness of the graphene according to the density of TSW defects. Finally, a multiphase micromechanics model incorporating the weakened interface between graphene and PP matrix is applied to study the stress-strain relation of poly-dispersed nanocomposites with random graphene orientation. The two rivalling effects of the degradation of the graphene and improvement of the interfacial shear load transfer are evaluated from parametric studies on the effect of the aspect ratio and the volume

fraction of the defected graphene on overall stress-strain relation of poly-dispersed nanocomposites.
This research is supported by a Basic Science Research Program grant (15-113-701-010) through the Agency for Defense Development of Korea

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(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room9)

[SY-H11] Linear and non-linear viscoelastic properties of model fractal-like aggregates polymer nanocomposites

○Samy MERABIA[1], Yang WANG[1], François DETCHEVERRY[1], Marc COUTY[2], Gaëtan MAUREL[2] （1.CNRS and Universite Lyon 1, France, 2.MFP Michelin, Clermont-Ferrand , France）

Dispersing solid fillers into a polymer matrix is a common strategy to enhance and tailor its properties. Polymer nanocomposites (PNCs) so obtained with fractal-like aggregates have exceptional rheological behavior that have long been exploited in the tire industry. However, due to disparity of time and length scales, our understanding of the relation between nanocomposites structure and rheology remains far from complete.
In this contribution, we propose a mesoscopic model to describe the dynamics and the rheology of aggregate PNCs. While aggregates are described explicitly as groups of interacting particles, we use for the polymer matrix an implicit description based on generalized Langevin equation, that captures the average effect of a viscoelastic medium. These two-level description allows us to simulate large PNCs systems containing dozens of aggregates.
We focus on the linear and non-linear viscoelastic properties of PNCs. We characterize the influence of aggregate size, rigidity and volume fraction. We show that compared to nanoparticles, aggregates may display levels of reinforcement considerably larger. We also demonsrate that the stress relaxation of aggregates display long relaxation times, which originates in the slow rotation of the aggregates. As concerns non linear properties, we concentrate on the Payne effect characterized by a drop of the storage modulus for small deformation amplitudes. We relate the Payne effect to the deformation and alignment of the aggregates under the imposed deformation direction. We also discuss memory effects, and in particular the slow recover kinetics subsequent to a first deformation. All these considerations may help in building connections between the macroscopic mechanical response of the PNCs and the mesoscopic morphology of the nanofillers.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room9)

[SY-H11] Topological defect structure in the self-assembly of semiflexible polymers under spherical confinement

○Mihir Khadilkar, Arash Nikoubashman （Johannes GutenBerg University Mainz, Germany, Germany）

Static and dynamic properties of macromolecules are often strongly affected in confinement, due to the enforced constraints on polymer motion and conformation. Moreover, for semiflexible polymers like DNA and actin, the confinement effects also compete with the enthalpic costs of bending. Using coarse-grained molecular dynamics simulations, we explore the phase behavior of semiflexible polymers confined to spheres and thin spherical shells. We observe a disordered-to-nematic ordering transition as a function of chain stiffness accompanied by the emergence of topological defects on the surface. Each of the configuration

variables including chain length, packing density, chain stiffness and shell thickness uniquely affects the phase behavior, including the nature and relative orientation of the defects. Systemic trends observed could pave the way for a better understanding of the links between topological defects and elastic properties of the macromolecules. Further, controlling the nature and locations of these defects could also be crucial in understanding other multiscale biological processes involving these biomolecules like chromosomal packing of DNA and gene regulation.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room9)

[SY-H11] Molecular dynamics simulation of the detachment force between graphene and epoxy resin

○Kazuki Mori[1], Makoto Yabe[2], Yuji Kohno[2], Jun Koyanagi[3] (1.ITOCHU Techno-Solutions Corporation, Japan, 2.Yokohama National University, Japan, 3.Tokyo University of Science, Japan)

We introduced a computational method to investigate the shear detachment strength at a carbon fiber/epoxy resin interface using molecular dynamics simulations. In the computational model, the graphene molecular structure was assumed to be that of a simple carbon fiber. The interaction energies calculated for the epoxy bulk phase were in good agreement with the experimental data in our previous work [1], however, the estimates of surface energy between carbon fiber and epoxy resin were missing. In this work, we calculated the surface energy and estimated the correlation between surface energy and shear detachment strength of the carbon fiber/epoxy resin interface. All calculations were performed using Exabyte.io platform [2]. The calculated surface energy was confirmed to be related to the experimental shear strength: the surface energy increased with increase in the resin density near graphene. In addition, molecular structures of bulk resin and the resin near graphene surface regions were found to be different. Our results suggest that the carbon fiber and epoxy resin have strong interaction at the interface. In the vicinity of graphene, the resin molecular structure deformed into a flattened state. We propose this to happen due to the influence of CH/π orbitals. The CH/π interaction is a weak interaction (0.1 kcal/mol), however, the compound effect of the numerous weak interaction forces leads to the rise of a strong interaction at the surface between graphene and resin. Because of this, the carbon composite becomes a high-strength material. We further simulated the stress-strain curve of the graphene/epoxy composite model because the above interaction might be related to tensile stress. We found that the crack formation started from the epoxy interface layer and progressed to the bulk epoxy layer.

