

Wed. Oct 31, 2018

Room1

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

[SY-C5] Symposium C-5

Chair: Christopher Woodward (Air Force Research Laboratory, United States of America)

9:45 AM - 11:00 AM Room1

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

○Giacomo Po¹, Suneel Kodambaka², Jeffrey M Wheeler³, Davide Sangiovanni⁴ (1.University of California Los Angeles, Mechanical Engineering Department, United States of America, 2.University of California Los Angeles, Materials Science and Engineering Department, United States of America, 3.Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Mechanics of Materials and Nanostructures, Swaziland, 4.Department of Physics, Chemistry and Biology, Linköping University, Sweden)

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

○Julien Guenole¹, Fatim-Zahra Mouhib¹, Christoffer Zehnder¹, James Gibson¹, Blazej Grabowski², Sandra Korte-Kerzel¹ (1.Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Germany, 2.Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany)

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

○Jonathan Amodeo¹, Emile Maras² (1.MATEIS, Univ. Lyon 1, France, 2.SRMP, DEN, CEA, Gif-sur-Yvette, France)

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

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

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

[SY-C6] Symposium C-6

Chair: Jaime Marian (Dept. of Materials Science and Engineering, University of California Los Angeles, United States of America)

11:15 AM - 12:30 PM Room1

[SY-C6] Effect of interstitial solutes on the structure and

mobility of screw dislocations in bcc metals

Berengere Lüthi¹, Lisa Ventelon¹, David Rodney², Emmanuel Clouet¹, Bernard Legrand¹, Fabienne Berthier³, ○Francois Willaime⁴ (1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, France, 2.Institut Lumière Matière, CNRS-Université Claude Bernard Lyon 1, France, 3.Synthèse, Propriétés et Modélisation des Matériaux /Institut de Chimie Moléculaire et des Matériaux d'Orsay, Université Paris-Saclay, France, 4.DEN-Département des Matériaux pour le Nucléaire, CEA, Université Paris-Saclay, France)

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

○Tomohito Tsuru^{1,2}, Mitsuhiro Itakura¹, Masatake Yamaguchi^{1,2}, Tomoaki Suzudo¹, Masato Wakeda³, Shigenobu Ogata^{2,4}, Daryl C Chrzan⁵ (1.Japan Atomic Energy Agency, Japan, 2.ESISM, Kyoto University, Japan, 3.National Institute for Materials Science, Japan, 4.Osaka University, Japan, 5.University of California, Berkeley, United States of America)

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

○Simen Nut Hansen Eliassen¹, Normand Mousseau³, Mickaël Trochet³, Yanjun Li¹, Jesper Friis², Inga Gudem Ringdalen² (1.Dept. of Materials Science and Engineering, Norwegian Univ. of Science and Technology, Norway, 2.SINTEF Materials and Chemistry, Norway, 3.Dept. of Physics, Univ. de Montréal, Canada)

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

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

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

[SY-C7] Symposium C-7

Chair: David Rodney (Institut Lumière Matière, Université Lyon 1, France)

2:00 PM - 3:30 PM Room1

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

○Vasily V Bulatov¹, Alexander Stukowski², Luis A Zepeda-Ruiz¹, Tomas Oppelstrup¹ (1.Lawrence

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

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

○Javier Varillas^{1,2}, Jan Očenášek², Jorge Alcalá¹ (1.New Technologies Research Centre, University of West Bohemia in Pilsen, Czech Republic, 2.Department of Materials Science and Metallurgical Engineering, InSup, ETSEIB. Universitat Politècnica de Catalunya, Spain)

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

○Tomoaki Suzudo¹, Takashi Onitsuka², Ken-ichi Fukumoto² (1.Japan Atomic Energy Agency, Japan, 2.Fukui Univ., Japan)

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

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

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

○Ali Rida¹, Matthieu Micoulaut², Emmanuelle Rouhaud¹, Ali Makke^{1,3} (1.University of Technology of Troyes, France, 2.Sorbonne Université, France, 3.EPF, Engineering school, France)

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

[SY-C8] Symposium C-8

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

4:00 PM - 5:30 PM Room1

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

○Pierre-Antoine Geslin^{1,2,3}, David Rodney⁴ (1.Mateis lab, INSA Lyon/CNRS, France, 2.Institute for Materials Research, Tohoku University, Japan, 3.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan, 4.Institut Lumière Matière, Université Lyon 1, France)

[SY-C8] Tension of fluctuating dislocation lines

○Max Boleininger¹, Thomas D Swinburne², Laurent Dupuy³, Sergei L Dudarev¹ (1.Culham Centre for Fusion Energy, UK, 2.Theoretical Division T-1, Los

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

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

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

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

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

[SY-C8] Molecular dynamics simulations of dislocation dynamics

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

Room2

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E5] Symposium E-5

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

9:45 AM - 11:00 AM Room2

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

Vahid Tari¹, Ricardo A Lebensohn², Reeru Pokharel², Rachel E Lim¹, Darren C Pagan³, Yufeng Shen¹, Joel V Bernier⁴, Robert M Suter¹, ○Anthony D Rollett¹ (1.Carnegie Mellon University, United States of America, 2.Los Alamos National Laboratory, United States of America, 3.Cornell High Energy Synchrotron Source, United States of America, 4.Lawrence Livermore National Laboratory, United States of America)

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

○Jiaming Zhu¹, Yipeng Gao², Dong Wang³, Tong-Yi Zhang⁴, Yunzhi Wang² (1.City University of Hong Kong, Hong Kong, 2.Ohio State University, United States of America, 3.Xi'an Jiaotong University, China, 4.Shanghai University, China)

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

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

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

○Evgeniya Kabliman¹, Johannes Kronsteiner¹, Ernst
Kozeschnik² (1.Light Metals Technologies Ranshofen,
Center for Low-Emission Transport, Austrian Institute of
Technology, Austria, 2.Institute of Materials Science and
Technology, TU Wien, Austria)

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E6] Symposium E-6

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

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

○Ying-Jun Gao (Guangxi University, China)

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

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

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

○Michael Budnitzki (TU Bergakademie Freiberg,
Germany)

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

○Masaki Tanaka¹, Yelm Okuyama¹, Tatsuya Morikawa¹,
Toshiyuki Manabe² (1.Kyushu Univ., Japan, 2.Nippon
Steel &Sumitomo Corporation, Japan)

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

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

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E7] Symposium E-7

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

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

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

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

○Tetsuya Ohashi (Kitami institute of technology,
Japan)

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

○Daisuke Matsunaka¹, Yoji Shibutani² (1.Dept. of
Mechanical Systems Engineering, Shinshu Univ., Japan,
2.Dept. of Mechanical Engineering, Osaka Univ., Japan)

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

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

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

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

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E8] Symposium E-8

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

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

○Jun-Ping Du^{1,2}, W.T. Geng³, Kazuto Arakawa⁴,
Shigenobu Ogata^{2,1} (1.Elements Strategy Initiative for
Structural Materials, Kyoto University, Japan,
2.Department of Mechanical Science and
Bioengineering, Osaka University, Japan, 3.University of
Science and Technology Beijing, China, 4.Department of
Materials Science, Faculty of Science and Engineering,
Shimane University, Japan)

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

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

Lu (Department of Physics, Beihang University, China)

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

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

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

○Qinye Li¹, Lizhong He¹, Chenghua Sun^{2,3}, Xiwang Zhang¹ (1.Monash University, Australia, 2.Swinburne University of Technology, Australia, 3.Dongguan University of Technology, China)

[SY-E8] **First-principles Investigation on the Stability and Oxygen Adsorption Behavior of a $\text{Ti}_2\text{AlNb/TiAl}$ Interface**

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

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

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

Room3

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

[SY-F5] **Symposium F-5**

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

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

○Tomohiro Takaki¹, Shinji Sakane¹, Munekazu Ohno², Yasushi Shibuta³, Takayuki Aoki⁴ (1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.The University of Tokyo, Japan, 4.Tokyo Institute of Technology, Japan)

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

○Michael Kellner^{1,2}, Johannes Hötzer^{1,2}, Markus Linnenberg¹, Marco Seiz¹, Britta Nestler^{1,2} (1.Institute of Applied Materials - Computational Materials Science (IAM-CMS), Karlsruhe Institute of Technology, Germany, 2.Institute of Digital Materials Science (IDM), Karlsruhe University of Applied Science, Germany)

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

field model using thermodynamics data estimated by machine learning

○Sukeharu Nomoto¹, Hiroshi Wakameda¹, Masahito Segawa¹, Toshiyuki Koyama², Akinori Yamanaka³
(1.ITOCHU techno-Solutions Cooperation, Japan, 2.Materials Design Innovation Engineering, Nagoya Univ., Japan, 3.Department of Mechanical Systems Engineering, Tokyo University of Agriculture and Technology, Japan)

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

○Juba Hama¹, Benoît Appolaire², Yann Le Bouar¹, Alphonse Finel¹ (1.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay F-92322 Châtillon, France, 2.IJL, UMR 7198 CNRS-Université de Lorraine, 54000 Nancy, France)

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

[SY-F6] **Symposium F-6**

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

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

○Ingo Steinbach (Ruhr-University Bochum, Germany)

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

○Marius Gintalas¹, Miguel A. Santajuana², Carlos Garcia-Mateo², David San-Martin², Jose A. Jiménez², Wim Van Haver³, Pedro E. J. Rivera-Díaz-del-Castillo⁴ (1.The University of Cambridge, Department of Materials Science &Metallurgy, 27 Charles Babbage Road, Cambridge CB3 0FS, UK, 2.Materialia research group, Department of Physical Metallurgy, Spanish National Centre for Metallurgical Research (CENIM-CSIC), Avda. Gregorio del Amo 8, Madrid E-28040, Spain, 3.NV Bekaert SA, Bekaertstraat 2, Zvevegem B-8550, Belgium, 4.The University of Lancaster, Department of Engineering, Engineering Building, Lancaster University, Gillow Ave, Bailrigg, Lancaster LA1 4YW, UK)

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

○Maeva Cottura¹, Benoît Appolaire¹, Alphonse Finel², Yann Le Bouar² (1.Institut Jean Lamour, France, 2.LEM - CNRS/Onera, France)

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

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

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

[SY-F7] Symposium F-7

Chair: Tomohiro Takaki (Kyoto Institute of Technology, Japan)

2:00 PM - 3:30 PM Room3

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

○ Benoit Appolaire^{1,2}, Anna Ask³, Samuel Forest³, Kais Ammar³ (1. Institut Jean Lamour, Univ. de Lorraine, France, 2. LEM, CNRS-Onera, France, 3. Centre des Matériaux, Mines ParisTech, France)

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

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

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

○ Masahito Segawa¹, Nomoto Sukeharu¹, Akinori Yamanaka² (1. ITOCHU Techno-Solutions Corporation, Japan, 2. Division of Advanced Mechanical Systems Engineering, Institute of Engineering, Tokyo University of Agriculture and Technology, Japan)

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

○ Chamara Kumara¹, Donyong Deng², Johan Moverare², Per Nylén¹ (1. Department of Engineering Science, University West, Sweden, 2. Department of Management and Engineering, Linköping University, Sweden)

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

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

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

[SY-F8] Symposium F-8

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

4:00 PM - 5:30 PM Room3

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

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

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

○ Dongdong Zhao¹, Sylvain Gouttebroze², Jesper Friis³, Yanjun Li¹ (1. Norwegian University of Science and Technology (NTNU), 7491, Trondheim, Norway, 2. SINTEF Materials and Chemistry, 0314 Oslo, Norway, 3. SINTEF Materials and Chemistry, 7491 Trondheim, Norway)

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

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

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

○ Jae-Hyeok Shim¹, Magdalena Speicher², Mahesh Chandran³, Woo-Sang Jung¹ (1. Korea Institute of Science and Technology, Korea, 2. Materials Testing Institute, Germany, 3. Indo-Korea Science and Technology Centre, India)

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

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

Room4

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

[SY-N1] Symposium N-1

Chair: Danny Perez (Los Alamos National Laboratory, United States of America)

9:45 AM - 10:45 AM Room4

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

○ Arthur F Voter (Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, United States of America)

States of America)

[SY-N1] Atomistic processes at interfaces on extended timescales○Jutta Rogal¹ (1. Ruhr University Bochum, Germany)

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

[SY-N2] Symposium N-2

Chair: Erik Bitzek (FAU Erlangen-Nuernberg, Germany)

11:15 AM - 12:15 PM Room4

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

○Nikolas Provatas (McGill University, Canada)

[SY-N2] The Phase Field Method: Crystal Structures and Facets○Peter Voorhees¹, Eli Alster¹, Nana Ofuri-Opoku^{1,3}, David Montiel², Katsuyo Thornton², James Warren³
(1. Northwestern University, United States of America, 2. University of Michigan, United States of America, 3. National Institute for Standards and Technology, United States of America)**[SY-N2] Using free energy calculations and statistical mechanics to probe the brittle to ductile transition of bcc metals**○Thomas Swinburne¹ (1. CINaM, CNRS/Aix-Marseille Univ., France)

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

[SY-N3] Symposium N-3

Chair: Arthur F. Voter (Los Alamos National Lab, United States of America)

2:00 PM - 3:30 PM Room4

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

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

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

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

[SY-N3] Hydrogen diffusion in TiH_x: insights from PRD accelerated QMD○Ivan Novoselov^{1,2}, Alexey Yanilkin¹ (1. Dukhov

Research Institute of Automatics, Russia, 2. Moscow

Institute of Physics and Technology, Russia)

[SY-N3] Shape fluctuation of metallic nanoclusters: observations from long-timescale simulations○Rao Huang¹, Li-Ta Lo², Arthur F. Voter², Danny Perez²
(1. Xiamen University, China, 2. Los Alamos National Lab, United States of America)

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

[SY-N4] Symposium N-4

Chair: Laurent Karim Beland (Queen's University, Canada)

4:00 PM - 5:30 PM Room4

[SY-N4] Multiscale diffusion method for simulations of long-time defect evolution with application to dislocation climb○Kristopher Baker¹, William Curtin² (1. Knolls Atomic Power Laboratory, United States of America, 2. Swiss Federal Institute of Technology, Switzerland)**[SY-N4] Accelerated Quantum Molecular Dynamics**○Enrique Martinez Saez¹, Christian Negre², Romain Perriot², Danny Perez², Eduard Kober², Marc Cawkwell², Arthur F. Voter², Anders Niklasson² (1. Material Science and Technology Division, MST-8, Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America, 2. Theoretical Division, T-1, Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America)**[SY-N4] On the effect of hydrogen on vacancy diffusion**○Sebastian Echeverri Restrepo¹, Anthony T Paxton²
(1. Department of Metallic Materials & Ceramics, SKF, Netherlands, 2. Department of Physics, King's College London, UK)**Room5**

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

[SY-O5] Symposium O-5

Chairs: Hitoshi Washizu (University of Hyogo, Japan), Sophie Loehle (TOTAL Marketing & Services, Solaize, France)

9:45 AM - 11:00 AM Room5

[SY-O5] On the formation of superlubricious layers during boundary lubrication of diamond and diamond-like carbon○Michael Moseler^{1,2} (1. Fraunhofer Institute for Mechanics of Materials IWM, Germany, 2. University of

Freiburg, Germany)

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

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

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

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

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

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

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

[SY-O6] Symposium O-6

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

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

○Lucia Nicola^{1,2} (1.Delft University of Technology, Netherlands, 2.University of Padova, Italy)

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

○Kerstin Falk¹, Konstantinos Gkagkas², Gianpietro Moras¹, Michael Moseler^{1,3} (1.Dept. of Tribology, Fraunhofer IWM, Freiburg, Germany, 2.Toyota Motor Europe, Technical Center, Zaventem, Belgium, 3.Dept. of Physics, University of Freiburg, Germany)

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

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

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

Rafael Pereira de Matos¹, Sophie Loehlé², Clotilde Minfray¹, ○Manuel Cobian¹ (1.LTDS ECL, Université de Lyon, France, 2.TOTAL Marketing & Services, Solaize, France)

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

[SY-O7] Symposium O-7

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

[SY-O7] Toward Exascale Atomistic Simulations of Interfaces

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

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

○Yusuke Ootani¹, Jingxiang Xu¹, Naoki Takahashi¹, Koshi Adachi², Momoji Kubo¹ (1.Institute for Materials Research, Tohoku University, Japan, 2.Department of Mechanical Systems Engineering, Graduate School of Engineering, Tohoku University, Japan)

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

○Masahiro Saito¹, Jingxiang Xu¹, Yusuke Ootani¹, Nobuki Ozawa¹, Koshi Adachi², Momoji Kubo¹ (1.Institute for Materials Research, Tohoku Univ., Japan, 2.Graduate School of Engineering, Tohoku Univ., Japan)

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

○Gianpietro Moras¹, Andreas Klemen¹, Thomas Reichenbach¹, Adrien Gola², Hiroshi Uetsuka³, Michael Moseler^{1,4}, Lars Pastewka^{1,5} (1.Fraunhofer Institute for Mechanics of Materials IWM, Germany, 2.Institute for Applied Materials, Karlsruhe Institute of Technology, Germany, 3.Asahi Diamond Industrial Co. Ltd., Japan, 4.Institute of Physics, University of Freiburg, Japan, 5.Department of Microsystems Engineering, University of Freiburg, Germany)

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

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

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

[SY-O8] Symposium O-8

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

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

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

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

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

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

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

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

○Eiji Tomiyama^{1,2}, Takeshi Iwasaki³, Hitoshi Washizu²
(1. Research Organization for Information Science and Technology, Japan, 2. Graduate School of Simulation Studies, Univ. of Hyogo, Japan, 3. Lubricants Research Laboratory, Idemitsu Kosan Co., Ltd., Japan)

Room6

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A5] Symposium A-5

Chair: Sinisa Dj Mesarovic (Washington State University, United States of America)

9:45 AM - 11:00 AM Room6

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

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

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

○Dominik Steinberger¹, Shyamal Roy¹, Dan Mordehai², Stefan Sandfeld¹ (1. Chair of Micromechanical Materials Modelling, TU Bergakademie Freiberg, Germany, 2. Department of Mechanical Engineering, Technion - Israel Institute of Technology, Israel)

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

kinematics.