[1] K. Mori, N. Matsumoto, S. Nomoto, K. Tsuruta, OJCM (2017) 7, 179-184
[2] https://exabyte.io/

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room9)

[SY-H11] Relation between deformation and electrical conductivity for electroconductive polymer nanocomposites with highly segregated structure

○Oleg V. Lebedev[1], Sergey Abaimov[1], Alexander Ozerin[2], Anton Trofimov[1], Iskander Akhatov[1] (1.Center for Design, Manufacturing and Materials, Skolkovo Institute of Science and Technology, Russia, 2.Laboratory of the Structure of Polymer Materials, N.S. Enikolopov Institute of Synthetic Polymer Materials of RAS, Russia)

Polymer composites with highly non-uniform distribution of nanoscale filler in a matrix (filler forming a so-called segregated structure) possess many interesting properties, such as very low percolation threshold and distinct non-linear piezoresistance effect. To study the dependence of the loss in electrical conductivity on the uniaxial deformation and 3D expansion degree, multiscale finite-element analysis was conducted for polymer matrix containing carbon nanotubes. At the first stage of this work, a uniform distribution of dense-packed and entangled nanotubes was created within a thin planar RVE with polyethylene properties. The response of RVE’s electrical conductivity to a variety of loading conditions was studied to simulate the response of different parts of a segregated structure on the nano-level to the external loading applied at macro-level. In particular, the planar RVE was oriented at different angles relatively to the axis of macroscopic uniaxial loading and progressively deformed to observe non-linear effects. For each pair angle/deformation, a value of effective electrical conductivity was calculated by an external procedure (Python script), accounting for the Kirchhoff's circuit laws. In the result, an analytical functional dependence of the electrical conductivity on RVE’s angle and degree of deformation was developed and compared with the experimental results obtained for uniaxially-deformed electroconductive nanocomposite. At the second stage, a finite-element micro-level model of the segregated structure, recreated from the experimentally observed filler distribution in a composite, was created. The elements of the volume corresponding to the segregated highly filled areas were modeled as having effective electroconductive properties that obey the previously developed conductivity and angle/deformation analytic relation. The micro-level model was uniaxially deformed and thermally treated to introduce expansion of the matrix, and for each degree of deformation or expansion the effective electrical conductivity of the material was calculated. For the obtained dependencies, an analytical expression was developed and was compared with the experimental results for a composite with highly segregated structure.

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

[SY-H12] Symposium H-12

Fri. Nov 2, 2018 11:15 AM - 12:00 PM Room9

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

[SY-B9] Symposium B-9

Chair: Michael Tonks(University of Florida, United States of America)

Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room10

[SY-B9] Ab Initio Modeling of Self-Interstitial and Vacancy Migration in Zirconium

○Emmanuel Clouet[1], Céline Varvenne[2] （1.CEA Saclay, France, 2.CNRS - Aix-Marseille University, France）

[SY-B9] Atomistic modelling of point defect clusters in zirconium and impact on the microstructure evolution and crystal growth under irradiation

Benjamin CHRISTIAEN[3], Christophe DOMAIN[3,2], ○Ludovic THUINET[1,2], Antoine AMBARD[3,2], Alexandre LEGRIS[1,2] （1.UMET, UMR CNRS 8207, Lille university, F-59655 Villeneuve d’ Ascq, France, 2.EM2VM, EDF-CNRS, France, 3.EDF R&D, MMC, Les Renardieres, F-77810 Moret-sur-Loing, France）

[SY-B9] Modeling of dislocation climb assisted glide in crystal plasticity models

○Alankar Alankar, Vikram Phalke, Ritesh Dadhich, Ashish Mishra （IIT Bombay, India）

[SY-B9] The role of oxide grain boundaries in the oxidation of zirconium alloy fuel cladding

○Maria S Yankova[1], Felicity Baxter[1,2], Alistair Garner[1], Philipp Frankel[1], Christopher P Race[1] （1.Materials Performance Centre, School of Materials, University of Manchester, UK, 2.Corrosion and Materials Science, Wood. PLC, UK）

[SY-B9] Advances in X-ray Diffraction Line Profile Analysis of Dislocation Loops in Zr - Insights from Atomistic Modelling.