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

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A6] Symposium A-6

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

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

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

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

○Emma Griffiths¹, Jana Wilmers², Swantje Bargmann², BD Reddy¹ (1. University of Cape Town, South Africa, 2. University of Wuppertal, Germany)

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

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

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

○Roland PELLENQ¹, Pierre-Louis Valdenaire¹, Christophe Bichara³, Franz Ulm¹, Jean-Marc Leyssale²
(1. <MSE>2, MIT- CNRS - AMU, United States of America, 2. ISM, CNRS - Bordeaux U., France, 3. CINaM, CNRS - Aix-Marseille U., France)

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A7] Symposium A-7

Chair: Michael Zaiser (FAU University of Erlangen-Nuremberg, Germany)

2:00 PM - 3:30 PM Room6

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

○Thomas Hochrainer (TU Graz, Austria)

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

○Katrin Schulz¹, Markus Sudmanns¹, Kolja Zoller¹, Peter Gumbsch^{1,2} (1. Karlsruhe Institute of Technology, Germany, 2. Fraunhofer Institute for Mechanics of Materials, Germany)

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

○Michael Zaiser, Ronghai Wu (FAU University of

Erlangen-Nuremberg, Germany)

[SY-A7] 2D continuum theory of dislocations

○Istvan Groma (Eotvos Lorand University, Hungary)

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

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

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A8] Symposium A-8

Chair: Thomas Hochrainer(TU Graz, Austria)

4:00 PM - 5:30 PM Room6

[SY-A8] Pattern formation in doubly curved thin shells○Eleni Katifori¹, Desislava Todorova¹, Octavio Albarran², Lucas Goehring² (1.University of Pennsylvania, United States of America, 2.Max Planck Institute, Germany)**[SY-A8] Phase-field model for microstructure change in L1₀ type ordering with lattice distortion**○Ryuichiro Oguma¹, Long-Qing Chen², Syo Matsumura³ (1.Fukuoka Univ., Japan, 2.The Pennsylvania State Univ., United States of America, 3.Kyushu Univ., Japan)**[SY-A8] Coupling multi-component phase field models for oxide systems to thermodynamic databases - breaking the curse of dimensionality**○Inge Bellemans¹, Nico Vervliet², Lieven De Lathauwer^{2,3}, Nele Moelans⁴, Kim Verbeken¹ (1.Department of Materials, Textiles and Chemical Engineering, Ghent University, Belgium, 2.Department of Electrical Engineering, KU Leuven, Belgium, 3.Group Science, Engineering and Technology, KU Leuven - Kulak, Belgium, 4.Department of Materials Engineering, KU Leuven, Belgium)**[SY-A8] A Sharp Phase Field Method**○Alphonse FINEL¹, Yasunori YAMADA², Yann LE BOUAR¹, Benoît DABAS¹, Benoît APPOLAIRE¹, Tetsuo MOHRI² (1.Laboratoire d'Etude des Microstructures, CNRS, ONERA, France, 2.Institute for Materials Research, Tohoku University, Japan)**Room7**

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

[SY-I5] Symposium I-5

Chairs: Stephen M Foiles(Sandia National Laboratories, United States of America), Mitra L Taheri(Drexel University, United States of America)

9:45 AM - 11:00 AM Room7

[SY-I5] Heterogeneous disconnections nucleation**mechanisms during grain boundary migration**○Nicolas Combe^{1,2}, Frederic Mompou¹, Marc Legros¹ (1.CEMES Toulouse, France, 2.Univ. Toulouse, UPS, France)**[SY-I5] Motion of Grain Boundaries Based on Disconnections**○Chaozhen Wei^{1,2}, Luchan Zhang⁵, Yang Xiang², Jian Han⁴, Spencer Thomas⁴, kongtao Chen⁴, David J. Srolovitz^{3,1} (1.HKUST Jockey Club Institute for Advanced Study, Hong Kong University of Science and Technology, Hong Kong, 2.Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong, 3.Materials Science and Engineering, Mechanical Engineering and Applied Mechanics, Computer and Information Science, University of Pennsylvania, United States of America, 4.Materials Science and Engineering, University of Pennsylvania, United States of America, 5.Department of Mathematics, National University of Singapore, Singapore)**[SY-I5] Dislocation-mediated boundary motion, dislocation-boundary interaction, and their effect on the mechanical behavior in fcc materials**○Bob Svendsen^{1,2}, Jaber Rezaei Mianroodi², Juan Li³, Christoph Kirchlechner³, Gerhard Dehm³ (1.Material Mechanics, RWTH Aachen University, Germany, 2.Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Germany, 3.Structure and Nano-/Micromechanics of Materials, Max-Planck-Institut für Eisenforschung GmbH, Germany)

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

[SY-I6] Symposium I-6

Chairs: Garritt Tucker(Colorado School of Mines, United States of America), Chuang Deng(University of Manitoba, Canada)

11:15 AM - 12:30 PM Room7

[SY-I6] Migration mechanisms of faceted vicinal grain boundaries○Sherri Hadian¹, Blazej Grabowski¹, Mike W Finnis², Jörg Neugebauer¹ (1.Max-Planck-Institut fuer Eisenforschung, Germany, 2.Imperial College London, UK)**[SY-I6] Multiscale model for the structure and energy of low-angle general grain boundaries in Al, Cu and Ni**○Shuyang Dai¹, Yang Xiang², David Joseph Srolovitz³

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

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

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

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

[SY-I7] Symposium I-7

Chairs: Nicolas Combe(CEMES Toulouse, France), Brandon Runnels(University of Colorado Colorado Springs, United States of America)

2:00 PM - 3:30 PM Room7

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

○Chris P Race (University of Manchester, UK)

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

○Ali Al-Hadi I. Kobaissy¹, Georges Ayoub², Mu'Tasem Shehadeh¹ (1.Department of Mechanical Engineering, American University of Beirut, Lebanon, 2.Department of Industrial and Manufacturing Systems Engineering, University of Michigan-Dearborn, United States of America)

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

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

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

○Saryu Fensin¹, Timothy Frolov² (1.Los Alamos National Lab, United States of America, 2.Lawrence Livermore National Laboratory, United States of America)

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

[SY-I8] Symposium I-8

Chair: Srikanth Patala(North Carolina State University, United States of America)

4:00 PM - 5:00 PM Room7

[SY-I8] New Approaches for Understanding

Nanocrystalline Mechanics: Physical Microstructures, Grain Boundary Descriptors and Deformation Mechanisms

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

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

○Alexandre Dimanov¹, Jean Raphanel¹, Michel Bornert², Eva Héripré³, Mathieu Bourcier¹, Ababacar Gaye², Alexandre El Sabbagh¹, Wolfgang Ludwig⁴, Andrew King⁵ (1.LMS, CNRS-UMR7649, Ecole Polytechnique, France, 2.Laboratoire Navier, CNRS-UMR8205, Ecole des Ponts, France, 3.MSSMAT, CNRS-UMR8579, Centrale-Supélec, France, 4.MATEIS, UMR5510, INSA-Lyon, France, 5.SOLEIL Synchrotron, Beam line Psiché, France)

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

○Nikhil Chandra Admal¹, Javier Segurado^{2,1}, Jaime Marian¹ (1.University of California Los Angeles, United States of America, 2.IMDEA, Spain)

Room8

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

[SY-G1] Symposium G-1

Chairs: Byeongchan Lee(KyungHee Univ., Korea), Keonwook Kang(Yonsei University, Korea)

9:45 AM - 11:00 AM Room8

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

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

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

○Hyunggyu Lee¹, Byeongchan Lee², Keonwook Kang¹ (1.yonsei university, Korea, 2.kyung hee university, Korea)

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

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

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

○Jean-Michel Scherer^{1,2}, Samuel Forest², Jacques Besson², Benoit Tanguy¹, Jérémy Hure¹ (1.DEN-Service d'Etudes des Matériaux Irradiés, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette cedex, France, France, 2.MINES ParisTech, PSL-Research University, Centre des

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

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

[SY-G2] Symposium G-2

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

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

○Han Henri ZHAO¹, Bing Hou² (1.Ecole Normale Paris-Saclay, France, 2.School of aeronautics, NWPU, , China)

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

○Janghyuk Moon¹, Kyeongjae Cho², Maenghyo Cho³ (1.School of Energy System Engineering, Chung-Ang Univ., Korea, 2.Department of Materials Science and Engineering, University of Texas at Dallas, United States of America, 3.School of Mechanical &Aerospace Engineering, Seoul National University, Korea)

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

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

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

○Hussein M Zbib¹, Mehdi Hamid¹, Rahul Panat², Sadeq Saleh² (1.Washington State university, United States of America, 2.Carnegie Mellon University, United States of America)

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

○Mihkel Veske¹, Andreas Kyritsakis¹, Kyrre Ness Sjobak², Vahur Zadin³, Flyura Djurabekova¹ (1.Helsinki Institute of Physics, University of Helsinki, Finland, 2.Department of Physics, University of Oslo, Norway, 3.Institute of Technology, University of Tartu, Estonia)

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

[SY-G3] Symposium G-3

Chairs: Seunghwa Ryu(Korea Advanced Institute of Science and

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

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

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

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

Jae-Wan Lee¹, Jimin Choi¹, Keonwook Kang¹, Soonho Song¹, ○Won-Suk Ohm¹, Jung Su Park² (1.Yonsei University, Korea, 2.Agency for Defense Development, Korea)

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

○Jimin Choi¹, Sanghyuk Yoo¹, Soonho Song¹, Jung Su Park², Keonwook Kang¹ (1.Yonsei Univ., Korea, 2.Agency for Defense Development, Korea)

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

○Roman Kositski¹, Dominik Steinberger², Stefan Sandfeld², Dan Mordehai¹ (1.Department of Mechanical Engineering, Technion - Israel Institute of Technology, 32000 Haifa, Israel, 2.Chair of Micromechanical Materials Modelling (MiMM), Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, 09599 Freiberg, Germany)

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

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

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

[SY-G4] Symposium G-4

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

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

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

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

○Junyoung Park¹, Jaehee Lyu¹, Shibutani Yoji² (1.Dept. of Mechanical Design Engineering, Kumoh National Institute of Technology, Korea, 2.Dept. of Mechanical Engineering, Osaka University, Japan)

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

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

Room9

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

[SY-H3] Symposium H-3

Chair: Hansohl Cho (Los Alamos National Laboratory, United States of America)

9:45 AM - 11:00 AM Room9

[SY-H3] Polydomain liquid crystal elastomers1

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

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

○William Goncalves¹, Takuya Mabuchi², Takashi Tokumasu¹ (1.Institute of Fluid Science, Tohoku University, Sendai, Miyagi 980-8577, Japan, 2.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Sendai, Miyagi 980-8577, Japan)

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

○Emanuele Locatelli¹, Daniele Parisi^{2,3}, Maria Merola², Domenico Truzzolillo⁴, Mario Gauthier⁵, Christos N. Likos¹, Dimitris Vlassopoulos^{2,3} (1.Faculty of Physics, University of Vienna, Austria, 2.Institute of Electronic Structure and Laser, FORTH, Greece, 3.Department of Materials Science and Technology, University of Crete, Greece, 4.Laboratoire Charles Coulomb, UMR 5221 CNRS - Université de Montpellier, France, 5.Faculty of Science, University of Waterloo, Canada)

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

[SY-H4] Symposium H-4

Chair: Meredith Silberstein (Cornell University, United States of America)

11:15 AM - 12:30 PM Room9

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

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

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

○Chrystelle A. Bernard¹, Tiana Deplancke⁴, Olivier Lame⁴, Kazuhiro Ogawa³, Jean-Yves Cavallé² (1.Frontier Research Institute for Interdisciplinary Sciences (FRIS), Tohoku Univ., Japan, 2.Engineering Science Lyon Tohoku joint lab for Materials under Extreme Conditions (ELYTMaX) UMI3757, Tohoku Univ., Japan, 3.Fracture and Reliability Research Institute (FRI), Tohoku Univ., Japan, 4.Materials Engineering and Science (MATEIS), CNRS, INSA-Lyon, UMR5510 Univ. de Lyon, France)

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

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

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

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

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

[SY-H5] Symposium H-5

Chair: Alexey Lyulin (Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands)

2:00 PM - 3:30 PM Room9

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

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

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

○Ryota Osawa¹, Yoshiteru Aoyagi² (1.Dept. of Mechanical Engineering, Tohoku Univ., Japan, 2.Tohoku Univ., Japan)

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

○Sumit Basu (Indian Institute of Technology Kanpur,

India)

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

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

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

[SY-H6] Symposium H-6

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

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

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

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

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

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

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

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

○Yaguang Sun¹, Hua Yang², Yafang Guo¹ (1.Dept. of
Mechanics, Beijing Jiaotong Univ., China, 2.State Key
Lab. for Geomechanics and Deep Underground
Engineering, China Univ. of Mining and Tech., China)

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

Arjan E. Boerema¹, Patrick R. Onck¹, Erik Van der
Giessen¹, Stefanos Papanikolaou² (1.Univ. of
Groningen, Netherlands, 2.West Virginia Univ., United
States of America)

Room10

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

[SY-B1] Symposium B-1

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

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

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

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

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

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

○Marcin Roland Zemla¹, Jan Stanislaw Wrobel¹, Marek
Muzyk¹, Tomasz Wejrzanowski¹, Duc Nguyen-Manh²,
Sergei L. Dudarev², Luca Messina³, Par Olsson³,
Christophe Domain⁴ (1.Faculty of Materials Science
and Engineering, Warsaw University of Technology,
Woloska 141, 02-507 Warsaw, Poland, 2.CCFE, Culham
Centre for Fusion Energy, Abingdon, Oxon OX14 3DB,
UK, 3.KTH Royal Institute of Technology, Nuclear
Engineering, 106 91 Stockholm, Sweden, 4.Dép
artement Matériaux et Mécanique des Composants,
EDF-R&D, Les Renardières, F-77250 Moret sur Loing,
France)

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

○Jesper Byggmatar¹, Fredric Granberg¹, Andrea E
Sand¹, Kai Nordlund¹ (1. Department of Physics,
University of Helsinki, Finland)

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

○Fredric Granberg¹, Haixuan Xu², Kai Nordlund¹
(1.Department of Physics, University of Helsinki,
Finland, 2.Department of Materials Science and
Engineering, University of Tennessee, United States of
America)

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

[SY-B2] Symposium B-2

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

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

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

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

- [SY-B2] Influence of vibrational entropy on the concentrations of uranium vacancies in UO_2
[○]Jean-Paul Crocombette¹, Fabien Bruneval¹, Aurélien Soulié¹, Mihai-Cosmin Marinica¹, Samuel Murphy²
 (1.CEA Saclay, France, 2.Lancaster University, UK)

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

- [SY-B2] **Intragranular bubble impact on nuclear fuel thermomechanical properties**
 Fabienne Ribeiro¹, Mehdi Colbert¹, [○]Jack Arayro¹, Guy Tréglia² (1.Institut de Radioprotection et de Sécurité Nucléaire/PSN-RES/SEMIA/LPTM, France, France, 2.Centre Interdisciplinaire de Nanoscience de Marseille, CNRS, France, France)

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

- [SY-B3] **Symposium B-3**
 Chair: Kazuto Arakawa(Shimane University, Japan)
 2:00 PM - 3:15 PM Room10

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

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

- [SY-B3] **Molecular dynamics simulation study of the interaction of Re with interstitial defects in tungsten bulk**
 Yangchun Chen¹, Jingzhong Fang¹, Ning Gao², Hong-Bo Zhou³, Wangyu Hu⁴, Fei Gao^{4,5}, [○]Huiqiu Deng^{1,4}
 (1.School of Physics and Electronics, Hunan University, China, 2.Institute of Modern Physics, Chinese Academy of Sciences, China, 3.Department of Physics, Beihang University, China, 4.College of Materials Science and Engineering, Hunan University, China, 5.Department of Nuclear Engineering and Radiological Science,

University of Michigan, United States of America)

- [SY-B3] **Hydrogen super-saturated layers in plasma loaded tungsten: a global model combining Density Functional Theory data, Thermodynamic and Kinetic models**

[○]Yves Ferro, Etienne Hodille (Aix-Marseille University, France)

- [SY-B3] **Mobility of small vacancy and interstitial prismatic dislocation loops in BCC tungsten**
[○]Jan Fikar¹, Roman Gröger¹, Robin Schaublin²
 (1.Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic, Switzerland, 2.Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, Switzerland)

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

- [SY-B4] **Symposium B-4**
 Chair: Gary S Was(University of Michigan, United States of America)
 4:00 PM - 5:15 PM Room10

- [SY-B4] **Kinetics of Precipitation in Fe-Cr and Fe-Cr-C alloys under Irradiation**

[○]Frederic Soisson (CEA Saclay, France)

- [SY-B4] **The complex problem of the experimental validation of atomistic and microstructural evolution models**

[○]Lorenzo Malerba (CIEMAT, Energy, Environment and Technology Research Centre, Spain)

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

- [SY-B4] **Oxygen diffusion in bcc Fe under the influence of foreign atoms and vacancies**

[○]Xiaoshuang Wang, Matthias Posselt, Jürgen Faßbender (Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany)

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

[SY-C5] Symposium C-5

Chair: Christopher Woodward (Air Force Research Laboratory, United States of America)

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

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

○Giacomo Po¹, Suneel Kodambaka², Jeffrey M Wheeler³, Davide Sangiovanni⁴ (1.University of California Los Angeles, Mechanical Engineering Department, United States of America, 2.University of California Los Angeles, Materials Science and Engineering Department, United States of America, 3.Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Mechanics of Materials and Nanostructures, Swaziland, 4.Department of Physics, Chemistry and Biology, Linköping University, Sweden)

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

○Julien Guenole¹, Fatim-Zahra Mouhib¹, Christoffer Zehnder¹, James Gibson¹, Blazej Grabowski², Sandra Korte-Kerzel¹ (1.Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Germany, 2.Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany)

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

○Jonathan Amodio¹, Emile Maras² (1.MATEIS, Univ. Lyon 1, France, 2.SRMP, DEN, CEA, Gif-sur-Yvette, France)

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

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

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

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

Invited

[○]Giacomo Po¹, Suneel Kodambaka², Jeffrey M Wheeler³, Davide Sangiovanni⁴ (1.University of California Los Angeles, Mechanical Engineering Department, United States of America, 2.University of California Los Angeles, Materials Science and Engineering Department, United States of America, 3.Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Mechanics of Materials and Nanostructures, Swaziland, 4.Department of Physics, Chemistry and Biology, Linköping University, Sweden)

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

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

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

[○]Julien Guenole¹, Fatim-Zahra Mouhib¹, Christoffer Zehnder¹, James Gibson¹, Blazej Grabowski², Sandra Korte-Kerzel¹ (1.Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Germany, 2.Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany)

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

We propose here a numerical atomistic approach at the cross-road of experiments and *ab initio* simulations, to shed light on the responsible mechanisms for the plasticity in hexagonal Mg₂Ca (C14) Laves phases. Elastic and plastic properties of bulk Laves phase are investigated by both first principle and classical atomistic simulations. Molecular dynamics/statics simulations with a robust MEAM interatomic potential are performed to study the propagation of dislocations, by a combination of nudge-elastic-band (NEB) methods and nano-mechanical tests. In particular, the cross-slip to pyramidal slip planes, the propagation of dislocations in the basal plane by the so called synchroshear mechanism [3,4] and the influence of temperature on slip systems activation, are investigated at the atomic scale. All these results are finally correlated and discussed by considering experimental findings, especially from micro-pillar compression

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

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

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

[○]Jonathan Amodeo¹, Emile Maras² (1.MATEIS, Univ. Lyon 1, France, 2.SRMP, DEN, CEA, Gif-sur-Yvette, France)

Micro- and nano-sized structures have attracted substantial interest due to their special mechanical behavior: they generally show an increased yield strength compared with the bulk material as well as an improved ductility. Among them, nanoparticles (NPs) which are generally used for their shape-dependent functional properties also appear as perfect candidates for submicronic plasticity investigations due to their broad range of sizes and their variety of shapes. While metallic and silicon NPs have been widely investigated since almost two decades, less is known about the strength of ceramic NPs maybe due to the brittleness of their bulk counterparts.