○Chris P Race, Rory Hulse, Tamas Ungar （University of Manchester, UK）

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room10)

[SY-B9] Ab Initio Modeling of Self-Interstitial and Vacancy Migration in Zirconium

○Emmanuel Clouet[1], Céline Varvenne[2] (1.CEA Saclay, France, 2.CNRS - Aix-Marseille University, France)

Irradiation in hexagonal close-packed zirconium leads to the creation of point-defects, both vacancies and self-interstitials. Migration and clustering of these point-defects control the microstructure evolution under irradiation. In particular, the faster diffusion of self-interstitial in the basal planes than along the c axis is often assumed to explain the self-organization of the microstructure observed in irradiated Zr as well as the breakaway growth visible for high irradiation dose. As no direct experimental measurement characterizing a possible diffusion anisotropy is possible, at least for the self-interstitial, ab-initio calculations appear as a suitable alternative.
We model with ab initio calculations all possible configurations of the self interstitial and calculat with NEB the different migration barriers between these configurations [1]. The attempt frequencies corresponding to the different migration events are deduced from phonon calculations thanks to the harmonic approximation and the transition state theory. We thus fully characterize the migration of both the self-interstitial and the vacancy. The obtained ab initio data is validated by modeling internal friction in irradiated zirconium and comparing the low temperature peaks with the ones observed in experiments [2]. Once this validation step performed, diffusion coefficients are calculated and diffusion anisotropy is characterized.

[1] C. Varvenne, F. Bruneval, M.-C. Marinica and E. Clouet, Phys. Rev. B 88, 134102 (2013).
[2] R. Pichon, E. Bisogni and P. Moser, Radiation Effects 20, p. 159 (1973).

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room10)

[SY-B9] Atomistic modelling of point defect clusters in zirconium and impact on the microstructure evolution and crystal growth under irradiation

Benjamin CHRISTIAEN[3], Christophe DOMAIN[3,2], ○Ludovic THUINET[1,2], Antoine AMBARD[3,2], Alexandre LEGRIS[1,2] (1.UMET, UMR CNRS 8207, Lille university, F-59655 Villeneuve d' Ascq, France, 2.EM2VM, EDF-CNRS, France, 3.EDF R&D, MMC, Les Renardieres, F-77810 Moret-sur-Loing, France)

Zirconium alloys are used to manufacture fuel cladding as well as fuel assemblies of pressurized water nuclear reactors. Under irradiation, they show a dimensional change commonly called growth. Experimental observations have shown that above a threshold dose, these alloys are subject to accelerated growth called "breakaway". It has been well established that the irradiation formation of and <c> dislocation loops is directly responsible for the growth of irradiated zirconium alloys and that the appearance of <c> loops is correlated with this growth acceleration. However, the nucleation mechanisms of the <c> loops are still poorly understood. In order to improve our understanding, atomic-scale calculations based on the density functional theory (DFT) and empirical potentials are used to determine the properties of clusters of point defects (vacancies as well as self-interstitials) in terms of formation energy, binding energy and eigenstrain, of prime importance to assess their influence on the deformation of the material. In particular, DFT simulations of dislocation loops in large supercells allow to revisit their energies used as input parameters of mesoscale models (Object KMC), resulting in prediction of growth and its acceleration. Moreover, pyramids of stacking

faults are studied in more detail and their characterization sheds light on their plausible role in the nucleation sequence of <c> loop, which allows to propose an original scenario for their appearance.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room10)

[SY-B9] Modeling of dislocation climb assisted glide in crystal plasticity models

○Alankar Alankar, Vikram Phalke, Ritesh Dadhich, Ashish Mishra （IIT Bombay, India）

We present crystal plasticity modeling of climb assisted glide in fcc, bcc and hcp metals. Dislocation density is divided into edge and screw characters. Dislocation density evolution takes care of non-schmid effect and the effect of screw dislocation core assymetry in hcp metals. A chemical stress component due to non-equilibrium vacancy concentration acts on edge dislcoations and is called drag-stress. This chemical stress component depends strongly on crystallographic orientation as well if the vacancy concentration is low. Evolution of chemical stress and thus dislocation climb rate is discussed as a function of dislocation density, strain, crystallographic orientation and temperature. Model is calibrated against data from literature. The model is able to predict mechanical behavior under conditions of creep. Also, depending on whether creep occurs or not, the model is able predict crystallographic texture during deformation. Such model has been used for modeling of irradiation in Zr and zircaloys.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room10)

[SY-B9] The role of oxide grain boundaries in the oxidation of zirconium alloy fuel cladding

○Maria S Yankova[1], Felicity Baxter[1,2], Alistair Garner[1], Philipp Frankel[1], Christopher P Race[1] （1.Materials Performance Centre, School of Materials, University of Manchester, UK, 2.Corrosion and Materials Science, Wood. PLC, UK）

Oxidation of the Zr alloy fuel cladding in light water reactors is one of the key degradation mechanisms, limiting the amount of fuel burned. The structural and electronic properties of monoclinic and tetragonal zirconia grain boundaries strongly affect the transport of species through the oxide layer. Improving the understanding of oxygen transport through the oxide grain boundaries, and its interaction with dopant point defects, is an important factor in achieving a more mechanistic knowledge and better control of the corrosion process. We are exploiting a combination of density functional theory (DFT) simulation, scanning precession electron diffraction in the transmission electron microscope (SPED-TEM) and novel Python-based texture analysis to obtain an improved mechanistic understanding of the oxide microstructure. We have investigated the effect of oxygen defects and key alloying elements such as Sn and Nb on the structural and electronic properties of representative oxide grain boundaries using DFT. We have investigated dopant-oxygen vacancy binding which can have a significant effect on oxygen conductivty. We have characterised the grain boundary misorientation distribution in non-irradiated and irradiated oxides with estimates on the relative boundary energetics. We have further used the results of our DFT calculations to test a range of empirical potentials for the Zr-O system to establish their suitability for computational modelling of zirconia at microstructural length-scales.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room10)

[SY-B9] Advances in X-ray Diffraction Line Profile Analysis of Dislocation Loops in Zr - Insights from Atomistic Modelling.

○Chris P Race, Rory Hulse, Tamas Ungar （University of Manchester, UK）

Irradiation-induced growth (IIG) of Zr-alloy nuclear fuel cladding can limit the service life of nuclear fuel. It involves a macroscopic shape change driven by the formation and growth of populations of dislocation loops.

Efforts to create Zr-alloys that are resistant to IIG thus rely on accurate determination of the size distribution and number density of dislocation loops in irradiated candidate alloys. X-ray diffraction (XRD) can, in principle, provide this information via an analysis of changes to the diffraction peak shapes. Such methods are well developed in the study of plastic deformation, but the different character of the defects formed under irradiation complicates the analysis. An improved understanding of the effect of dislocation loops on the diffraction peak shapes is therefore required.

We have constructed atomistic models of controlled defect populations in Zr and generated theoretical XRD profiles. We have compared these with experimental profiles and analysed changes in lineshape in terms of contributions from the strain fields of individual defects. In particular, we are able to explain the appearance of features in the experimental profiles that are peculiar to irradiated material. We show that these new features contain information about the character of the dislocation loops in irradiated material.

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

[SY-B10] Symposium B-10

Chair: Frederic Soisson(CEA Saclay, France)

Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room10

[SY-B10] Sink strengths of point defects near tilt grain boundaries: A phase field model

○Pengchuang Liu[1], Songlin Zheng[2], Pengcheng Zhang[1], Sanqiang Shi[3], Kaiguo Chen[2]
（1.Institute of Materials, China academy of engineering physics, China, 2.Institute of Fluid Physics, China academy of engineering physics, China, 3.Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hong Kong）

[SY-B10] Modelling swelling and growth under irradiation using the phase field method

○Daniel Schwen, Andea M. Jokisaari （Dept. of Fuels Modeling and Simulation, Idaho National Laboratory, United States of America）

[SY-B10] Phase-field modelling of dislocation loop evolution under irradiation : application to radiation induced segregation prediction near the dislocation cores

○Gabriel Franck BOUOBDA MOLADJE[1], Ludovic THUINET[1], Alexandre LEGRIS[1], Charlotte BECQUART[1], Maylise NASTAR[2], Frédéric SOISSON[2] （1.CNRS, université de Lille, France, 2.CEA, Université Paris-Saclay, France）

[SY-B10] Theoretical derivation of the ABVI model from cluster expansion Hamiltonian

○Antonio Fernandez Caballero[1,2], Jan Wrobel[3], Paul Mummery[1], Duc Nguyen-Manh[2] （1.School of Mechanical, Aerospace and Civil Engineering, University of Manchester, UK, 2.Department of Materials Science and Scientific Computing, CCFE, United Kingdom Atomic Energy Authority, Abingdon OX14 3DB, UK, UK, 3.Faculty of Materials Science and Engineering, Warsaw University of Technology, Ul. Wołoska 141, 02-507 Warsaw, Poland, Poland）

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room10)

[SY-B10] Sink strengths of point defects near tilt grain boundaries: A phase field model

○Pengchuang Liu[1], Songlin Zheng[2], Pengcheng Zhang[1], Sanqiang Shi[3], Kaiguo Chen[2] （1.Institute of Materials, China academy of engineering physics, China, 2.Institute of Fluid Physics, China academy of engineering physics, China, 3.Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hong Kong）

Dislocations and grain boundaries are perfect sinks for point defects (PDs), the ability of sinks to absorb point defects is a critical factor for the irradiation damage behaviors of materials. Phase field (PF) method was used to describe low angle tilt grain boundaries which composed of edge dislocations. Evolution processes of tilt grain boundaries and PDs were coupled in a same PF model. We considered the climbing mechanism rather than fixed dislocations. Sink strengths of grain boundaries were computed based on the obtained steady-state average PDs concentrations. We studied the saturation properties of tilt grain boundaries and obtained the relations between sink strengths and dislocation densities. PDs generation rate represents the irradiation intensity, it is also undemanding to take into account in this PF model. Elastic interactions of point defects and dislocations have great impacts on the sink properties of tilt grain boundaries. We compared the effects of different eigenstrains and applied stresses and got the connections between sink strengths and climbing speeds of dislocations. A physical phase-field model was built, which covered material processes to study sink properties of tilt grain boundaries without additional assumptions. We compared the calculated results with the theoretical and existing ones, clarified the inherent differences between them, results are favorable for designing extremely radiation tolerant materials.