In the light of recent but preliminary in situ TEM observations, we investigate here the mechanical behavior of $\langle 100 \rangle$ -oriented MgO nanocubes. First, incipient plasticity mechanisms are investigated using molecular dynamics simulations (MD) of virtual nanocompression tests at constant strain rate. Results show that the plastic deformation of MgO nanocubes starts with the nucleation from the surface of perfect $\frac{1}{2}\langle 110 \rangle\{110\}$ dislocations under ultra-high stresses, one order of magnitude larger than what is generally observed in fcc metals. However, as MD simulations can only be carried out at strain rates several orders of magnitude larger than experimental ones, we used the nudged-elastic-band method to calculate the activation energy for the nucleation of the dislocation as a function of stress, particle size and dislocation nucleation site. With the help of the transition state theory, the nucleation stress can then be estimated as a function of temperature and experimental strain rate. We find that due to the large stiffness of the activation energy vs. stress curve, the strain rate has a much smaller influence on the nucleation stress than what is found for metallic nanocrystals and therefore, that the nucleation stress estimated using MD is close to that corresponding to experimental strain rate.

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

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

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

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

[SY-C6] Symposium C-6

Chair: Jaime Marian (Dept. of Materials Science and Engineering, University of California Los Angeles, United States of America)

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

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

Berengere Lüthi¹, Lisa Ventelon¹, David Rodney², Emmanuel Clouet¹, Bernard Legrand¹, Fabienne Berthier³, [○]Francois Willaime⁴ (1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, France, 2.Institut Lumière Matière, CNRS-Université Claude Bernard Lyon 1, France, 3.Synthèse, Propriétés et Modélisation des Matériaux /Institut de Chimie Moléculaire et des Matériaux d'Orsay, Université Paris-Saclay, France, 4.DEN-Département des Matériaux pour le Nucléaire, CEA, Université Paris-Saclay, France)

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

[○]Tomohito Tsuru^{1,2}, Mitsuhiro Itakura¹, Masatake Yamaguchi^{1,2}, Tomoaki Suzudo¹, Masato Wakeda³, Shigenobu Ogata^{2,4}, Daryl C Chrzan⁵ (1.Japan Atomic Energy Agency, Japan, 2.ESISM, Kyoto University, Japan, 3.National Institute for Materials Science, Japan, 4.Osaka University, Japan, 5.University of California, Berkeley, United States of America)

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

[○]Simen Nut Hansen Eliassen¹, Normand Mousseau³, Mickaël Trochet³, Yanjun Li¹, Jesper Friis², Inga Gudem Ringdalen² (1.Dept. of Materials Science and Engineering, Norwegian Univ. of Science and Technology, Norway, 2.SINTEF Materials and Chemistry, Norway, 3.Dept. of Physics, Univ. de Montréal, Canada)

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

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

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

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

Invited

Berengere Lüthi¹, Lisa Ventelon¹, David Rodney², Emmanuel Clouet¹, Bernard Legrand¹, Fabienne Berthier³,
 ○Francois Willaime⁴ (1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, France, 2.Institut Lumière Matière, CNRS-Université Claude Bernard Lyon 1, France, 3.Synthèse, Propriétés et Modélisation des Matériaux /Institut de Chimie Moléculaire et des Matériaux d'Orsay, Université Paris-Saclay, France, 4.DEN-Département des Matériaux pour le Nucléaire, CEA, Université Paris-Saclay, France)

There is ample experimental evidence of the effects of solute interactions with dislocations, such as Cottrell atmospheres and dynamical strain ageing (DSA). In this work we investigated, using Density Functional Theory (DFT) electronic structure calculations, the interaction between interstitial solute atoms, in particular carbon, and screw dislocation cores in body centered cubic (bcc) metals, in particular iron.

First considering carbon in bcc Fe, our calculations evidence a strong attractive interaction of carbon with screw dislocation cores inducing an unexpected reconstruction towards a hard-core configuration, which is unstable in pure metals. The carbon atoms are at the center of regular trigonal prisms formed by the Fe atoms. Around this decorated core, the 4th nearest neighbor octahedral sites are found to be also highly attractive for carbon. The complex thermodynamic behavior of carbon segregation on these dislocation sites, as function of temperature and bulk carbon concentration, is modelled using mean field and Monte Carlo methods. The parameters of the Hamiltonian, fitted to DFT calculations, account for the C-C repulsions between neighboring sites. It is concluded that in the temperature range corresponding to the occurrence of DSA, the carbon atoms occupy every other prismatic sites, while the other sites are essentially empty. This configuration is then used to study the kink-pair mechanism suggested by in situ straining experiments. The results obtained for the kink-pair formation energy and single kink migration energies are consistent with the activation energy of the end of DSA regime.

The solute segregation on dislocation-core prismatic sites was investigated for other solutes in Fe and for C in other bcc metals. A behavior similar to Fe-C is exhibited for B, N and O in Fe and for C in group 6 metals, Mo and W, but with solute-solute interactions between prismatic sites which can be either attractive or repulsive. By way of contrast, the configuration of lowest energy in group 5 consists of the dislocation in its easy core and the carbon atom in a fifth nearest neighbor octahedral site. We show that this group dependence is consistent with the carbon local environment in the stable stoichiometric carbide structures, namely cubic NaCl-type for group 5 and hexagonal WC-type for group 6.

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

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

○Tomohito Tsuru^{1,2}, Mitsuhiro Itakura¹, Masatake Yamaguchi^{1,2}, Tomoaki Suzudo¹, Masato Wakeda³,
 Shigenobu Ogata^{2,4}, Daryl C Chrzan⁵ (1.Japan Atomic Energy Agency, Japan, 2.ESISM, Kyoto University, Japan, 3.National Institute for Materials Science, Japan, 4.Osaka University, Japan, 5.University of California, Berkeley, United States of America)

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

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

In the present study, we implemented first-principles calculations to obtain corresponding data to the fundamental properties of dislocation motion. We will discuss the effect of transmutation product on solid solution softening in BCC tungsten and the change in slip system caused by a specific solute in HCP titanium.

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

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

[○]Simen Nut Hansen Eliassen¹, Normand Mousseau³, Mickaël Trochet³, Yanjun Li¹, Jesper Friis², Inga Gudem Ringdalen² (1.Dept. of Materials Science and Engineering, Norwegian Univ. of Science and Technology, Norway, 2.SINTEF Materials and Chemistry, Norway, 3.Dept. of Physics, Univ. de Montréal, Canada)

Multicrystalline silicon (mc-Si) is widely used for solar cell applications due to the low production costs and high efficiency. However, the crystallization processes of mc-Si induces different kinds of defects in the structure which reduces the overall conversion efficiency. Regions containing a high density of defects such as dislocations are especially detrimental. The origin of dislocations is an ongoing debate. Previous studies indicates that generation of dislocations in mc-Si can occur at $\Sigma 3$ grain boundaries; however, a detailed atomistic description of the mechanisms governing the generation of dislocations is lacking. To cast light on the mechanisms behind generation of dislocations, we have deployed the kinetic Activation-Relaxation Technique (k-ART), an off-lattice Kinetic Monte Carlo code with an on-the fly cataloging of events. K-ART allows us to construct an extensive description of the energy landscape around defects and obtain the energy barriers of diffusion pathways. Furthermore, this is achievable at a time scale and in a temperature regime relevant to experimental observations. In this work, we have constructed a model structure containing an asymmetric and a symmetric $\Sigma 3$ grain boundary which are joined together to form a kink. We present here an energy pathway for generation of dislocations from the kink with the associated energy barriers, and how the energy barriers is affected when the system is subjected to a shear force.

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

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

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

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

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

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

[SY-C7] Symposium C-7

Chair: David Rodney (Institut Lumiere Matiere, Universite Lyon 1, France)

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

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

○ Vasily V Bulatov¹, Alexander Stukowski², Luis A Zepeda-Ruiz¹, Tomas Oppelstrup¹ (1. Lawrence Livermore National Laboratory, United States of America, 2. Darmstadt University, Germany)

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

○ Javier Varillas^{1,2}, Jan Očenášek², Jorge Alcalá¹ (1. New Technologies Research Centre, University of West Bohemia in Pilsen, Czech Republic, 2. Department of Materials Science and Metallurgical Engineering, InSup, ETSEIB. Universitat Politècnica de Catalunya, Spain)

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

○ Tomoaki Suzudo¹, Takashi Onitsuka², Ken-ichi Fukumoto² (1. Japan Atomic Energy Agency, Japan, 2. Fukui Univ., Japan)

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

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

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

○ Ali Rida¹, Matthieu Micoulaut², Emmanuelle Rouhaud¹, Ali Makke^{1,3} (1. University of Technology of Troyes, France, 2. Sorbonne Université, France, 3. EPF, Engineering school, France)

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

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

Invited

○Vasily V Bulatov¹, Alexander Stukowski², Luis A Zepeda-Ruiz¹, Tomas Oppelstrup¹ (1.Lawrence Livermore National Laboratory, United States of America, 2.Darmstadt University, Germany)

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

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

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

○Javier Varillas^{1,2}, Jan Očenášek², Jorge Alcalá¹ (1.New Technologies Research Centre, University of West Bohemia in Pilsen, Czech Republic, 2.Department of Materials Science and Metallurgical Engineering, InSup, ETSEIB. Universitat Politècnica de Catalunya, Spain)

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

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

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

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

○Tomoaki Suzudo¹, Takashi Onitsuka², Ken-ichi Fukumoto² (1.Japan Atomic Energy Agency, Japan, 2.Fukui Univ., Japan)

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

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

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

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

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

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

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

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

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

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

○Ali Rida¹, Matthieu Micoulaut², Emmanuelle Rouhaud¹, Ali Makke^{1,3} (1.University of Technology of Troyes, France, 2.Sorbonne Université, France, 3.EPF, Engineering school, France)

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

[SY-C8] Symposium C-8

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

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

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

○ Pierre-Antoine Geslin^{1,2,3}, David Rodney⁴ (1. Mateis lab, INSA Lyon/CNRS, France, 2. Institute for Materials Research, Tohoku University, Japan, 3. Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan, 4. Institut Lumière Matière, Université Lyon 1, France)

[SY-C8] Tension of fluctuating dislocation lines

○ Max Boleininger¹, Thomas D Swinburne², Laurent Dupuy³, Sergei L Dudarev¹ (1. Culham Centre for Fusion Energy, UK, 2. Theoretical Division T-1, Los Alamos National Laboratory, United States of America, 3. DEN-Service de Recherches Métallurgiques Appliquées, CEA, France)

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

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

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

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

[SY-C8] Molecular dynamics simulations of dislocation dynamics

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

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

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

Invited

○Pierre-Antoine Geslin^{1,2,3}, David Rodney⁴ (1.Mateis lab, INSA Lyon/CNRS, France, 2.Institute for Materials Research, Tohoku University, Japan, 3.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan, 4.Institut Lumière Matière, Université Lyon 1, France)

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

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

[SY-C8] Tension of fluctuating dislocation lines

○Max Boleininger¹, Thomas D Swinburne², Laurent Dupuy³, Sergei L Dudarev¹ (1.Culham Centre for Fusion Energy, UK, 2.Theoretical Division T-1, Los Alamos National Laboratory, United States of America, 3.DEN-Service de Recherches Métallurgiques Appliquées, CEA, France)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

[SY-C8] Molecular dynamics simulations of dislocation dynamics

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

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

[SY-E5] Symposium E-5

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

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

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

Vahid Tari¹, Ricardo A Lebensohn², Reemu Pokharel², Rachel E Lim¹, Darren C Pagan³, Yufeng Shen¹, Joel V Bernier⁴, Robert M Suter¹, [○]Anthony D Rollett¹ (1.Carnegie Mellon University, United States of America, 2.Los Alamos National Laboratory, United States of America, 3.Cornell High Energy Synchrotron Source, United States of America, 4.Lawrence Livermore National Laboratory, United States of America)

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

[○]Jiaming Zhu¹, Yipeng Gao², Dong Wang³, Tong-Yi Zhang⁴, Yunzhi Wang² (1.City University of Hong Kong, Hong Kong, 2.Ohio State University, United States of America, 3.Xi'an Jiaotong University, China, 4.Shanghai University, China)

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

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

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

[○]Evgeniya Kabliman¹, Johannes Kronsteiner¹, Ernst Kozeschnik² (1.Light Metals Technologies Ranshofen, Center for Low-Emission Transport, Austrian Institute of Technology, Austria, 2.Institute of Materials Science and Technology, TU Wien, Austria)

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

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

Invited

Vahid Tari¹, Ricardo A Lebensohn², Reeru Pokharel², Rachel E Lim¹, Darren C Pagan³, Yufeng Shen¹, Joel V Bernier⁴, Robert M Suter¹, [○]Anthony D Rollett¹ (1.Carnegie Mellon University, United States of America, 2.Los Alamos National Laboratory, United States of America, 3.Cornell High Energy Synchrotron Source, United States of America, 4.Lawrence Livermore National Laboratory, United States of America)

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

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

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

[○]Jiaming Zhu¹, Yipeng Gao², Dong Wang³, Tong-Yi Zhang⁴, Yunzhi Wang² (1.City University of Hong Kong, Hong Kong, 2.Ohio State University, United States of America, 3.Xi'an Jiaotong University, China, 4.Shanghai University, China)

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

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

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

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

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

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

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

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

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

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

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

○Evgeniya Kabliman¹, Johannes Kronsteiner¹, Ernst Kozeschnik² (1.Light Metals Technologies Ranshofen, Center for Low-Emission Transport, Austrian Institute of Technology, Austria, 2.Institute of Materials Science and Technology, TU Wien, Austria)

When material deformation occurs at elevated temperatures, one has to take into account the simultaneous evolution of grain, sub-grain structure and microchemistry (dissolution and precipitation of phase particles). In the present work, we present current results on the implementation of a computational strong coupling scheme between material deformation and microchemistry/microstructure evolution. For this purpose, we introduce a Dyna2Micro Material Model, which is implemented into a Finite Element Code (LS-DYNA or LSTC) and allows a simultaneous calculation of the (sub)-grain structure and phase kinetics at every integration point and time step. Dynamic processes, such as, work hardening and recovery are calculated by using a dislocation based model (MD² Model) implemented into a user defined subroutine, while the phase dissolution and precipitation is calculated by the thermo-kinetic software package MatCalc. Computational efficiency is realized by a new remote control feature implemented in MatCalc specially developed for this project as command interface between the user subroutine and a running MatCalc session. The simulations are checked by simulation of multi-step hot compression tests using a 3D axisymmetric cylindrical model of samples according to the experimental set up. For the material, we choose an Al-Cu-Mg alloy, where precipitation and dissolution of Al₂Cu and Al₂CuMg is considered. The whole simulation process from solidification, pre-heat treatment, deformation and post heat treatment is then controlled by the SProC (Smart Process Control) Toolkit.

[SY-E6] Symposium E-6

Chairs: Ying-Jun Gao(Guangxi University, China), Masaki Tanaka(Kyushu Univ., Japan)

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

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

○Ying-Jun Gao (Guangxi University, China)

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

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

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

○Michael Budnitzki (TU Bergakademie Freiberg, Germany)

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

○Masaki Tanaka¹, Yelm Okuyama¹, Tatsuya Morikawa¹, Toshiyuki Manabe² (1.Kyushu Univ., Japan, 2.Nippon Steel &Sumitomo Corporation, Japan)

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

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

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

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

○Ying-Jun Gao (Guangxi University, China)

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

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

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

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

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

[1] M. Hassani, P. Engels and F. Varnik, Wall effects on spatial correlations of non-affine strain in a 3D model glasses (Europhysics Letters 2018, in press).

[2] A. Nicolas and J.-L. Barrat, A mesoscopic model for the rheology of soft amorphous solids, with application to microchannel flows, Faraday Discuss. 167, 567 (2013).

[3] F. Varnik, S. Mandal, V. Chikkadi, D. Denisov, P. Olsson, D. Vagberg, D. Raabe, and P. Schall, Correlations of plasticity in sheared glasses, Phys. Rev. E 89, 040301 (2014).

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

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

○Michael Budnitzki (TU Bergakademie Freiberg, Germany)

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

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

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

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

○Masaki Tanaka¹, Yelm Okuyama¹, Tatsuya Morikawa¹, Toshiyuki Manabe² (1.Kyushu Univ., Japan, 2.Nippon Steel & Sumitomo Corporation, Japan)

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

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

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

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

Against highly complex hierarchical material systems as in high Cr heat-resistant ferritic steels exhibiting inhomogeneous recovery-triggered accelerated creep rupture, the present study tackles a series of problems about their practically-feasible multiscale modeling and simulations based on FTMP. The targeted system here is composed of martensite laths with high-dense dislocations (Scale A), lath blocks/packets (Scale B) embedded within a prior austenitic grain (Scale C). The objectives are (a) reproduction of the experimentally-observed accelerated degradation of the creep strength due to inhomogeneous recovery of the microstructures under relatively low stress conditions, and (b) identification of the minimal conditions for (a)

to occur, focusing on the interactions between Scales A and B. Creep analyses, considering the interior high-dense dislocations evaluated by the spontaneously-evolved incompatibility tensor field in Scale B, are conducted for single lath block models first. They exhibit pronounced local instability due to local recovery brought about by the interaction incompatibility field. Thus-developed models are further combined to construct single packets and embedded packet models, respectively, and the same series of analyses are performed on them. The fluctuating incompatibility field in Scale A, concurrently enhanced by the interaction term, is demonstrated to promote the local recovery. We further clarify the contributions of the projection directions of the incompatibility tensor in evaluating the Scale A dislocation density. The projection to the slip plane normal direction is turned out to play exclusively-dominant roles, implying the critical contribution of the climb-related elementary processes to the enhanced localized recovery. An attempt is also made to replace the above recovery model to improve the consistency of the current approach.