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room10)

[SY-B10] Modelling swelling and growth under irradiation using the phase field method

○Daniel Schwen, Andea M. Jokisaari （Dept. of Fuels Modeling and Simulation, Idaho National Laboratory, United States of America）

In extreme environments with high point defect production rates, some materials can experience macroscopic dimensional changes due to the mechanisms of swelling and growth. Both processes are related to preferential absorption of different point defect species at different sinks. In the case of swelling this entails the creation of voids which act as vacancy sinks, while interstitials are absorbed at dislocations or grain boundaries where new lattice sites are created, leading to a total volume increase of the sample. Growth occurs if anisotropic interstitial and vacancy fluxes with differing spatial orientations lead to lattice site creation and removal along non-parallel lattice planes, leading to a volume conserving shape change. Prediction of swelling and growth behavior requires an understanding of the defect transport and reaction processes at the mesoscale. The phase field method has been established as a standard modeling technique on these length scales.

In this work we develop a modified set of phase field equations that allow for the local and anisotropic creation and destruction of lattice sites at sinks using a tensor field describing the local lattice site changes. We apply this method to study the effects of microstructure on swelling and growth behavior in polycrystalline materials, in the presence of applied mechanical loading, and microstructural features such as

precipitates.

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room10)

[SY-B10] Phase-field modelling of dislocation loop evolution under irradiation : application to radiation induced segregation prediction near the dislocation cores

○Gabriel Franck BOUOBDA MOLADJE[1], Ludovic THUINET[1], Alexandre LEGRIS[1], Charlotte BECQUART[1], Maylise NASTAR[2], Frédéric SOISSON[2] （1.CNRS, université de Lille, France, 2.CEA, Université Paris-Saclay, France）

Understanding and predicting the microstructural evolution of metallic alloys constituting the reactor vessels are crucial issues for safety in the nuclear industry. Under irradiation, point defects (PD) are created and diffuse towards microstructural defects such as dislocations. These microstructural defects will evolve according to their ability to absorb PD, also known as sink strength. Dislocation climb is one consequence of PD absorption and leads to growth or shrinkage of dislocation loops. Phase field (PF) models have already been proposed to describe dislocation climb when only vacancies are considered, which couple non-conservative dislocation motion and vacancy diffusion through an absorption term. To simulate growth/shrinkage of dislocation loops under irradiation in metallic alloys where vacancies but also self-interstitials are created, a new formulation of these models is required, and this will constitute the first part of the presented work. In particular, it will be shown that such a formulation is not a straigthforward generalization of the existing models. Thanks to this new PF model, well-known phenomena observed under irradiation, such as radiation induced segregation, will be studied near the dislocation cores. The particular influence of climb and elastic interactions between PDs and dislocations, generally ignored in RIS calculations, will be discussed in detail.

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room10)

[SY-B10] Theoretical derivation of the ABVI model from cluster expansion Hamiltonian

○Antonio Fernandez Caballero[1,2], Jan Wrobel[3], Paul Mummery[1], Duc Nguyen-Manh[2] （1.School of Mechanical, Aerospace and Civil Engineering, University of Manchester, UK, 2.Department of Materials Science and Scientific Computing, CCFE, United Kingdom Atomic Energy Authority, Abingdon OX14 3DB, UK, UK, 3.Faculty of Materials Science and Engineering, Warsaw University of Technology, Ul. Wołoska 141, 02-507 Warsaw, Poland, Poland）

In nuclear fusion research, degradation of material microstructure and nanostructure by radiation damage is of interest both from experimentally and modelling perspectives. Modelling from first principles can be used to rationalize mechanisms behind degradation phenomena caused by the simplest type of damage produced by radiation: vacancies and interstitials and their clusters. Recent studies found that density functional theory and kinetic monte carlo can be used to investigate radiation induced segregation and precipitation[1] incorporating both vacancy and interstitial into Ising-like ABVI model Hamiltonian[2]. The kinetic processes of solute transport both by vacancies and interstitials can be captured by a Hamiltonian parametrised by

bond energies and derived from DFT.

In this work, we treat multi-body defect-solute or solute-solute interactions as cluster entities from the cluster expanded Hamiltonian of the alloy system containing point defects. Binding energies for elements within defect cluster are expressed in terms of effective interactions parameters found from the cluster expansion of the Hamiltonian of the system containing vacancies and interstitials. Local effects from defect surroundings are incorporated by offseting the binding enery by the cluster expanded reference energy depending on chemical compositions of the surroundings[3,4]. This model can be used to investigate the kinetic simulations of segregation and precipitation of binary alloys under irradiation.