[SY-E7] Symposium E-7

Chairs: Daisuke Matsunaka(Shinshu Univ., Japan), Shiyu Du(Chinese Academy of Sciences, China)

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

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

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

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

[○]Tetsuya Ohashi (Kitami institute of technology, Japan)

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

[○]Daisuke Matsunaka¹, Yoji Shibutani² (1.Dept. of Mechanical Systems Engineering, Shinshu Univ., Japan, 2.Dept. of Mechanical Engineering, Osaka Univ., Japan)

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

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

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

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

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

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

Invited

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

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

1. Chachamovitz D, Mordehai D. Sci Rep 2018;8:3915

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

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

[○]Tetsuya Ohashi (Kitami institute of technology, Japan)

Density evolution of atomic vacancies during plastic slip deformation is evaluated by crystal plasticity analyses where evolution of dislocation density is calculated by the model of Kocks and Mecking¹ and the dislocation mean free path is given by an effective average distance of forest dislocations and a microstructure length scale^{2, 3}. We slightly modified the model by Essmann and Mughrabi⁴ for the evolution of atomic vacancy density and implemented to the crystal plasticity software code. Analysis results⁵ show that the vacancy density sometimes reaches at the order of $10^{24} / \text{m}^3$, which is at the order of 10^{-4} in terms of concentration. Increase rate of the atomic vacancy is shown to depend largely on the microstructure length scale and slip multiplication on different systems.

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

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

○Daisuke Matsunaka¹, Yoji Shibutani² (1.Dept. of Mechanical Systems Engineering, Shinshu Univ., Japan, 2.Dept. of Mechanical Engineering, Osaka Univ., Japan)

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

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

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

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

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

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

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

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

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

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

Carbon nanotubes (CNT) possess excellent mechanical properties in terms of axial elastic stiffness and rupture strength. It is therefore an obvious question whether these properties can be harnessed for structural applications by using such nanoparticles as fillers in low-melting lightweight metals such as Al or Mg nanocomposite. To this end, homogeneous dispersion of CNT in the metal matrix and strong interfacial bonding are essential factors since agglomerated nanoparticles with weak bonding into the surrounding metal matrix might act as flaws which actually deteriorate, rather than improve, the mechanical properties of composites. However, good dispersion and strong interfacial bonding are hindered by the low affinity of CNT to Al or Mg. To overcome this problem, interface engineering approaches such as coating CNT with an appropriate metal such as Nitweight, or by decorating them with metal nanoparticles, may offer a promising approach towards the efficient fabrication of lightweight metal-CNT nanocomposites.

In this work we study how metal coated or metal decorated carbon nanotubes affect the mechanical properties of aluminium/CNT composites. In particular we look at the pullout behaviour of pristine as well as Ni coated or Ni decorated CNT from an aluminium matrix. Our result shows that Ni coating produces an extended interface (“intephase”) where a significant amount of energy is dissipated during CNT pull-out, leading to a high pull-out force. We then investigate the interaction of embedded CNT with and without coating/decoration with cracks and with dislocations during simulated tensile tests. We discuss the results in view of promising approaches for engineering CNT-metal interfaces such as to achieve high strength and high toughness of the metal-CNT composites.

[SY-E8] Symposium E-8

Chairs: Hao Wang(Institute of Metal Research, CAS, China), Jun-Ping Du(Kyoto University, Japan)

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

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

○Jun-Ping Du^{1,2}, W.T. Geng³, Kazuto Arakawa⁴, Shigenobu Ogata^{2,1} (1.Elements Strategy Initiative for Structural Materials, Kyoto University, Japan, 2.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 3.University of Science and Technology Beijing, China, 4.Department of Materials Science, Faculty of Science and Engineering, Shimane University, Japan)

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

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

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

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

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

○Qinye Li¹, Lihong He¹, Chenghua Sun^{2,3}, Xiwang Zhang¹ (1.Monash University, Australia, 2.Swinburne University of Technology, Australia, 3.Dongguan University of Technology, China)

[SY-E8] First-principles Investigation on the Stability and Oxygen Adsorption Behavior of a Ti₂AlNb/TiAl Interface

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

[SY-E8] DFT predictions of hydrogen storage properties of Mg₇TiX₂ (X= F, O, S, P and Cl)

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

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

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

○Jun-Ping Du^{1,2}, W.T. Geng³, Kazuto Arakawa⁴, Shigenobu Ogata^{2,1} (1.Elements Strategy Initiative for Structural Materials, Kyoto University, Japan, 2.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 3.University of Science and Technology Beijing, China, 4.Department of Materials Science, Faculty of Science and Engineering, Shimane University, Japan)

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

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

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

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

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

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

vacancy diffusion will also be markedly reduced by biaxial strain. Consequently, our finding suggests that anisotropic strain will significantly enhance vacancy mobility in W and promote the formation and growth of hydrogen/helium bubbles.

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

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

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

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

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

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

○Qinye Li¹, Lizhong He¹, Chenghua Sun^{2,3}, Xiwang Zhang¹ (1.Monash University, Australia, 2.Swinburne University of Technology, Australia, 3.Dongguan University of Technology, China)

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

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

[SY-E8] **First-principles Investigation on the Stability and Oxygen Adsorption Behavior of a Ti₂AlNb/TiAl Interface**

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

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

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

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

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

Stability and reversibly de/hydrogenation properties of presumed Mg_7TiX_2 (X= F, O, S, P and Cl) were predicted using Density Functional Theory. Hypothetical Mg_7TiX_2 and its hydride are energetically stable with respect to the individual elements involved and they may be synthesized experimentally. The stability of alloy highly relate to the formation energy of Mg-X compound because that distance of Ti-X is large than that of Mg-X. The considered systems possess preferable hydrogen adsorbing capacity, and their hydrogen adsorption energies lie in the range from -0.5 eV to -0.05 eV. The dehydrogenation of the $\text{Mg}_7\text{TiX}_2\text{H}_{14}$ were calculated and found that H-Mg bond and Ti-Mg bond have significant effect on dehydrogenation process. The study of desorption energy of X atoms found that P atoms are less stable than H atoms and will escape from system before H atoms that lead system collapse, thus Mg_7TiP_2 is not available to hydrogen storage. Our studies indicated that Mg_7TiX_2 (X= F, O, S and Cl) can realize reversible hydrogen storage properties.

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

[SY-F5] Symposium F-5

Chair: Ingo Steinbach(Ruhr-University Bochum, Germany)

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

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

○Tomohiro Takaki¹, Shinji Sakane¹, Munekazu Ohno², Yasushi Shibuta³, Takayuki Aoki⁴ (1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.The University of Tokyo, Japan, 4.Tokyo Institute of Technology, Japan)

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

○Michael Kellner^{1,2}, Johannes Hötzer^{1,2}, Markus Linnenberg¹, Marco Seiz¹, Britta Nestler^{1,2} (1.Institute of Applied Materials - Computational Materials Science (IAM-CMS), Karlsruhe Institute of Technology, Germany, 2.Institute of Digital Materials Science (IDM), Karlsruhe University of Applied Science, Germany)

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

○Sukeharu Nomoto¹, Hiroshi Wakameda¹, Masahito Segawa¹, Toshiyuki Koyama², Akinori Yamanaka³ (1.ITOCHU techno-Solutions Cooperation, Japan, 2.Materials Design Innovation Engineering, Nagoya Univ., Japan, 3.Department of Mechanical Systems Engineering, Tokyo University of Agriculture and Technology, Japan)

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

○Juba Hama¹, Benoît Appolaire², Yann Le Bouar¹, Alphonse Finel¹ (1.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay F-92322 Châtillon, France, 2.IJL, UMR 7198 CNRS-Université de Lorraine, 54000 Nancy, France)

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

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

Invited

○Tomohiro Takaki¹, Shinji Sakane¹, Munekazu Ohno², Yasushi Shibuta³, Takayuki Aoki⁴ (1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.The University of Tokyo, Japan, 4.Tokyo Institute of Technology, Japan)

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

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

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

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

○Michael Kellner^{1,2}, Johannes Hötzer^{1,2}, Markus Linnenberg¹, Marco Seiz¹, Britta Nestler^{1,2} (1.Institute of Applied Materials - Computational Materials Science (IAM-CMS), Karlsruhe Institute of Technology, Germany, 2.Institute of Digital Materials Science (IDM), Karlsruhe University of Applied Science, Germany)

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

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

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

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

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

○Sukeharu Nomoto¹, Hiroshi Wakameda¹, Masahito Segawa¹, Toshiyuki Koyama², Akinori Yamanaka³
(1.ITOCHU techno-Solutions Cooperation, Japan, 2.Materials Design Innovation Engineering, Nagoya Univ., Japan, 3.Department of Mechanical Systems Engineering, Tokyo University of Agriculture and Technology, Japan)

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

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

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

○Juba Hamma¹, Benoît Appolaire², Yann Le Bouar¹, Alphonse Finel¹ (1.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay F-92322 Châtillon, France, 2.IJL, UMR 7198 CNRS-Université de Lorraine, 54000 Nancy, France)

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

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

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

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

[SY-F6] Symposium F-6

Chair: Benoit Appolaire(Institut Jean Lamour, Univ. de Lorraine, France)

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

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

○Ingo Steinbach (Ruhr-University Bochum, Germany)

[SY-F6] Characterisation and modelling of drawn martensite

○Marius Gintalas¹, Miguel A. Santajuana², Carlos Garcia-Mateo², David San-Martin², Jose A. Jimé nez², Wim Van Haver³, Pedro E. J. Rivera-Diaz-del-Castillo⁴ (1.The University of Cambridge, Department of Materials Science &Metallurgy, 27 Charles Babbage Road, Cambridge CB3 0FS, UK, 2.Materialia research group, Department of Physical Metallurgy, Spanish National Centre for Metallurgical Research (CENIM-CSIC), Avda. Gregorio del Amo 8, Madrid E-28040, Spain, 3.NV Bekaert SA, Bekaertstraat 2, Zwevegem B-8550, Belgium, 4.The University of Lancaster, Department of Engineering, Engineering Building, Lancaster University, Gillow Ave, Bailrigg, Lancaster LA1 4YW, UK)

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

○Maeva Cottura¹, Benoît Appolaire¹, Alphonse Finel², Yann Le Bouar² (1.Institut Jean Lamour , France, 2.LEM - CNRS/Onera, France)

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

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

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

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

Invited

○Ingo Steinbach (Ruhr-University Bochum, Germany)

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

The quenching simulation reproduces the martensite transformation under consideration of the Kurdjumov-Sachs relationship. Based on these results, tempering is simulated. Diffusion is enabled at elevated temperatures and cementite carbides are nucleated, which decreases carbon composition in the martensite, which also decreases the tetragonal distortion. A virtual tension test provides then information about strain hardening, damage as well as the macroscopic response of the material to the loading. Different microstructures, as resulting from different alloy composition and different tempering conditions are compared regarding their mechanical performance.

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[2] Microstructure Design of Tempered Martensite by Atomistically Informed Full-Field Simulation: From Quenching to Fracture, Efim Borukhovich, Guanxing Du, Matthias Stratmann, Martin Boeff, Oleg Shchyglo, Alexander Hartmaier, Ingo Steinbach, Materials 9 (8), 673

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

[SY-F6] Characterisation and modelling of drawn martensite

○Marius Gintalas¹, Miguel A. Santajuana², Carlos Garcia-Mateo², David San-Martin², Jose A. Jiménez², Wim Van Haver³, Pedro E. J. Rivera-Díaz-del-Castillo⁴ (1.The University of Cambridge, Department of Materials Science & Metallurgy, 27 Charles Babbage Road, Cambridge CB3 0FS, UK, 2.Materialia research group, Department of Physical Metallurgy, Spanish National Centre for Metallurgical Research (CENIM-CSIC), Avda. Gregorio del Amo 8, Madrid E-28040, Spain, 3.NV Bekaert SA, Bekaertstraat 2, Zwevegem B-8550, Belgium, 4.The University of Lancaster, Department of Engineering, Engineering Building, Lancaster University, Gillow Ave, Bailrigg, Lancaster LA1 4YW, UK)

There has been an extensive work on microstructural refinement via severe plastic deformation, which leads to improved strength in metallic materials. However, due to the complexity of the microstructural changes involved, the mechanisms responsible for the strength enhancement of the cold deformed martensite have not been completely revealed. This work summarises advanced experimental and modelling activities carried out on heavily drawn martensite. These include slow heating high resolution dilatometry, high resolution transmission electron microscopy and high resolution X-ray diffraction conducted with both synchrotron and lab x-ray sources. The purpose of employing various characterisation techniques is to collect data to gain a comprehensive understanding on the microstructural evolution with respect to applied strain. The modelling work aims to propose a novel martensite strength model to describe the relationship between microstructure and mechanical properties, including the effects of applied strain upon severe plastic deformation. The strengthening model is validated using stress-strain data of martensite drawn at various strain levels.

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

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

○Maeva Cottura¹, Benoît Appolaire¹, Alphonse Finel², Yann Le Bouar² (1.Institut Jean Lamour , France, 2.LEM - CNRS/Onera, France)

Many materials used in everyday life have a complex internal structure organized at different scales with a texture of grains, and a complex pattern of thermodynamic phases at lower scale. This microstructure strongly impacts the movement of crystalline defects in the materials and therefore controls the mechanical behaviour. The phase field method has emerged as a well-suited method for tackling microstructure evolutions during phase transformations when elastic coherency stresses are generated. In addition, in many materials and especially at high temperature, the microstructure evolution is coupled with plasticity, and there is currently a great research effort to extend the phase field method to take this coupling into account. In this context, we will show how to couple a classical phase field model (for the description of the phase transformation) with a crystal plasticity model based on dislocation densities. The latter model uses a storage-recovery law for the dislocation density of each glide system and a hardening matrix to account for the short-range interactions between dislocations. The proposed model will be applied to study rafting of ordered precipitates observed in Ni-based superalloys. We will present 3D calculations of microstructure evolution under [100], [110] and [111] creep loading as well as different shear creep tests.

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

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

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

We investigate the role of coherency strains and applied load on phase growth and morphological evolution in binary diffusion couples using the phase field method. We employ the Kim-Kim-Suzuki model for the chemical contribution in the free energy. The elastic energy contribution to the free energy is evaluated using a suitable interpolation scheme considering the elastic heterogeneity between the different phases. When

elastic stresses are considered, we observe bending and splitting of the phase layers for mechanically constrained, partially constrained and relaxed systems. The interface remains planar in the absence of elastic stresses. In addition, we study the role of volume fraction of the phases and finite size of the system on the microstructure evolution.

[SY-F7] Symposium F-7

Chair: Tomohiro Takaki(Kyoto Institute of Technology, Japan)

Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3

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

○Benoit Appolaire^{1,2}, Anna Ask³, Samuel Forest³, Kais Ammar³ (1.Institut Jean Lamour, Univ. de Lorraine, France, 2.LEM, CNRS-Onera, France, 3.Centre des Materiaux, Mines ParisTech, France)

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

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

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

○Masahito Segawa¹, Nomoto Sukeharu¹, Akinori Yamanaka² (1.ITOCHU Techno-Solutions Corporation, Japan, 2.Division of Advanced Mechanical Systems Engineering, Institute of Engineering, Tokyo University of Agriculture and Technology, Japan)

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

○Chamara Kumara¹, Dunyong Deng², Johan Moverare², Per Nylén¹ (1.Department of Engineering Science, University West, Sweden, 2.Department of Management and Engineering, Linköping University, Sweden)

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

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

 (Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3)

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

Invited

○Benoit Appolaire^{1,2}, Anna Ask³, Samuel Forest³, Kais Ammar³ (1.Institut Jean Lamour, Univ. de Lorraine, France, 2.LEM, CNRS-Onera, France, 3.Centre des Materiaux, Mines ParisTech, France)

Elaborating a unified field framework to model concurrent viscoplastic deformation and recrystallization and grain growth in metal polycrystals has remained a formidable issue. In this work, we will present such a unified framework relying on the enhancement of a Cosserat crystal plasticity model with an order parameter to account for diffuse, mobile grain boundaries in analogy with phase field models. The Cosserat directors are taken to represent the lattice orientation of the grains. In order to introduce an evolution law for reorientation during grain boundary migration, the skew-symmetric part of the Cosserat deformation tensor is associated with a dissipative stress. The formulation in terms of the Cosserat deformation provides a natural way to couple reorientation due to deformation and reorientation due to grain boundary migration. In the absence of displacements and for a particular choice of free energy function the model can be considered a generalization to three dimensions of the Kobayashi-Warren-Carter (KWC) orientation phase field model (2000, 2003).

The proposed 3D anisotropic constitutive framework couples the changing orientation at a material point due to migrating grain boundaries (which is essential to the KWC model) to the lattice reorientation due to displacements and plastic slip. Due to the coupling of the Cosserat directors and the elastic reorientation, the bulk rotation of the grains which is inherent to the KWC model (and considered an artefact here although it can nevertheless be desirable in certain cases) can be controlled and even suppressed.

In this contribution, we will explain the main features of this framework and we will illustrate its capabilities with several cases that could not be handled convincingly by other models.

 (Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3)

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

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

We develop a phase-field model for the simulation of chemical diffusion limited microstructure evolution, with a special focus on precipitation growth and ripening in multi-component alloys. Further, the model accounts for elastic effects, which result from the lattice-misfit between the precipitate particles and the parent matrix-phase. To be able to simulate particle growth and ripening in one dimension, we introduce an extra optional driving-force term, which mimics the effect of the curved particle/matrix interface in one dimension. As a case study, we consider the gamma'-precipitation growth and ripening under the influence of realistic heat treatment time-scales in the multi-component Ni-base single crystalline cast alloy CMSX-4. The respectively required temperature-dependent thermodynamic and kinetic input parameters are obtained from CALPHAD calculations using the commercial software-package ThermoCalc. The required temperature-dependent elastic parameters are measured in-house at the chair of Metals and Alloys, using resonance ultrasound spectroscopy for the anisotropic and inhomogeneous stiffness-tensor and high temperature X-ray diffraction for the lattice misfit.

We study the kinetics of growth and ripening of statistically many interacting precipitated particles as function of the temperature and time in one and two dimensions, with the explicit consideration of up to 8 independent chemical components. Furthermore, the model is applied to calculate the detailed shape-evolution of a few interacting gamma'-particles in two and three dimensions with periodic boundary conditions. Relations to the shapes of gamma'-particles in respectively heat treated experimental microstructures are discussed.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3)

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

○Masahito Segawa¹, Nomoto Sukeharu¹, Akinori Yamanaka² (1.ITOCHU Techno-Solutions Corporation, Japan, 2.Division of Advanced Mechanical Systems Engineering, Institute of Engineering, Tokyo University of Agriculture and Technology, Japan)

Multi-phase-field (MPF) method incorporating CALPHAD database has attracted much attention as a powerful numerical tool for simulating microstructure evolutions in various metallic materials. Transformation modes and diffusion behavior of substitutional solute atoms strongly depend on temperature and chemical compositions of the alloy especially in multi-component steels, i.e. an Fe-C-Mn ternary alloy. Therefore, we need to use a robust MPF model which can simulate the transition of transformation mode and the complex diffusion behavior. Recently, the MPF model with finite interface dissipation has been proposed (Hereafter, the MPF model is called as the non-equilibrium MPF (NEMPF) model). The attractive advantages of the NEMPF model are its computational efficiency and flexibility for simulating microstructure evolutions under strong non-equilibrium interface condition without the equal chemical potential assumption. In the previous study, we investigated the cyclic $\gamma \rightarrow \alpha$ and $\alpha \rightarrow \gamma$ transformations in Fe-C-Mn-Si alloys using the NEMPF model coupled with CALPHAD database. The one-dimensional simulations of the cyclic phase transformation revealed that the switching of the polarities of Mn and Si spikes formed at the α / γ interface caused the stagnant stage where the phase transformation was suppressed. In this study, the two-dimensional simulation of cyclic phase transformation in Fe-C-Mn-Si alloy is performed using the NEMPF model in order to gain a deeper understanding of the mechanism of the stagnant stage and the transition of transformation modes.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3)

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

○Chamara Kumara¹, Donyong Deng², Johan Moverare², Per Nylén¹ (1.Department of Engineering Science, University West, Sweden, 2.Department of Management and Engineering, Linköping University, Sweden)

Electron Beam Melting (EBM) is a powder bed additive manufacturing process where powder material is being melted selectively by a layer-by-layer approach using an electron beam. It has some unique features when it comes to manufacturing of components in high-performance superalloys such as alloy 718 that are commonly used in gas turbines. EBM has high deposition rate due to high beam energy and speed, comparatively low residual stresses and limited problems with oxidation. However, due to the layer-by-layer melting approach and high powder bed temperature, the resultant microstructure of as-built EBM Alloy 718

is observed to have a microstructure gradient starting from the top of the sample. The aim of this study was to use modelling to create a deeper understanding of microstructure development during EBM and the homogenization that occurs during manufacturing in Alloy 718. A multi-component phase field modelling approach combined with thermodynamic modelling was used to predict the experimentally observed microstructure gradient. Of particular interest was to study the element segregation during the solidification and the subsequent “in-situ” homogenization heat treatment that occur due to the elevated powder bed temperature. The predicted element composition was then used in thermodynamic modelling to predict the changes in the CCT and TTT diagrams for Alloy 718. This helps to explain the observed phase evolution within the microstructure. The results indicate that the approach can be a valuable tool both for creating process understanding and for process development including subsequent homogenization and heat treatment.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room3)

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

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

Laser melting deposition is a complicated physical and chemical metallurgical process. In this paper, the phase field model of alloy solidification is coupled to laser melting deposition process, and a finite element model of heat transfer is established. By studying the variation of the spacing of dendrite Fe_2B of Fe-B alloy powder under the conditions of laser melt deposition, the robustness and accuracy of the coupled model were verified. Experiments show that under different temperature gradient conditions, the size and spacing of the dendrite Fe_2B of the cross-section morphology of the Fe-B alloy deposited by laser melting deposition have changed significantly. The quantitative phase field simulation of the heat transfer finite element model under local steady state conditions confirms this behavior. This work demonstrates the potential of the phase-field method to simulate laser melting deposition techniques and analyze the potential of alloy solidification under complex heat transfer conditions.

[SY-F8] Symposium F-8

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

Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3

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

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

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

○Dongdong Zhao¹, Sylvain Gouttebroze², Jesper Friis³, Yanjun Li¹ (1.Norwegian University of Science and Technology (NTNU), 7491, Trondheim , Norway, 2.SINTEF Materials and Chemistry, 0314 Oslo, Norway, 3.SINTEF Materials and Chemistry, 7491 Trondheim, Norway)

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

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

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

○Jae-Hyeok Shim¹, Magdalena Speicher², Mahesh Chandran³, Woo-Sang Jung¹ (1.Korea Institute of Science and Technology, Korea, 2.Materials Testing Institute, Germany, 3.Indo-Korea Science and Technology Centre, India)

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

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

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3)

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

Invited

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

In the past 20 years, significant progress has been made in the development of state parameter-based modeling approaches for the simulation of microstructure evolution, in particular, with respect to precipitation kinetics, recrystallization, recovery, grain growth, dislocation density evolution in the course of thermo-mechanical treatment, as well as the mutual interactions of all mechanisms. Once, the relevant state parameters and their evolution are known, it is straightforward, however not trivial, to deduct from these the stress strain response of the microstructure as a function of temperature and strain rate. In this presentation, an overview of these models is given as well as some implementation details in the thermokinetic software package MatCalc. Finally, an example is discussed, where the precipitation microstructure and its interaction with deformation in the course of compression testing is simulated and compared to corresponding experimental data.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3)

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

○Dongdong Zhao¹, Sylvain Gouttebroze², Jesper Friis³, Yanjun Li¹ (1.Norwegian University of Science and Technology (NTNU), 7491, Trondheim, Norway, 2.SINTEF Materials and Chemistry, 0314 Oslo, Norway, 3.SINTEF Materials and Chemistry, 7491 Trondheim, Norway)

A newly developed modelling framework which accounts for grain boundary (GB) segregation and precipitation in multi-component Al alloys subjected to cooling and subsequent heat treatments is presented. Within this framework, both the equilibrium and non-equilibrium segregation mechanisms are considered to predict the solute and vacancy segregations towards GBs. In the model of non-equilibrium segregation, GBs are considered as ideal sinks for vacancy annihilation. The CALPHAD (CALculations of PHase Diagrams) approach is implemented to supply the important thermodynamic and kinetic data of multi-component Al alloys as input for the model. The present framework is expected to predict the solute and vacancy segregations at GBs in multi-component Al alloys during typical heat treatment (e.g. quenching, ageing) processes. It is shown that the variation of vacancy and solute segregation behavior at GBs as a function of heat treatment or microstructure variables, i.e. solution/ageing temperature, cooling rate, grain size, can be well described within the present model. Based on the segregation of solute elements, preliminary precipitation behavior at GBs and bulk are predicted using the Kampmann-Wagner numerical approach. The simulation results have been compared with experimental observations. This work is supposed to provide a preliminary theoretical understanding towards the GB segregation and precipitation in multi-component Al alloys subjected to various cooling and subsequent heat treatment processes.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3)

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

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

Aging is commonly performed after forming process to obtain better mechanical properties and electrical conductivity of Al-Mg-Si alloys (AA6xxx series) applied in the electrical wire. In this work, the nucleation, growth, coarsening and dissolution of different precipitate phases (Mg_xSi_y) during aging treatment is simulated based on a Kampmann-Wagner Numerical (KWN) type precipitation model. By coupling with the CALPHAD, the thermodynamics of the metastable precipitate phases is well treated. Furthermore, the precipitation model is linked to an electrical conductivity model to predict the evolution of electrical conductivity based on the volume fraction, size and spatial distribution of different precipitates, solid solution level, etc. The modeling results are compared to the transmission electron microscopy (TEM) experimental results and electrical conductivity measurements. It is revealed that the present model can well address the influence of alloy composition, aging temperature and aging time on the microstructure and electrical conductivity of Al-Mg-Si alloys.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3)

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

○Jae-Hyeok Shim¹, Magdalena Speicher², Mahesh Chandran³, Woo-Sang Jung¹ (1.Korea Institute of Science and Technology, Korea, 2.Materials Testing Institute, Germany, 3.Indo-Korea Science and Technology Centre, India)

There is an urgent need to improve the thermal efficiency of fossil fuel power plants by raising the operation temperature and pressure in order to reduce CO₂ emission as well as the cost of fuel. Plant operation at higher temperatures inevitably requires the development of heat-resistant alloys with a higher creep strength. There has recently been an increasing interest in applying advanced heat-resistant alloys to fossil fuel power plants in order to raise their operation temperature. The important role of precipitation in the achievement of good creep properties of heat-resistant alloys has long been recognized. One of the most effective ways for improving the creep properties is to uniformly distribute fine precipitates with a good long-term stability at elevated temperatures. The experimental investigation of the long-term precipitate evolution behavior in heat-resistant alloys have not often been performed, although it is important in understanding the creep properties. In addition to experimental approaches, there have recently been a few attempts to simulate the precipitation kinetics in heat-resistant alloys. The purpose of this study is to simulate the long-term precipitate evolution in various heat-resistant alloys such as ferritic/martensitic and austenitic steels and nickel alloys using the MatCalc software, which operates based on the classical nucleation theory and evolution equations derived from the thermodynamic extremum principle that maximizes the dissipation rate of the total Gibbs energy of the system. The simulation results, such as the precipitation sequence and the precipitate size, will be compared with experimental observations.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room3)

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

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

Metal additive manufacturing is disrupting the traditional approaches in the manufacturing sector. However, there are uncertainties associated with the qualification of fabricated components owed to the difficulty in predicting the process-structure relationship in the PSPP linkage. Understanding the process-structure linkage includes understanding the (a) liquid-solid phase transformation and (b) solid-solid phase transformation. Previously solidified layers are affected by the thermal cycles during the melting of the subsequent layers. During processing in AM, the conditions are highly non-isothermal, non-equilibrium and understanding this highly transient condition is crucial to understand the precipitation kinetics. The temperature of the substrate can also be varied in the machine. This affects the solid-state phase transformation of a given alloy system. Multiple phases can simultaneously precipitate from the product phase as a function of thermal cycle. In this work, we develop a model based on simultaneous transformation kinetics theory and the developed phenomenological model is then coupled with the numerical thermal model to predict the solid-state phase transformation and volume fraction of multiple phases as a function of thermal cycles and processing conditions. Numerical thermal model is used to predict the thermal cycles as a function of input processing conditions. The thermal cycle is then discretized into set of small isothermal steps. The extent of simultaneous precipitation/dissolution of the phases will be calculated at each of the discretized time step. Volume fraction of each of the phases is then updated and similar procedure is repeated for rest of the discretized isothermal time steps. Appropriate thermodynamic framework, database will be used to calculate the thermodynamic properties as a function of alloy system and is used as the input to the model. It is a semi-empirical model and the input from experimental results are used to calibrate the model. Some of the other calibration parameters include nucleation site densities and surface energies. Advantages and limitations of this approach will be discussed in detail.

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

[SY-N1] Symposium N-1

Chair: Danny Perez (Los Alamos National Laboratory, United States of America)

Wed. Oct 31, 2018 9:45 AM - 10:45 AM Room4

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

○ Arthur F Voter (Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, United States of America)

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

○ Jutta Rogal¹ (1. Ruhr University Bochum, Germany)

(Wed. Oct 31, 2018 9:45 AM - 10:45 AM Room4)

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

Invited

○Arthur F Voter (Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, United States of America)

Many important materials processes take place on time scales that far exceed the roughly one microsecond accessible to molecular dynamics simulation. Typically, this long-time evolution is characterized by a succession of thermally activated infrequent events involving defects in the material. In the accelerated molecular dynamics (AMD) methodology, known characteristics of infrequent-event systems are exploited to make reactive events take place more frequently, in a dynamically correct way. For certain processes, this approach has been remarkably successful, offering a view of complex dynamical evolution on time scales of microseconds, milliseconds, and sometimes beyond. We have recently made advances in all three of the basic AMD methods (hyperdynamics, parallel replica dynamics, and temperature accelerated dynamics (TAD)), exploiting both algorithmic advances and novel parallelization approaches. I will describe these advances, present some examples of our latest results, and discuss what should be possible when exascale computing arrives in roughly four years.

(Wed. Oct 31, 2018 9:45 AM - 10:45 AM Room4)

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

Invited

○Jutta Rogal¹ (1. Ruhr University Bochum, Germany)

Obtaining atomistic insight into the fundamental processes during phase transformations and their dynamical evolution up to experimental timescales remains one of the great challenges in materials modelling. In particular, if the mechanisms of the phase transformations are governed by so-called rare events the timescales of interest will reach far beyond the applicability of regular molecular dynamics simulations. In addition to the timescale problem the simulations provide a vast amount of data in the high-dimensional phase space. A physical interpretation of these data requires the projection into a low-dimensional space and the identification of suitable reaction coordinates.

In this presentation, I will give an example of our analysis of the atomistic processes at a complex phase boundary during a solid-solid phase transformation. The migration of the phase boundary proceeds via concerted multi-atom processes on a complex energy landscape. Here, we employ an adaptive kinetic Monte Carlo (AKMC) approach together with driven adiabatic free energy dynamics (d-AFED) to investigate such processes at the interface between the body-centered cubic and A15 phase in molybdenum.

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

[SY-N2] Symposium N-2

Chair: Erik Bitzek (FAU Erlangen-Nuernberg, Germany)

Wed. Oct 31, 2018 11:15 AM - 12:15 PM Room4

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

○Nikolas Provatas (McGill University, Canada)

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

○Peter Voorhees¹, Eli Alster¹, Nana Ofuri-Opoku^{1,3}, David Montiel², Katsuyo Thornton², James Warren³ (1.Northwestern University, United States of America, 2.University of Michigan, United States of America, 3.National Institute for Standards and Technology, United States of America)

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

○Thomas Swinburne¹ (1.CINaM, CNRS/Aix-Marseille Univ., France)

(Wed. Oct 31, 2018 11:15 AM - 12:15 PM Room4)

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

Invited

○Nikolas Provatas (McGill University, Canada)

This talk will study several closely connected density functional type theories that employ both short and long range, rotationally invariant, multi-point particle interactions. Collectively, these models give rise to a class of *structural phase field crystal (XPFC)* models. These XPFC models allow for numerous microstructural phenomena to be studied that couple important physics emergent at the atomic scale with phase transformation kinetics occurring on diffusional time scales. Results from recent solidification studies conducted using XPFC modelling in pure materials and alloys will be presented and compared to experiments and other theory. These include multi-step nucleation in solidification, void formation in nano-confined liquid pools during rapid cooling, solute drag, and dislocation-assisted nucleation in solid-state precipitation in alloys. Coupling of the base phase field theory with heat transfer will also be demonstrated for the study of latent heat effects in solidification. We close by discussing coarse graining methods for deriving practical phase field theories from phase field crystal models for meso-scale modelling applications.

(Wed. Oct 31, 2018 11:15 AM - 12:15 PM Room4)

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

○Peter Voorhees¹, Eli Alster¹, Nana Ofuri-Opoku^{1,3}, David Montiel², Katsuyo Thornton², James Warren³

(1.Northwestern University, United States of America, 2.University of Michigan, United States of America, 3.National Institute for Standards and Technology, United States of America)

Phase field crystal (PFC) method allows the atomic scale motion and defect formation to be determined on diffusive timescales. A major challenge with the method is to devise free energy functions that can yield complicated crystal structures. We introduce a phase-field crystal model that creates an array of complex three- and two-dimensional crystal structures via a numerically tractable three-point correlation function. This approach successfully yields energetically stable simple cubic, diamond cubic, simple hexagonal, graphene layers, and CaF₂ crystals, as well as the particularly complex and technologically important perovskite crystal structure. Highly anisotropic interfaces play an important role in the development of material microstructure. We examine the capability of the PFC model to quantitatively describe faceted interfaces by coarse graining the PFC model to attain both its complex amplitude formulation, and its corresponding phase field limit. Using this formulation, we find that the model yields Wulff shapes with missing orientations, the transition to missing orientations, and facet formation. We demonstrate, in two dimensions, how the resultant model can be used to study the growth of crystals with varying degrees of anisotropy in the phase-field limit.

(Wed. Oct 31, 2018 11:15 AM - 12:15 PM Room4)

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

Invited

○Thomas Swinburne¹ (1.CINaM, CNRS/Aix-Marseille Univ., France)

The fracture response of bcc metals is known to be controlled by dislocation mobility, which in turn is dependent on the slow, thermally activated nucleation of kink pairs on screw dislocations. We present a general, efficient scheme to calculate free energy barriers in large crystalline systems[1] which we apply to the kink nucleation process, finding significant anharmonic contributions at low homologous temperatures. A statistical mechanical approach is then used to study kink-limited dislocation motion through a field of obstacles[2]. We identify a crossover obstacle density below which the activation energy for plastic flow is half the free energy barrier for kink pair nucleation. Our results show striking agreement with fracture experiments across a wide range of bcc metals and are applied to interpret experimental data on irradiation induced embrittlement.