[1] *G. Martin, 1980, Phys. Rev. B 21, 2122*

[2] *C. Huang and J. Marian, 2016, J. Phys.: Condens. Matter 28 425201*

[3] *J.S. Wrobel, D. Nguyen-Manh, K.J. Kurzydlowski, S.L. Dudarev, 2017, Journal of Physics: Condensed Matter, 29 145403.*

[3] *A. Fernandez-Caballero, J.S. Wrobel, P.M. Mummery, D. Nguyen-Manh, 2017, J. Phase Equilibrium and Diffusion, 38 391-403.*

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K4] Symposium K-4

Chairs: Tetsuo Mohri(IMR, Tohoku University, Japan), Akihiro Nakatani(Dept. of Adaptive Machine Systems, Osaka Univ., Japan)

Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room11

[SY-K4] Disclination dipole model of kink deformation in layered solid

○Akihiro Nakatani[1], Xiao-Wen Lei[2] （1.Dept. of Adaptive Machine Systems, Osaka Univ., Japan, 2.Dept. of Mechanical Engineering, Univ. of Fukui, Japan）

[SY-K4] Large-scale coarse-grained molecular dynamics simulations on fracture processes of lamellar structure in crystalline polymers

○Yuji Higuchi （The University of Tokyo , Japan）

[SY-K4] Grain boundary sliding within the entropy production rate theory

○Tetsuo Mohri （IMR, Tohoku University, Japan）

[SY-K4] Molecular Dynamics Simulation on Intergranular Cracking Mechanism of Iron Material in High Temperature Pressurized Water Environment

○Qian Chen, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Materials Research, Tohoku University, Japan）

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room11)

[SY-K4] Disclination dipole model of kink deformation in layered solid

Invited

○Akihiro Nakatani[1], Xiao-Wen Lei[2] （1.Dept. of Adaptive Machine Systems, Osaka Univ., Japan, 2.Dept. of Mechanical Engineering, Univ. of Fukui, Japan）

Kink deformation is commonly observed in layered solid for a wide variety of scales from atomistic layers to geological structures, and their structural similarity means possibility of universal application of deformable body mechanics. In our previous works, the deformation mechanism of kink deformation in a layered solid with a single-slip system has been studied and it is shown that the fundamental process of kink deformation is represented by disclination dipole model.
In this study, first, we review the relationship between generalized continuum theories and the disclination dipole dynamics from a multiscale point of view.
Secondly, nucleation of kink deformation under a compressive force in the direction parallel to the layers is studied using configulational force of disclination dipole based on instability theory, in which the deformation mechanism is discussed from the viewpoint of the instability theory with the Maxwell's equal area rule.
Third, we use cellular automaton as a discretized model of disclination dipole theory, in which each layer is divided into segments and the amount of Frank vector of each segment is encoded using integers. In this study, total strain energy is calculated as sum of the local bending strain energy of each layer and inter-layer energy, in which the local strain energy density is evaluated as a linear function of square of curvature and inter-layer energy is assumed to be expressed by a form of Lennard-Jones 12-6 potential. The Metropolis Monte Carlo Method is adopted to evolve the state of the material system. The result of this scheme is verified on the classical problem of buckling of Euler's column with comparing analytical solution. After that, simulation of kinking deformation is examined for various values of the inter-layer strength parameter.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room11)

[SY-K4] Large-scale coarse-grained molecular dynamics simulations on fracture processes of lamellar structure in crystalline polymers

○Yuji Higuchi （The University of Tokyo , Japan）

Understanding the fracture processes of crystalline polymers such as polyethylene by molecular theory is one of the big challenges, which contributes to the increase in the toughness of polymeric materials in industry. To reveal the fracture process, coarse-grained molecular dynamics simulation is effective; however the fracture processes of the most fundamental crystal structure, lamellar structure consisting of amorphous and crystalline layers, in polyethylene has not been revealed. The reason is the difficulty of the construction of the lamellar structure due to the small simulation size in the order of 10^4 beads. Thus, we propose a crystallization method for the large-scale lamellar structure in the order of 10^6 beads and perform the fracture simulation.

In the fracture process of the lamellar structure by coarse-grained molecular dynamics simulation, mechanical properties are consistent with the experiment, confirming the validity of the simulation results. We also reveal that the movement of chain ends from amorphous layers to crystalline layers causes the deformation and void generation in the amorphous region, indicating that the chain ends act as defect [1, 2].

In the large scale simulations, the buckling of crystalline layer and its fragmentations are observed, which can be compared directly with the experimental observation by electronic microscope. Our large-scale coarse-grained molecular dynamics simulations are useful to reveal the fracture process of polymers at molecular level. We develop the above molecular technology which can reveal the fracture processes of polymeric materials at the molecular level and successfully apply it to the fracture process of double network gels [3].

[1] Y. Higuchi et al., Macromolecules 50, 3690-3702 (2017).
[2] Y. Higuchi, Polym. J. in press (2018).
[3] Y. Higuchi et al., Macromolecules in press (2018).

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room11)

[SY-K4] Grain boundary sliding within the entropy production rate theory

○Tetsuo Mohri （IMR, Tohoku University, Japan）

It is a challenging task to clarify the underlying principle of deformation behavior of an alloy. In high temperatures, an alloy undergoes various deformation modes driven by dislocations movement, grain boundary sliding etc. Under a given strain rate (tensile test) or a given stress (creep test), how does an alloy adjust internal structures to accommodate externally imposed deformation conditions such as deformation rate and applied stress? This is the question the author addresses in the present paper. By taking a grain boundary sliding as an example, we formulated deformation behavior in terms of average rotation rate of a grain and density of rotating grains based on entropy production rate theory within the linear regime. The physical implications of grain boundary sliding at an extremum of entropy production rate are main focus of the discussion, and thermodynamic similarity between grain boundary sliding and dislocations driven deformation is addressed. Furthermore, it will be briefly touched upon how to extend the formulation of grain boundary sliding for an alloy to larger scale deformation phenomena.