[1] TD Swinburne and M-C Marinica, Physical Review Letters 120 (13), 135503

[2] TD Swinburne and SL Dudarev, Physical Review Materials 2 (7), 073608

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

[SY-N3] Symposium N-3

Chair: Arthur F. Voter (Los Alamos National Lab, United States of America)

Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room4

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

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

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

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

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

○Ivan Novoselov^{1,2}, Alexey Yanilkin¹ (1.Dukhov Research Institute of Automatics, Russia, 2.Moscow Institute of Physics and Technology, Russia)

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

○Rao Huang¹, Li-Ta Lo², Arthur F. Voter², Danny Perez² (1.Xiamen University, China, 2.Los Alamos National Lab, United States of America)

 (Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room4)

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

Invited

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

There has been significant emphasis recently on the synthesis of fivefold-twinned Ag and Cu nanowires, which are considered to be excellent candidates for transparent conductors in flexible and stretchable electronic devices. A fundamental understanding of nanowire growth is important in achieving optimal syntheses. Nanowires grow from fivefold-twinned seeds and our work shows that likely shapes for these structures include {111} end facets and “notches”, {100} side facets, and {110} facets between the notches and the ends. We find that the density of islands on the {111} facets of growing wires is lower than that on {100} facets and that islands are likely to nucleate on {111} facets near {110}-{111} facet boundaries. Our climbing-image nudged-elastic band calculations of diffusion barriers based on embedded-atom method potentials indicate that diffusion in the {111} notches and on the {110} “steps” is significantly faster than diffusion on {100} facets. Thus, these structures become “superhighways” that channel atom diffusion to the wire ends to increase wire aspect ratios. Small islands facilitate trapping of atoms on {111} facets. We use finite Markov chains to model nanowire growth and to predict net atom fluxes from nanowire sides to the ends. These simulations predict anisotropic nanowires similar to those seen experimentally.

 (Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room4)

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

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

Atomistic simulations are a key component to understand reaction chemistry in materials; for instance, the detonation chemistry of energetic materials under pressure, which is characterized by rapid breaking and remaking of covalent bonding, and where intermediate products and reaction rates are difficult to characterize in experiments.

While accurate methods exist to study systems of relevant size with explicit electronic contributions critical to the description of bonds, e.g. density functional tight-binding (DFTB), the timescale of the simulation is often limited to a few hundreds of picoseconds. This restrains the study to systems in which reactions occur relatively quickly. In the case of detonation chemistry, this implies high pressure and temperature. In order to consider less extreme conditions, one can benefit from the rare occurrence of chemical reactions to use accelerated molecular dynamics methods such as parallel replica dynamics (PRD).

In this work, we describe efforts to combine the DFTB code LATTE, developed at LANL, with the PRD method, in order to perform accelerated QMD (AQMD) simulations of reactive chemistry. AQMD was first applied to the study of liquid benzene, a prototypical reactive hydrocarbon that has been studied both experimentally and theoretically. AQMD allowed to perform simulations reaching several nanoseconds, and thus the observation of reactions at pressures below 20 GPa. Importantly, these simulations unraveled the precursor reaction to polymerization: the formation of Diels-Alder dimers.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room4)

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

[○]Ivan Novoselov^{1,2}, Alexey Yanilkin¹ (1.Dukhov Research Institute of Automatics, Russia, 2.Moscow Institute of Physics and Technology, Russia)

TiH_x is of practical interest due to high volume concentration of hydrogen, and for many applications its diffusion properties should be established with confidence. We investigate the mechanisms of diffusion, and calculate corresponding rates in the framework of quantum molecular dynamics (QMD). However, time scales accessible to conventional QMD are very limited. It therefore can be employed only at very high temperatures, where no experimental data is available. In order to explore diffusion at lower temperatures, we accelerate QMD simulations via parallel replica dynamics algorithm (PRD). Application of PRD allows to reveal different mechanisms of hydrogen diffusion in TiH_x , and also makes it possible to perform direct comparison with experiment

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room4)

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

Invited

[○]Rao Huang¹, Li-Ta Lo², Arthur F. Voter², Danny Perez² (1.Xiamen University, China, 2.Los Alamos National Lab, United States of America)

Metallic nanoclusters are functional materials with many applications owing to their unique physical and chemical properties, which are sensitively controlled by their shapes and structures. An in-depth understanding of their morphology stability is therefore of crucial importance. It has been well documented by transmission electron microscopy (TEM) studies that metallic nanoclusters can interconvert between different isomers. However, the relevant mechanisms remain elusive because the timescales of such shape fluctuations are too short to be resolved experimentally and yet too long for conventional atomistic simulations. By employing a recently introduced Accelerated Molecular Dynamics method, Parallel Trajectory Splicing, we present simulations that reached timescales of milliseconds and thus provide a clear description of the dynamic process of the experimentally observed shape fluctuation in metallic nanoclusters. We observe transformations back and forth between face-centered-cubic (fcc) and structures with five-fold symmetry (decahedron or icosahedron). These transitions occur following either by a partial-dislocation-mediated twinning mechanism or by a surface-reconstruction driven process. The identified pathway is in remarkable agreement with the existing microscopy results and serves as further evidence that shape fluctuation can occur directly through thermal activation, without involving melting or other external factors.

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

[SY-N4] Symposium N-4

Chair: Laurent Karim Beland(Queen's University, Canada)

Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room4

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

○Kristopher Baker¹, William Curtin² (1.Knolls Atomic Power Laboratory, United States of America, 2.Swiss Federal Institute of Technology, Switzerland)

[SY-N4] Accelerated Quantum Molecular Dynamics

○Enrique Martinez Saez¹, Christian Negre², Romain Perriot², Danny Perez², Eduard Kober², Marc Cawkwell², Arthur F. Voter², Anders Niklasson² (1.Material Science and Technology Division, MST-8, Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America, 2.Theoretical Division, T-1, Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America)

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

○Sebastian Echeverri Restrepo¹, Anthony T Paxton² (1.Department of Metallic Materials & Ceramics, SKF, Netherlands, 2.Department of Physics, King's College London, UK)

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room4)

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

Invited

[○]Kristopher Baker¹, William Curtin² (1.Knolls Atomic Power Laboratory, United States of America, 2.Swiss Federal Institute of Technology, Switzerland)

In many problems of interest to materials scientists and engineers, the evolution of crystalline extended defects (dislocations, cracks, grain boundaries, interfaces, voids, precipitates) is controlled by the flow of point defects (interstitials/substitutional atoms and/or vacancies) through the crystal into the extended defect. Accurate modeling of this process requires atomistic methods in and around the extended defect, but the flow of point defects into and out of the extended defect region can be treated by coarse-grained methods. This talk presents a multiscale algorithm to provide this coupling, which was first documented in the manuscript "Multiscale diffusion method for simulations of long-time defect evolution with application to dislocation climb," published in 2016 in the *Journal of the Mechanics and Physics of Solids*, Number 92, pages 297-312. Specifically, direct accelerated molecular dynamics (AMD) of extended defect evolution is coupled to a diffusing point defect concentration field that captures the long spatial and temporal scales of point defect motion in the presence of the internal stress fields generated by the evolving extended defect. The algorithm is applied to study vacancy absorption into an edge dislocation in aluminum where vacancy accumulation in the core leads to nucleation of a double-jog that then operates as a sink for additional vacancies; this corresponds to the initial stages of dislocation climb modeled with explicit atomistic resolution. The method is general, so it can be applied to many other problems associated with nucleation, growth, and reactions due to accumulation of point defects in crystalline materials.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room4)

[SY-N4] Accelerated Quantum Molecular Dynamics

[○]Enrique Martinez Saez¹, Christian Negre², Romain Perriot², Danny Perez², Eduard Kober², Marc Cawkwell², Arthur F. Voter², Anders Niklasson² (1.Material Science and Technology Division, MST-8, Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America, 2.Theoretical Division, T-1, Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America)

The accurate study of the long-term evolution of rare events is extraordinarily challenging as computations are arduous and quantum-based molecular dynamics simulation times are limited to, at most, hundreds of ps. Here, the Extended Lagrangian Born-Oppenheimer molecular dynamics formalism is used in conjunction with Parallel Replica Dynamics to obtain an accurate tool to describe the long-term dynamics of reactive benzene. Langevin dynamics has been employed at different temperatures to calculate the first reaction times in a periodic benzene sample at different pressures. We have also studied the long-term behavior of vacancy complexes, which compare satisfactorily with experimental observations. Our coupled engine runs for times on the order of ns (two to three orders of magnitude longer than traditional techniques) and is capable of detecting reactions characterized by rates significantly lower than we could study before.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room4)

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

○Sebastian Echeverri Restrepo¹, Anthony T Paxton² (1.Department of Metallic Materials & Ceramics, SKF, Netherlands, 2.Department of Physics, King's College London, UK)

Although it is widely recognised that even small amounts of hydrogen (H) can cause embrittlement in iron (Fe) and in (high strength) steels, the fundamental mechanisms that cause it are not yet completely understood. To contribute to a better understanding of the fundamental behaviour of hydrogen in metals, in the present work we used parallel replica dynamics (PRD) to study the effect that different amounts of atomic H have in the diffusion of a single vacancy in body centred cubic (BCC) Fe. Using PRD we calculated, for the first time, the diffusion of hydrogen vacancy complexes at temperatures and time scales that are not reachable using classical methods. These calculations showed that the diffusivity of a vacancy-H complex is not only dependent of the migration barriers, but also that the addition of one H atom reduces the diffusivity of a vacancy in BCC Fe and the subsequent addition of more H atoms has the opposite effect.

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

[SY-O5] Symposium O-5

Chairs: Hitoshi Washizu(University of Hyogo, Japan), Sophie Loehle(TOTAL Marketing & Services, Solaize, France)

Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room5

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

○Michael Moseler^{1,2} (1.Fraunhofer Institute for Mechanics of Materials IWM, Germany, 2.University of Freiburg, Germany)

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

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

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

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

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

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

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room5)

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

Invited

○Michael Moseler^{1,2} (1.Fraunhofer Institute for Mechanics of Materials IWM, Germany, 2.University of Freiburg, Germany)

Ultralubricity and superlubricity has been observed for diamond and tetrahedral amorphous carbon (ta-C) coatings lubricated with water and unsaturated organic friction modifiers, respectively. Although spectroscopic characterization suggests that lubricity is connected to the formation of oxygen-containing surface layers, the underlying tribo-chemical mechanisms and the detailed structures of these layers remain elusive. This talk presents atomistic calculations on various scales that elucidate the mechano-chemical processes for the formation of oxygen functional groups and aromatic protective layers [1,2].

In the first part of this talk, quantum molecular dynamics calculations are presented that shed light on friction regimes for diamond lubricated by water and the different characteristic layers in the different regimes [1]. We find four universal friction regimes that are active on all low-index diamond surfaces: cold-welding&amorphisation, ether cold-welding without amorphisation, H/OH-termination, H/OH-termination with water layer coverage. In addition four special regimes are found: aromatic Pandey surface reconstruction for (111), ether/keto passivation for (110) and (001) as well as two mild cold-welding regimes for (110).

In the second part, combined experiments and multiscale simulations are presented that unveil the tribochemical mechanism leading to superlubricity of ta-C/ta-C tribopairs lubricated by unsaturated fatty acids [2]. Experiments show that superlow friction can be achieved by lubrication with unsaturated fatty acids. Atomistic simulations reveal that, due to the simultaneous presence of a carboxylic group and a C=C double bond, unsaturated fatty acids can concurrently chemisorb on both ta-C surfaces and bridge the tribogap. The resulting, sliding-induced mechanical strain triggers a cascade of molecular fragmentation reactions that release passivating hydroxyl, keto, hydrogen and olefinic groups to the ta-C surfaces. These findings provide design principles for novel organic friction modifiers that promote the formation of superlubricious amorphous carbon layers.

[1] T.Kuwahara, G.Moras, M.Moseler, **Phys. Rev. Lett.** 119 096101 (2017)

[2] T.Kuwahara, P.A.Romero, S.Makowski, V.Weihnacht, G.Moras, M.Moseler, under consideration (2018)

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room5)

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

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

Epoxy resin is commonly used as an adhesive for bonding metals. Recent industrial demands, e.g., light-weight multi-material cars and highly reliable pressure sensors, motivate researchers to improve the reliability and durability of bonded materials. One critical issue regarding adhesive bonding is the weakening of its bonding strength by the water that migrates from a moist environment along the interface. When bonding naturally surface-oxidized aluminum with epoxy resin, the adhesion strength reduces by about 40 % in a moist environment. Surface treatment techniques, such as sealing with polyvinyl chloride, only delay such adhesion weakening.

Despite the importance of this issue, adhesion weakening is not well understood. To understand the mechanisms at the electronic structure level, we perform atomic dynamics simulations on various Al and epoxy resin interface systems with water molecules inserted in the contact region. In accordance with experimental conditions, the Al layer is surface oxidized to a depth of 10 Å while the bisphenol-A type epoxy molecule has both OH and ether groups. Shear deformations are simulated using the hybrid quantum-classical method in which about 1,500 atoms at the contact region are treated with density-functional theory.

For the first time, calculated adhesion strengths compare well with the experimental values. Former simulations gave one order of magnitude larger adhesion strength than the experimental value. Three types of chemical reactions that affect the adhesion strength are found to occur depending on the terminal functional groups of the Al oxide surface and the water layer formation. Separate calculations confirm small barrier energies for all the reaction processes.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room5)

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

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

Relating to recent rapid advancement in substrate-decoration technique such as the one using the Self-Assembled Monolayers, there exist strong demands to predict the adhesion free energy between a complex liquid and polymer-grafted substrate. In principle, the adhesion free energy can be evaluated through the molecular simulation by integrating the work required to separate the liquid from the substrate. In former methods for the work of adhesion, a planar shape potential is introduced and the work of adhesion is calculated through integrating the force exerted on the potential from liquid molecules when liquid molecules are separated from the solid surface by gradually shifting the potential origin. These methods work well for sufficiently flat solid substrate. However, they are inefficient for a polymer-grafted substrate because it becomes necessary to shift the potential over a long distance.

Motivated by that, we propose a novel method to efficiently evaluate the work of adhesion of the interface between a liquid and a polymer-grafted surface. In the present method, a set of spherical potentials whose centers are set at the atomic positions of either polymer or substrate are introduced instead of a planar

potential. It enables efficient separation of the liquid molecules from the polymer-grafted substrate.

Moreover, potential-parameter update schemes are carefully chosen to suppress sharp variation in the force exerted on the potential and thereby to minimize the number of integration points.

The present method is applied to the interface between a water and a gold substrate on which poly(ethylene oxide)s (PEOs) are grafted. Then, we find that the work of adhesion tends to become large at the intermediate density of PEO. This tendency is related to the number of water molecules accessible to oxygen atoms in PEO.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room5)

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

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

In order to control energy losses in mechanical systems, the study of friction in lubricated contacts has to be approached. Depending on the operating conditions and its chemical nature, the confined fluid can exhibit a limiting shear stress at high pressure [1, 2]. The physical origins of this phenomenon and its implications to friction are currently not completely understood [3]. In this study, an extensive Molecular Dynamics analysis of the shearing behavior of different types of molecules is performed. The behavior of the confined sheared system is explored and compared to the fluid bulk state. One of the main conclusion is that flow profile results from two competing forces in the molecular system, which is linked to the weakest interfaces being sheared. Additionally, the saturated shear stress response is found to be related to the concept of atomic mobility. With increasing pressure, the relaxation time of the material is increased. Thus, atomic mobility can be saturated for a range of high pressures, diffusion would not be allowed, and a solid-like behavior is displayed. Finally, a link between flow and friction behavior is discussed.

[1] Martinie, L. and Vergne, P., “ Lubrication at extreme conditions: a discussion about the limiting shear stress concept” , Tribol. Lett., 63, 2016.

[2] Ewen, J. P., Gattinoni, C., Zhang, J., Heyes, D. M., Spikes, H. A. and Dini D., “ On the effect of confined fluid molecular structure on nonequilibrium phase behaviour and friction” , Phys. Chem. Chem. Phys., 2017.

[3] Ndiaye, S. N., Martinie, L., Philippon, D., Devaux, N. and Vergne, P., “ A Quantitative Friction-Based Approach of the Limiting Shear Stress Pressure and Temperature Dependence” , Tribol. Lett., 65, 2017.

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

[SY-O6] Symposium O-6

Chairs: Yoshitaka Umeno(The University of Tokyo, Japan), Yoshinori Shiihara(Toyota Technological Institute, Japan)

Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room5

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

○ Lucia Nicola^{1,2} (1.Delft University of Technology, Netherlands, 2.University of Padova, Italy)

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

○ Kerstin Falk¹, Konstantinos Gkagkas², Gianpietro Moras¹, Michael Moseler^{1,3} (1.Dept. of Tribology, Fraunhofer IWM, Freiburg, Germany, 2.Toyota Motor Europe, Technical Center, Zaventem, Belgium, 3.Dept. of Physics, University of Freiburg, Germany)

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

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

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

Rafael Pereira de Matos¹, Sophie Loehlé², Clotilde Minfray¹, ○Manuel Cobian¹ (1.LTDS ECL, Université de Lyon, France, 2.TOTAL Marketing & Services, Solaize, France)

 (Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room5)

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

Invited

○Lucia Nicola^{1,2} (1.Delft University of Technology, Netherlands, 2.University of Padova, Italy)

When rough bodies are pressed against each other, a small contact area has to support all the load. This is why plastic deformation occurs even at moderate nominal contact pressure. Although indentation of elastic bodies by self-affine rough indenters has been studied extensively, little attention has so far been devoted to plasticity. This is mostly because capturing plasticity as well as contact with a self-affine rough surface is computationally quite challenging. Here, we succeed in achieving this goal by using Green's function dislocation dynamics, a modeling technique that combines discrete dislocation plasticity (DDP) with Green's function molecular dynamics (GFMD). As usual in DDP, plasticity is studied by tracking the nucleation and glide of each dislocation in the metal crystal. The dislocation image fields are instead calculated with GFMD, which allows to describe the self-affine rough surface using wavelengths spanning from 5 nanometers to 100 micrometers.

Simulations are performed varying various parameters of the surface roughness, including the Hurst exponent and the root-mean-square height. Results show that the plastic response is size-dependent. An important implication of the size-dependence is that, when bodies deform plastically, it is not possible to scale observables such as contact pressure and contact area with crystal size or root-mean-square height, as typically done for elastic contact problems.

 (Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room5)

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

○Kerstin Falk¹, Konstantinos Gkagkas², Gianpietro Moras¹, Michael Moseler^{1,3} (1.Dept. of Tribology, Fraunhofer IWM, Freiburg, Germany, 2.Toyota Motor Europe, Technical Center, Zaventem, Belgium, 3.Dept. of Physics, University of Freiburg, Germany)

Liquid crystals (LC) - well-known for their application in LC-displays - have recently raised interest also for lubrication applications: favorable friction properties (specific friction of the order 0.005) have been experimentally observed in different systems [1]. The special behavior is attributed to the anisotropic viscosity and compressibility, which LC exhibit in semi-ordered phases (i.e. nematic or smectic phase). The LC molecules' elongated shape allows them to align with the shear, which could simultaneously reduce friction and increase load support. Moreover, the complex phase behavior and dynamic properties might also be exploited to design novel tribological systems with tunable or self-regulating friction, so-called 'smart' lubricants [2,3].