(Fri. Nov 2, 2018 9:45 AM - 11:00 AM Room11)

[SY-K4] Molecular Dynamics Simulation on Intergranular Cracking Mechanism of Iron Material in High Temperature Pressurized Water Environment

○Qian Chen, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo （Institute for Materials Research, Tohoku University, Japan）

Iron-based materials are widely used in power plants, and usually serve in high temperature pressurized water environment. The severe water environment causes stress corrosion cracking (SCC), resulting in potentinally catastrophic accidents. It is therefore important to understand the chemical reaction dynamics at the iron-water interface and the SCC mechanism during failure process in order to improve corrosion resistance. However, it is difficult to achieve that by experimental observation, particularly in high temperature pressurized water. Thus, the SCC mechanism for iron-based materials in such an environment is still unclear. In this study, we employed molecular dynamics simulation to study the failure process in high temperature pressurized water environment. To investigate chemical reactions, a reactive force field was used in this study. Since intergranular cracking is more common than transgranular cracking during the

fracture processes of iron materials, a Σ5(310) grain boundary was modeled. To investigate the crack growth process under stress conditions, we applied external tension along the perpendicular direction of the pre-crack model with water arranged on the surface. The simulation results showed structural change due to plastic deformation around the pre-crack, and the structural change was found to be attributable to twinning by partial dislocations. In addition, small cracks were observed in the lateral direction of the pre-crack tip. To investigate the effect of high temperature pressurized water, we also simulated the model without water for comparison. It was revealed that crack propagation was promoted by suppressing structural relaxation due to the chemical reactions in the high temperature pressurized water condition.

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K5] Symposium K-5

Chairs: Masanori Kohyama(AIST, Japan), Masatake Yamaguchi(Japan Atomic Energy Agency, Japan)
Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room11

[SY-K5] Effects of a bulk-region size in the first-principles tensile test of a grain boundary

○Masanori Kohyama[1], Hao Wang[2], Shingo Tanaka[1] (1.AIST, Japan, 2.Shanghai Univ., China)

[SY-K5] Combined analysis of first-principles calculations and fracture mechanics experiments on intergranular embrittlement of an alloy steel

○Masatake Yamaguchi (Center for Computational Science and e-Systems, Japan Atomic Energy Agency, Japan)

[SY-K5] First-principles local energy analysis of grain boundary segregation of sp-elements on bcc Fe

○Kazuma Ito[1,2], Somesh Kr. Bhattacharya[3], Shingo Tanaka[3], Masanori Kohyama[3], Hideaki Sawada[2], Shigenobu Ogata[1] (1.Osaka University, Japan, 2.Nippon Steel &Sumitomo Metal Corporation, Japan, 3.National Institute of Advanced Industrial Science and Technology, Japan)

[SY-K5] Fast and scalable prediction of local energy at grain boundaries: Machine-learning based modeling of first-principles calculations

○Tomoyuki Tamura[1,2], Masayuki Karasuyama[1,2,3], Ryo Kobayashi[1,2], Ryuichi Arakawa[1], Yoshinori Shiihara[4], Ichiro Takeuchi[1,2,5] (1.Nagoya Institute of Technology, Japan, 2.Center for Materials Research by Information Integration (CMI2), Research and Services Division of Materials Data and Integrated System (MaDIS), National Institute for Materials Science (NIMS), Japan, 3.PRESTO, JST, Japan, 4.Toyota Technological Institute, Japan, 5.RIKEN Center for Advanced Intelligence Project, Japan)

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room11)

[SY-K5] Effects of a bulk-region size in the first-principles tensile test of a grain boundary

○Masanori Kohyama[1], Hao Wang[2], Shingo Tanaka[1] (1.AIST, Japan, 2.Shanghai Univ., China)

The first-principles tensile test (FPTT) of a grain boundary (GB) is a powerful tool to clarify intrinsic tensile strength and failure process of a GB, according to natural behaviors of electrons and atoms, corresponding to a slow tensile test at zero temperature [1]. This is quite effective to clarify the effects of segregated impurities [2]. This can provide intrinsic energy-strain and stress-strain curves of a GB, which should be useful to construct separation-energy curves for "cohesive zone model" in a continuum model as a multi-scale simulation technique. However, there are several unsolved issues in interpreting FPTT results compared to real mechanical properties of GBs. In the present study, we investigate the effects of the bulk-region size in the GB supercell, where usually two symmetric interfaces of a coincidence-site lattice (CSL) GB are alternately stacked between bulk slabs with some thickness. We show that the bulk-region thickness seriously affect the features of energy-strain and stress-strain curves around the failure point by comparing the FPTTs of the same Al GB with different bulk-region thicknesses, which are also analyzed by local-energy and local-stress techniques [3]. The difference is dominated by the relation between the Griffith and stress conditions for failure, depending on the bulk-region thickness. From this viewpoint, we re-interpret our previous FPTT results of Al GBs with various segregated impurities [2].