Here, we present a molecular dynamics simulations study of different LC lubricated model tribo-systems with the aim to characterize the LC rheological properties and investigate possible tuning mechanisms on a microscopic level. Shearing simulations of LC lubricating films with different structure characteristics, i.e. preferential molecule orientation, were performed for varying loads and shear rates. The response of the systems (velocity profiles, local viscosity and shear force) was evaluated and correlated to the fluid film

structure, which is influenced by the flow. Of particular interest are situations, where the inherent equilibrium structure of the LC film (induced by surface boundary conditions or external fields) is different from the shear direction, due to the competing forces for aligning the LC molecules in different directions.

[1] T. Amann, C. Dold and A. Kailer, *Tribology International* 65 (2013), p. 3

[2] C. Tadokoro, T. Nihira and K. Nakano, *Tribol Lett* 56 (2014), p. 239

[3] S. Itoh, Y. Imura, K. Fukuzawa and H. Zhang, *Langmuir* 31 (2015), p. 11360

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room5)

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

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

In solution, amphiphilic surfactants can form physisorbed boundary films on immersed surfaces. A film's structure and thereby its lubrication performance depend on numerous properties of all involved substances, such as the surface's potential, as well as surfactant and background electrolyte concentration. We investigate the dependency of the coefficient of friction on adsorption film topography in exemplary contact systems by means of classical all-atom molecular dynamics. For this purpose, the present study focuses on cationic CTAB at idealized aqueous solution-gold interfaces. Recent parametrizations of CTAB, originally intended for micelle modeling in bulk solution, are combined with representations of simple gold surfaces. The stability of differently shaped pre-assembled surface aggregates at various effective surfactant concentrations are compared against expected behavior as documented by abundant experimental contributions. We finally present friction tests in simple shear geometries of surfaces covered with pairwise identical CTAB film morphologies.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room5)

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

Rafael Pereira de Matos¹, Sophie Loehlé², Clotilde Minfray¹, [○]Manuel Cobian¹ (1.LTDS ECL, Université de Lyon, France, 2.TOTAL Marketing & Services, Solaize, France)

Amines molecules can be used as organic friction modifiers OFM in a lubricated contact working under in mixed/boundary regime.

Several experimental studies have been already done using steel against steel contact. Our aim is to propose

a computational simulation protocol to have a better understanding of what happens at atomic scale in the contact.

We study some physical properties (density, diffusivity) of amines

blended in Poly Alpha Olephin PAO using

molecular dynamics MD simulations employing the OPLS force field.

Green-Kubo formalism gives us access to diffusion coefficients of amines in the oil.

Then, we present ab-initio (DFT+U based) study of the adsorption of

this OFM on alpha-hematite Fe_2O_3 surface {01-12}.

The interactions between the amine molecule and the surface will be analysed and used to fit Lennard-Jones potential to model the interaction and open the way to new simulations using molecular dynamics.

We will conclude presenting simulations of the friction process applying stress and shear and computing a numerical coefficient of friction.

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

[SY-O7] Symposium O-7

Chairs: Lucia Nicola(Delft University of Technology, Netherlands), Shuji Ogata(Nagoya Institute of Technology, Japan)

Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5

[SY-O7] Toward Exascale Atomistic Simulations of Interfaces

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

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

○Yusuke Ootani¹, Jingxiang Xu¹, Naoki Takahashi¹, Koshi Adachi², Momoji Kubo¹ (1.Institute for Materials Research, Tohoku University, Japan, 2.Department of Mechanical Systems Engineering, Graduate School of Engineering, Tohoku University, Japan)

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

○Masahiro Saito¹, Jingxiang Xu¹, Yusuke Ootani¹, Nobuki Ozawa¹, Koshi Adachi², Momoji Kubo¹ (1.Institute for Materials Research, Tohoku Univ., Japan, 2.Graduate School of Engineering, Tohoku Univ., Japan)

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

○Gianpietro Moras¹, Andreas Klemenz¹, Thomas Reichenbach¹, Adrien Gola², Hiroshi Uetsuka³, Michael Moseler^{1,4}, Lars Pastewka^{1,5} (1.Fraunhofer Institute for Mechanics of Materials IWM, Germany, 2.Institute for Applied Materials, Karlsruhe Institute of Technology, Germany, 3.Asahi Diamond Industrial Co. Ltd., Japan, 4.Institute of Physics, University of Freiburg, Japan, 5.Department of Microsystems Engineering, University of Freiburg, Germany)

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

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

 (Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5)

[SY-O7] Toward Exascale Atomistic Simulations of Interfaces

Invited

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

Under the U.S. Department of Energy, Aurora/A21 early science program, our group will be one of the 10 initial users of the Nation's first exaflop/s computer that can perform 10^{18} mathematical operations per second, when it is introduced in 2021. To make quantum molecular dynamics (QMD) and reactive molecular dynamics (RMD) simulations exa-scalable, we have developed an extension of the divide-and-conquer algorithmic framework called divide-conquer-recombine. On today's supercomputing platform, for instance, the framework has achieved over 98% of the perfect speedup on 786,432 IBM Blue Gene/Q processors for 40 trillion electronic degrees-of-freedom QMD in the framework of density functional theory and 68 billion-atom RMD. Production simulations include (1) 16,616-atom QMD simulation of rapid hydrogen production from water using metallic alloy nanoparticles, (2) 6,400-atom nonadiabatic QMD simulation of photoexcitation dynamics for efficient solar cells, and (3) 112 million-atom RMD simulation of metacarbon synthesis by high temperature oxidation of SiC nanoparticles. We will discuss tribology and interfacial applications such as frictional heating of energetic molecular crystals.

 (Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5)

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

○Yusuke Ootani¹, Jingxiang Xu¹, Naoki Takahashi¹, Koshi Adachi², Momoji Kubo¹ (1.Institute for Materials Research, Tohoku University, Japan, 2.Department of Mechanical Systems Engineering, Graduate School of Engineering, Tohoku University, Japan)

It is known that silicon-based materials such as silicon carbide have low friction coefficients in water lubrication system. A tribofilm formed at a sliding interface is considered to reduce the friction coefficient, however detailed mechanism is still unclear because in-situ observation of the atomic scale sliding interface is difficult. Therefore, in this work, we investigated the structure, role and formation mechanism of the tribofilm of silicon-based materials by using molecular dynamics method. We performed sliding simulations of a SiO₂ substrate, which is a model of a native oxide layer of silicon-based materials, in water environment. We found that hydrolysis reaction of Si-O bond in SiO₂ surfaces occurred at contact areas of the surfaces as, $\text{Si-O} + \text{H}_2\text{O} \rightarrow \text{Si-OH} + \text{OH}$. The hydrolysis reaction was mediated by proton transfer process. Since the hydrolysis reaction dissociated Si-O bonds, Si-O bond network of the SiO₂ surfaces became sparse, and then, several SiO₂ clusters were removed from the surfaces as wear debris. The wear debris were dissolved in the water layer between two surfaces, forming a colloidal silica layer. On the other hand, the water molecules penetrated into the sparse SiO₂ surfaces and hydrate the surfaces, forming a hydrophilic silica gel layers on the SiO₂ surfaces. Therefore, at the sliding interface, the colloidal silica layer was sandwiched by two silica gel layers. The colloidal silica layer prevents the contact of the surfaces and reduces a friction force, whereas the hydrophilic silica gel layer holds the colloidal silica layer at the sliding interface. Thus, the colloidal silica and silica gel layer that formed by hydrolysis reaction reduces the friction coefficient of silicon-based materials in water lubrication systems.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5)

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

[○]Masahiro Saito¹, Jingxiang Xu¹, Yusuke Ootani¹, Nobuki Ozawa¹, Koshi Adachi², Momoji Kubo¹ (1.Institute for Materials Research, Tohoku Univ., Japan, 2.Graduate School of Engineering, Tohoku Univ., Japan)

Diamond-like carbon (DLC) has excellent friction properties such as low friction and high wear resistance. Thus, it is used as a solid lubricant material for engine parts. For this application, it is expected that DLC is used with the MoDTC friction modifier. When MoDTC is used as additives, a tribo-film of MoS₂ layers is formed at a sliding interface during friction, leading to low friction. It is known that frictional property of this system depends on many factors such as composition of additives, a structure of DLC, and so on. Thus, to improve the friction property, it is required to understand effects of these factors on friction behavior of the tribo-film. However, the friction behavior is unknown because *in situ* observation of the sliding interface is difficult. Thus, in order to investigate the friction behavior, we performed molecular dynamics simulation by using reactive force field, which takes into account the chemical reactions. In this study, we analyzed the influence of the defects in the MoS₂ layers on friction behavior of DLC by using a DLC/MoS₂ layers/DLC model. Here, we investigated the influence of the defects by comparing the friction behavior of the MoS₂ layers with and without grain boundaries. The friction simulation of the model without grain boundaries shows that the DLC/MoS₂ interface is the sliding interface. On the other hand, the simulation of the model with grain boundaries shows that the MoS₂/MoS₂ interface is the sliding interface since C-S bonds is formed between DLC and MoS₂ around grain boundaries. In addition, the MoS₂ layers with grain boundaries show higher friction force because the sliding between the MoS₂ layers is inhibited when a grain boundary attacks another grain boundary in neighboring layers. Then, we found that these friction behaviors caused by grain boundaries in the MoS₂ are major factors that increase friction force in this system. We will report the influence of other defects at the conference.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5)

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

[○]Gianpietro Moras¹, Andreas Klemenz¹, Thomas Reichenbach¹, Adrien Gola², Hiroshi Uetsuka³, Michael Moseler^{1,4}, Lars Pastewka^{1,5} (1.Fraunhofer Institute for Mechanics of Materials IWM, Germany, 2.Institute for Applied Materials, Karlsruhe Institute of Technology, Germany, 3.Asahi Diamond Industrial Co. Ltd., Japan, 4.Institute of Physics, University of Freiburg, Japan, 5.Department of Microsystems Engineering, University of Freiburg, Germany)

Silicon and diamond are brittle materials with the same crystal structure but opposite density change upon melting. Using molecular dynamics simulations, we show that both crystals can respond to shear deformation by undergoing mechanical amorphization. The resulting amorphous material has liquid-like structure, is denser than the crystal in silicon and less dense than the crystal in diamond. As a result, as normal pressure

increases, amorphization, which is often related to nanoscale wear, is enhanced in silicon but suppressed in diamond. Moreover, shear-induced amorphization of silicon yields a high-density, ductile amorphous material at pressures much lower than the polyamorphic transition (~ 14 GPa) observed upon hydrostatic compression. These results are potentially relevant for the friction properties of other crystals that densify upon melting and show polymorphism, like germanium and ice.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room5)

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

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

Simulations of materials and structures submitted to wear, machining, forming, forging, and impacts, to name but a few, often involve large deformations, damage, and failure. These phenomena are challenges for usual computational tools such as finite element modeling. When large deformations occur, finite element methods have limitations due to the need to remesh which is computationally expensive and sometimes fails.

Therefore, mesh-free methods such as Smooth Particle Hydrodynamics (SPH) are more suitable for these applications.

The use of SPH for the simulations of wear, tribology, and impacts problems in solids has recently gained momentum as large deformations and instability phenomena such as damage and fracture could be easily handled. However, little work exists on the implementation of damage in SPH. This is thought to be due to the approximation problems around surfaces. As damage and fracture develops in solids, this creates new surfaces around which the SPH approximation breaks down.

In this presentation, we present the results of simulations of wear response to show case a new implementation of damage in SPH that solves some of the problems due to the approximation break-downs close to surfaces. This implementation is built as an upgrade of the SPH package for solids available within LAMMPS called Smooth Mach Dynamics.

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

[SY-O8] Symposium O-8

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

Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room5

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

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

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

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

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

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

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

○Eiji Tomiyama^{1,2}, Takeshi Iwasaki³, Hitoshi Washizu² (1.Research Organization for Information Science and Technology, Japan, 2.Graduate School of Simulation Studies, Univ. of Hyogo, Japan, 3.Lubricants Research Laboratory, Idemitsu Kosan Co., Ltd., Japan)

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room5)

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

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

Intensive studies have been dedicated to the problem of boundary lubrication in recent years. Experimental studies have demonstrated a significant reduction in friction coefficients of steel that has nanostructured surfaces. It is conjectured that nanostructured metals have a large density of sites with strong attraction to lubricant molecules, resulting in reduced friction. The detailed mechanism of the phenomenon however remains unclear.

To reveal the mechanism of lubrication between metal surfaces, atomic- or molecular-level investigations are required for the effect of metal-molecule interaction on boundary lubrication. Coarse-grained molecular dynamics (CGMD) is a useful and efficient simulation method to tackle such problems. Indeed, a CGMD study of shear flow of lubricant molecules between metal surfaces showed that the more molecules were adsorbed on the surfaces, the lower the friction coefficient became. Nevertheless, molecular-level mechanisms are not fully understood regarding the experimentally presented effect of the surface nanostructure on the friction coefficient or the nature of structural ordering in shear flow.

In this study, we performed CGMD simulations with the aim to reveal the molecular-level friction mechanism in boundary lubrication between nanostructured steel surfaces. As lubricant molecules, polyethylene (nonpolar) and fatty acid (polar) were modeled by the coarse-grained method representing methylene (CH₂) and carboxyl (COOH) groups by individual particles. The effect of the surface nanostructure was mimicked by distributing atoms producing stronger attraction with the molecular groups. The effect of alignment of the strong potentials on the friction coefficient is apparent in the case of polar molecules. In both polar and nonpolar lubricants, the nanostructure enhances critical shear stress for separation of adsorbed lubricants from the surface. These results suggest salient influence of the surface nanostructure on the friction coefficient.

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room5)

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

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

As a low friction material, polymer brush has attracted attention in many areas because of its good frictional properties and biological compatibility. The frictional properties of polymer brush are improved by different chain topologies. However, the effects of the chain topologies on the wear of polymer brush are still not clear. To reduce the wear of the polymer brush, it is required to understand the wear behaviors and mechanism of different topological polymer brush. However, in-situ observation of the sliding interface at the molecular scale is difficult. Thus, we investigated the wear mechanism of polymer brush with different topological chain by using coarse-grained molecular dynamics (CGMD) method.

We perform friction simulations of linear polymer brush, cyclic polymer brush where the polymer chains have

cyclic structure, and crosslinked polymer brush where the polymer chains are connected with the neighboring polymer chain with crosslinker to understand the effect of chain topologies on the wear. We found that cyclic polymer brush and crosslinked polymer brush had smaller number of dissociation than linear polymer brush because the cyclic polymer brush and crosslinked polymer brush showed smaller frictional forces than that of linear polymer brush. We found that the cyclic polymer brush and crosslinked polymer brush had less interpenetrating beads than that of linear polymer brush. Therefore, the cyclic polymer brush and crosslinked polymer brush have smaller entanglements, leading to the low frictional force. We conclude that chain topologies of polymer brush can improve the wear resistance because they suppress the interpenetration at the sliding interface.

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room5)

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

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

In recent years, concentrated polymer brush (CPB), which is constructed by grafting polymer chains onto a substrate with high density, has been developed. CPB has attracted much attention for application to low friction materials as artificial joints because of its high wear resistance and biocompatibility. However, the graft of polymer chains onto substrate is complicated and takes much cost. As an alternative method analogous to CPB, bottlebrush polymer (BBP) known as macromolecules with polymeric side chains is candidate for low friction materials. Previous studies have revealed that BBPs with a cationic anchor block adsorbed on a negatively charged surface swell, which produces low friction force. However, the detail of friction mechanism of BBP is not clear. Furthermore, the effects of sliding speed and side chain length on friction properties are also unknown because the in-situ observation of the sliding interface is difficult. Thus, computational simulation is required. Herein, to reveal the mechanism during friction of BBP consisting of a cationic anchor block, we developed a coarse-grained molecular dynamics code which can consider chemical specificity of each monomer, and performed friction simulation in water solvent. The low friction coefficient was observed at the low load, but friction coefficient was increased at high load. We found that, at low load, water beads which coordinate to the side chain of BBP suppressed contact between BBPs on the counter surfaces, because side chains of BBP prefer to interact with the water beads. This swelling state of BBP facilitates shear between the opposite substrates. With high load, water beads were removed from the sliding interface, which reduces the number of water beads around BBP. Therefore, the contact between BBPs on a counter surface leads to high friction coefficient. The effects of side chain length and sliding speed on the friction properties will be discussed on the day.

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room5)

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

○Eiji Tomiyama^{1,2}, Takeshi Iwasaki³, Hitoshi Washizu² (1.Research Organization for Information Science and Technology, Japan, 2.Graduate School of Simulation Studies, Univ. of Hyogo, Japan, 3.Lubricants Research Laboratory, Idemitsu Kosan Co., Ltd., Japan)

Traction drive is a mechanism that transmits power by a rotor and lubricating oil. In order to evaluate the characteristics of the fluid molecules in the traction drive, we construct a simulation method to apply shear to the fluid confined between solids using LAMMPS, a molecular dynamics simulator.

In this simulation, conditions are set as follows. The boundary condition of the system is a periodic boundary condition in the horizontal direction. Fluid is composed of a single hydrocarbon compound and the number of atoms is about ten thousand. The solids are a model metal surface imitating (100) plane of α -iron, and their atomic motion is frozen. The force field parameter of fluid molecules uses the Dreiding force field. Apply a pressure of 0.8 GPa to 1.24 GPa in the direction perpendicular to the solid atoms. Furthermore, a constant slip of relative sliding speed 1 m/s to 50 m/s is applied. Then, the simulation time on the order of nanoseconds is passed and the steady state is set. With the above setting, an ensemble of constant pressure / constant shear state is created.