[1] M. Kohyama, Phil. Mag. Lett. 79, 659 (1999); Phys. Rev. B, 65, 184107 (2002)

[2] G. H. Lu et al., Phys. Rev. B, 73, 224115 (2006)

[3] H. Wang et al., Modell. Simul. Mater. Sci. Eng. 25, 015005 (2017)

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room11)

[SY-K5] Combined analysis of first-principles calculations and fracture mechanics experiments on intergranular embrittlement of an alloy steel

○Masatake Yamaguchi (Center for Computational Science and e-Systems, Japan Atomic Energy Agency, Japan)

A significant loss of fracture toughness (K_{Ic}) is induced by intergranular (grain boundary; GB) segregation of metalloid solute (Sb, Sn, and P) in a Ni-Cr steel. However, the atomistic mechanism has not been clarified from a multiscale point of view. From first-principles calculations, it is shown that segregated solute with higher energetic stability on fracture surfaces causes a larger linear reduction in the ideal work to intergranular fracture ($2\gamma_{int}$); i.e. the energy difference between a GB and its two fracture surfaces. The combined analysis with first-principles calculations and fracture mechanics experiments found several orders of magnitude more energy loss in K_{Ic} for a specific range in the $2\gamma_{int}$ within only a few tenths of J/m^2. These results illustrate that the GB of steel has the threshold energy of atomic cohesion under which catastrophic failure occurs [1]. [1] M. Yamaguchi and J. Kameda: Phil. Mag. 94, 2131-2149 (2014).

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room11)

[SY-K5] First-principles local energy analysis of grain boundary segregation of sp-elements on bcc Fe

○Kazuma Ito[1,2], Somesh Kr. Bhattacharya[3], Shingo Tanaka[3], Masanori Kohyama[3], Hideaki Sawada[2], Shigenobu Ogata[1] （1.Osaka University, Japan, 2.Nippon Steel &Sumitomo Metal Corporation, Japan, 3.National Institute of Advanced Industrial Science and Technology, Japan）

In polycrystalline materials, grain boundary segregation of impurity elements and alloying elements may have a great influence on the material properties. Particularly in steel materials, it is known that the sp-elements such as P and S segregate at the grain boundary, thereby remarkably lowering hot ductility and low temperature toughness. However, the microscopic mechanism of grain boundary segregation of these elements has not been fully clarified.

In this study, grain boundary segregation energies for sp-elements (Al,Si,P and S) in bcc Fe are calculated by first-principles calculations. Furthermore, to investigate the microscopic mechanism, the contribution of each physical origin to the grain boundary segregation energies is evaluated numerically by using first-principles local energy analysis. We will also discuss the relationship between the contribution of each physical origin and the geometric structure or the electronic state of the grain boundary.

(Fri. Nov 2, 2018 11:15 AM - 12:15 PM Room11)

[SY-K5] Fast and scalable prediction of local energy at grain boundaries: Machine-learning based modeling of first-principles calculations

○Tomoyuki Tamura[1,2], Masayuki Karasuyama[1,2,3], Ryo Kobayashi[1,2], Ryuichi Arakawa[1], Yoshinori Shiihara[4], Ichiro Takeuchi[1,2,5] （1.Nagoya Institute of Technology, Japan, 2.Center for Materials Research by Information Integration (CMI2), Research and Services Division of Materials Data and Integrated System (MaDIS), National Institute for Materials Science (NIMS), Japan, 3.PRESTO, JST, Japan, 4.Toyota Technological Institute, Japan, 5.RIKEN Center for Advanced Intelligence Project, Japan）

A GB is the interface between two grains or crystallites in a polycrystalline material, and the atomic configurations and chemical bonds near GB are distinct from those of the bulk crystal. Thus, the properties of materials with GBs can greatly differ from those of a single crystal. Since it is possible to improve various properties of materials significantly by GB engineering, it is of great importance to investigate physical and chemical properties of each atoms or local regions near GBs. By virtue of the development of efficient computational techniques of large-scale density functional theory (DFT) calculations and the rapid progress of parallel computers including supercomputers, we can deal with relatively large supercells for GB models. But, it needs much computational costs to perform DFT calculations with larger supercells, and it is impossible to cover all GB models.
We proposed a new scheme based on machine learning for the efficient screening in GB engineering. A set of results obtained from DFT calculations for a small number of GB systems is used as a training data set. In our scheme, by partitioning the total energy into atomic energies using a local-energy analysis scheme, we can increase the training data set significantly. We use atomic radial distribution functions and additional

structural features as atom descriptors to predict atomic energies and GB energies simultaneously using the least absolute shrinkage and selection operator (LASSO). In the test study with fcc-Al [110] symmetric tilt GBs, we could achieve enough predictive accuracy to understand energy changes at and near GBs at a glance, even if we collected training data from only ten GB systems. The present scheme can emulate time-consuming DFT calculations for large GB systems with negligible computational costs, and thus enable the fast screening of possible alternative GB systems.