The temperature dependency of the coefficient of traction is evaluated by changing the temperature of the fluid from -20 °C to 140 °C. The coefficient of traction also change with the change of temperature, and the tendency is at least qualitatively consistent with the experimental values.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A5] Symposium A-5

Chair: Sinisa Dj Mesarovic(Washington State University, United States of America)

Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room6

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

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

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

○Dominik Steinberger¹, Shyamal Roy¹, Dan Mordehai², Stefan Sandfeld¹ (1.Chair of Micromechanical Materials Modelling, TU Bergakademie Freiberg, Germany, 2.Department of Mechanical Engineering, Technion - Israel Institute of Technology, Israel)

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

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

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room6)

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

Invited

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

An essential part of the development of theory and simulations of microstructure evolution is the parameters used as input as well as the output, which should be comparable to experimental observations. An overview of the experimentally observed dislocation boundary evolution in metals of medium to high stacking fault energy are presented with emphasis on such parameters. In particular, the spatial distribution of boundaries in terms of boundary planes, spacings and misorientation angles are considered as a function of crystallographic grain orientation, deformation mode and strain. Based on the experimental observations relations to crystal plasticity and the Burgers vectors available for boundary formation are discussed.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room6)

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

○Dominik Steinberger¹, Shyamal Roy¹, Dan Mordehai², Stefan Sandfeld¹ (1.Chair of Micromechanical Materials Modelling, TU Bergakademie Freiberg, Germany, 2.Department of Mechanical Engineering, Technion - Israel Institute of Technology, Israel)

In general, data mining is the process of discovering patterns in large data sets, with the most common tasks being, anomaly detection, association rule learning, clustering, classification, regression and summarization. Within materials science, the most popular application so far is materials discovery, one of the goals of the well-known Materials Genome Initiative (<https://www.mgi.gov>).

In order to understand the convoluted interactions of dislocations that define the mechanical properties of metals to a large degree, a lot of data has been and is being generated, be it via experiments or simulations. Due to the complexity of the dislocation microstructure and its discrete nature aforementioned algorithms can not be applied ad-hoc. Thus, developing methods that enable their use are highly desirable.

In this presentation we want to outline the key aspects of the data mining framework for dislocation microstructures that we are currently developing. Among others, we will show examples of how quantitative comparisons of dislocation data—be it from experimental or computational methods—can be done. Aforementioned framework will be applied to a dataset consisting of hundreds of realizations of a numerical indentation experiment realized with discrete dislocation dynamics. Rate coefficient beneath the indenter will be extracted for the dislocation densities commonly found in continuous dislocation dynamics models. The resulting microstructures will be analyzed for common patterns and their correlation with the initially emerging structure to enable predicting the characteristics of the final state from the first initial steps.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room6)

[SY-A5] Lattice continua for polycrystal grains: Climb and glide of

dislocations, diffusion and grain boundary kinematics.

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

At high temperatures, the interior of each grain in a polycrystal suffers: (1) dislocation glide, (2) climb, and (3) diffusion of vacancies. Grain boundaries undergo: (4) growth/disappearance, as a result of vacancy diffusion, and, (5) crystallographic reorientation/mismatch, as a result of dislocations arriving to the boundaries either by glide or by climb. All the above deformation mechanisms are naturally described in the lattice continuum framework, whereby the lattice represents the material. Climbing edge dislocations are lattice sink/source which must be reflected in the continuity equation and the transport theorem. The interacting kinematics of dislocation glide and climb requires dual definition of crystallographic slip fields: the true slip and the apparent slip. The transport theorem for grains with lattice growing or disappearing lattice at different grain boundary faces results in the direct formulation of the boundary condition for vacancy diffusion flux in terms of the boundary velocity (different from the lattice velocity). The field equations for each grain are derived by means of the principle of virtual power. Additional boundary conditions result from the relative motion of the adjacent crystal faces: Change of tilt and twist angle and surface elastic mismatch are derived from the geometry of dislocations arriving to the boundary. The resulting polycrystal initial/boundary value problem consists of elasticity-plasticity-diffusion field equations in each crystalline domain with moving boundaries, coupled through the boundary conditions.

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Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A6] Symposium A-6

Chair: Emma Griffiths (University of Cape Town, South Africa)

Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room 6

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

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

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

○ Emma Griffiths¹, Jana Wilmers², Swantje Bargmann², BD Reddy¹ (1. University of Cape Town, South Africa, 2. University of Wuppertal, Germany)

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

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

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

○ Roland PELLENQ¹, Pierre-Louis Valdenaire¹, Christophe Bichara³, Franz Ulm¹, Jean-Marc Leyssale

² (1. <MSE>2, MIT- CNRS - AMU, United States of America, 2. ISM, CNRS - Bordeaux U., France, 3. CINaM, CNRS - Aix-Marseille U., France)

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room6)

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

Invited

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

The hierarchical self-assembly of triblock terpolymers in solution is a successful bottom-up methodology for constructing functional patchy nanoparticles with prescribed topology and shape. Currently, the design of such nanoparticles requires an iterative process to identify the experimental phase parameters needed to produce any target pattern. The broad use of this technology is therefore cumbersome and limited by an incomplete understanding of the mechanisms underlying patch transition. A detailed understanding of how thermodynamics and kinetics influence the topology of the assemblies is also missing. In this work, we present a set of rules for programming desired shapes of the nanoparticles and predicting the pathways by which they assemble. We investigate systematically the interplay between entropic and enthalpic parameters governing the self-assembly of ABC triblock copolymers in a selective solvent for the C block. We use a computational modeling at the mesoscale and thereby encompass the length and time scales associated with the motion and assembly of the polymer coils, while accurately approximating the chemically driven interactions. The phase diagram predicted by our model is consistent with experimentally identified characteristic nanoparticle shapes. We find that the effective volume fraction of the soluble block determines the size of a particle and the distribution of its patches via steric interactions. Moreover, we find that the relative fraction of the patch-forming block and its affinity with the core of a articles dictates the number and shape of its patches. As a major outcome, we construct a morphologically-based library of nanoparticles. That library can be used to hierarchically design mesoscale aggregates with specific morphologies. Our results provide insight regarding the mechanisms that determine nanometer scale objects in synthetic and naturally occurring systems.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room6)

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

○Emma Griffiths¹, Jana Wilmers², Swantje Bargmann², BD Reddy¹ (1.University of Cape Town, South Africa, 2.University of Wuppertal, Germany)

An important benefit of electroactive polymers is their large strain response due to certain stimuli such as an electric current. However, for sufficient mechanical use in electrochemical systems, they lack the necessary strength and stiffness. Metals on the other hand have sufficient strength and stiffness but are unable to function as piezoelectric materials [1]. By creating a metal-polymer composite, however, a stronger material with large strain capacity is created that can withstand larger actuation forces. Specifically, using polymer impregnated nanoporous structures, with their exceptional mechanical properties providing a reinforcing base [2,3], creates a composite material with superior actuator properties by having both sufficient strength and strain capabilities.

This work presents the chemoelectromechanical response of a gold-polymer nanocomposite model. A representative volume element is modelled using a linear version of the chemoelectromechanical theory developed by Wilmers et al. [4] and is implemented through a staggered explicit-implicit finite element

simulation in ABAQUS. Additionally the theory is enhanced by introducing an implicit solvent model to capture the effects of the crowding of ions due to saturation within the material. The micromechanical response of the composite is explored under an imposed electric field and thus providing information to be used in the optimization of microstructures for sensory and actuation applications.

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(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room6)

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

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

When it comes to talk about alternatives to non-renewable sources of energy, photovoltaics is one of the most promising choices for converting solar light into electricity with the use of solar cells. At present, there is wide variety of solar cell devices on the market and this variety will continue to grow because of the race for better conversion efficiency and the final product sustainability. Within recent years, the seemingly clear boundaries between photovoltaics of inorganic and organic solar cells have started to fade by the advent of metal-halide hybrid organic-inorganic perovskites (OIP). They are very promising candidates for future photovoltaic applications because they have wide-direct band gap, which can be tuned by either changing the organic cation, the metal atom, or the halide. Their power conversion efficiency now reached over 22%. At the same time, the level of our understanding of the origin of such performance is still insufficient. We believe that thin film morphology is a key factor determining the performance of bulk heterojunction organic solar cells, because of its influence on charge separation, charge transport and recombination losses in donor-acceptor blends. With this respect, we present both descriptive and predictive multiscale modeling of electronic and structural properties of blends of PCBM or hybrid OIP of the type $\text{CH}_3\text{NH}_3\text{PbX}_3$ ($\text{X}=\text{Cl}, \text{Br}, \text{I}$) with P3HT, P3BT or squaraine SQ2 dye sensitizer, including adsorption on TiO_2 clusters. Here, the multiscale nature of modeling means that in a set of simple hierarchical approaches we combine different methods for different scales (quantum mechanical, microscopic, mesoscopic) interpreted independently and that the information obtained at one level is transmitted to the next level as a required input. If necessary, new information is sometime transmitted back to the previous level for a feedback control. As the result, we arrive at a very reliable methodology that allows computing the microscopic structure of blends on the nanometer scale and getting insight on miscibility of its components at various thermodynamic conditions. The calculated nanoscale morphologies serve as an instrument in rational design of hybrid OIP. They are used in collaboration with experts who actually make prototypes or devices for practical applications.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room6)

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

[○]Roland PELLENQ¹, Pierre-Louis Valdenaire¹, Christophe Bichara³, Franz Ulm¹, Jean-Marc Leyssale²

(1.<MSE>2, MIT- CNRS - AMU, United States of America, 2.ISM, CNRS - Bordeaux U., France, 3.CINaM, CNRS - Aix-Marseille U., France)

The process by which organic matter decomposes deep underground to form petroleum and its underlying kerogen matrix has so far remained a no man's land to theoreticians, largely because of the geological (Millions of years) timescale associated with the process. Using a replica exchange accelerated molecular dynamics method initially developed in the context of the micro- to milli-second timescale for protein folding, we simulate the full transformation of cellulose and lignin (the main components of wood) into kerogen under prevailing geological conditions. We observe in sequence (i) the fragmentation of the cellulose crystal and production of water, (ii) the development of an aliphatic macromolecular phase, (iii) its aromatization, and (iv) its aggregation into a stiff porous aromatic carbon upon expulsion of the fluid phase. The composition of the solid residue along the maturation pathway strictly follows what is observed for natural type III kerogens and for artificially matured samples under closed conditions, providing further evidence of a kinetically controlled, irreversible, decomposition process in which the aliphatic (immature) phase is a metastable intermediate.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A7] Symposium A-7

Chair: Michael Zaiser (FAU University of Erlangen-Nuremberg, Germany)

Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room 6

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

○ Thomas Hochrainer (TU Graz, Austria)

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

○ Katrin Schulz¹, Markus Sudmanns¹, Kolja Zoller¹, Peter Gumbsch^{1,2} (1. Karlsruhe Institute of Technology, Germany, 2. Fraunhofer Institute for Mechanics of Materials, Germany)

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

○ Michael Zaiser, Ronghai Wu (FAU University of Erlangen-Nuremberg, Germany)

[SY-A7] 2D continuum theory of dislocations

○ Istvan Groma (Eotvos Lorand University, Hungary)

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

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

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6)

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

Invited

○Thomas Hochrainer (TU Graz, Austria)

During the last two decades, dislocation research saw a revival driven by new experimental techniques for small scale testing, high resolution characterization and the rise of large scale discrete dislocation simulations. This also stimulated intensive research in mesoscale theories of dislocations. Great advances were achieved on continuum models of dislocation interactions for strongly simplified straight-dislocation systems and continuum dislocation dynamics of single slip deformation. However, a transfer of the employed averaging methods to fully three-dimensional multiple slip deformation remains a challenge for various reasons.

In the current talk we shall highlight some challenges appearing on different levels of continuum dislocation modelling. At the most fundamental level it is yet unclear what continuum measures are suited for characterizing 3D networks of dislocations. The alignment tensors successfully used for dislocation distributions in single slip seem to be of limited value in networks consisting mostly of junctions and reaction products. It is likewise an open question how to describe the kinematics of dislocation networks, where reactions and junction formation or break-up imply permanent changes in the topology of the network and the characteristics of dislocations. Closely related is the challenge of capturing the averaged energetics, kinematics and dissipation of these dislocation interactions.

To overcome the named challenges possibly requires new mathematical tools or at least the adoption of concepts from other areas of physics and mathematics which were not yet (fully) exploited in dislocation theory. We shall discuss several ideas where we might find new impulses and promising tools for further successes in developing a mesoscale theory of dislocations. Expected key areas include discrete and differential topology, gradient flows, rough energy landscapes, and temporal and spatial statistics.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6)

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

○Katrin Schulz¹, Markus Sudmanns¹, Kolja Zoller¹, Peter Gumbsch^{1,2} (1.Karlsruhe Institute of Technology, Germany, 2.Fraunhofer Institute for Mechanics of Materials, Germany)

The striving for advanced materials with well-defined microstructures has led to an increasing effort towards a physically based description of the motion of dislocations as the cause of plastic deformation. Several dislocation based continuum theories have been introduced, but only recently rigorous techniques have been developed for performing meaningful averages over systems of moving, curved dislocations, yielding evolution equations for a dislocation density tensor, see [1].

Regarding a self-consistent coarsening of dislocation modeling in order to construct an efficient numerical implementation, several issues have to be solved including calculation of the stress field of a system of dislocations, representation of dislocation interactions and reactions as well as boundary conditions. Accurate solutions have been found for one and two dimensional systems [2, 3]. However, the analysis and

understanding of dislocation networks in three dimensions involves additional challenges such as the representation of dislocation multiplication.

In this presentation, we discuss the implications of a homogenization of dislocation interactions and reactions in the discrete-continuum transition regime. Based on the analysis of 3d discrete dislocation structures, we present a coarse-grained continuum formulation for dislocation multiplication due to cross-slip and glissile reaction events. The formulation is validated by the comparison with discrete dislocation dynamics simulations and discussed in the context of a continuum limit as lower application limit of a continuum approach.

[1]Hochrainer, T.; Sandfeld, S.; Zaiser, M.; Gumbsch, P.: Continuum dislocation dynamics: Towards a physical theory of crystal plasticity. *J. Mechan. Phys. Solids*. 63 (2014), p. 167-178.

[2] Schmitt, S., Gumbsch, P., Schulz, K.: Internal Stresses in a Homogenized Representation of Dislocation Microstructures. *J. Mechan. Phys. Solids*, 84 (2015), p. 528-544.

[3] Schulz, K., Sudmanns, M., Gumbsch, P.: Dislocation-Density based Description of the Deformation of a Composite Material. *Modell. Simul. Mater. Sci. Eng.*, 25 (2017), 064003.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6)

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

○Michael Zaiser, Ronghai Wu (FAU University of Erlangen-Nuremberg, Germany)

We analyze the stability of transport equations which describe dislocation dynamics in terms of fluxes of dislocation densities defined on scales above the dislocation spacing. We demonstrate that such transport equations exhibit a generic instability which emerges as soon as a dislocation flux function, which in the simplest case is identical with the shear strain rate on a given slip system, has a negative derivative with respect to the flowing dislocation density. The criterion for instability is equivalent to the condition that the stress required to sustain plastic flow at a given rate is an increasing function of dislocation density. We conclude that dislocation patterning of some kind is an almost trivial, and practically unavoidable, consequence of dislocation transport in conjunction with work hardening. Implications for the theory and interpretation of different types of dislocation patterns, and for density-based simulations of plastic flow in general, are discussed.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6)

[SY-A7] 2D continuum theory of dislocations

○Istvan Groma (Eotvos Lorand University, Hungary)

During the past 20 years, by a systematic course graining of the equation of motion of straight parallel edge dislocations a 2D continuum theory of dislocation has been developed. It is able to account for many important feature of the collective properties of dislocations, like size effect, hardening due to precipitates, dislocation density distribution next to boundaries, and dislocation patterning. The predictions of the theory

are directly compared to discrete dislocation dynamics simulations.

In spite of the success of the theory there are several open issues need to be addressed for further developing the current theory. In the talk the problems "blocking" the extension of the theory are discussed:

1. Do we need a continuum theory?
2. Why still in 2D? What we can learn from it?
3. Should we coarse grain the equations of motion of the dislocations or the energy of the discrete system to derive the continuum theory?
3. Numerical determination of the dislocation dislocation correlation function. Problems related to the the finite size effect observed.
4. What to do next to boundaries?
5. Phase field approach. Issues related to the nontrivial mobility function one has to introduce.
6. Slow, power law relaxation of the dislocation system.
7. How to incorporate stochastic effects.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room6)

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

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

Many dislocation dynamics simulation models were developed to understand plastic deformation of metals most of which are based on small deformation kinematics. In this talk, I will present a density-based dislocation dynamics model within the framework of finite deformation of crystals, focusing on crystal mechanics and the dislocation transport equations at finite deformation. The geometric coupling and non-linearity of the dislocation transport on various slip systems will be explained. The relevant crystal mechanics, thermodynamics, and constitutive closure questions will also be discussed. Collaboration: Giacomo Po, University of California-Los Angeles; Grethe Winther, Technical University of Denmark.

[SY-A8] Symposium A-8

Chair: Thomas Hochrainer(TU Graz, Austria)

Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room6

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

○Eleni Katifori¹, Desislava Todorova¹, Octavio Albarran², Lucas Goehring² (1.University of Pennsylvania, United States of America, 2.Max Planck Institute, Germany)

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

○Ryuichiro Oguma¹, Long-Qing Chen², Syo Matsumura³ (1.Fukuoka Univ., Japan, 2.The Pennsylvania State Univ., United States of America, 3.Kyushu Univ., Japan)

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

○Inge Bellemans¹, Nico Vervliet², Lieven De Lathauwer^{2,3}, Nele Moelans⁴, Kim Verbeken¹
(1.Department of Materials, Textiles and Chemical Engineering, Ghent University, Belgium, 2.Department of Electrical Engineering, KU Leuven, Belgium, 3.Group Science, Engineering and Technology, KU Leuven - Kulak, Belgium, 4.Department of Materials Engineering, KU Leuven, Belgium)

[SY-A8] A Sharp Phase Field Method

○Alphonse FINEL¹, Yasunori YAMADA², Yann LE BOUAR¹, Benoît DABAS¹, Benoît APPOLAIRE¹, Tetsuo MOHRI² (1.Laboratoire d'Etude des Microstructures, CNRS, ONERA, France, 2.Institute for Materials Research, Tohoku University, Japan)

 (Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room6)

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

Invited

[○]Eleni Katifori¹, Desislava Todorova¹, Octavio Albarran², Lucas Goehring² (1.University of Pennsylvania, United States of America, 2.Max Planck Institute, Germany)

Pattern formation in thin elastic shells has attracted increasing interest in both fundamental studies and practical applications. Examples include biological systems and engineering applications, such as the fabrication of flexible microelectronics. In this talk we explore the mechanical instabilities of an intrinsically curved thin shell deposited on a liquid surface. Here, the pattern formation is not a direct result of externally imposed strain, but is due to the geometric incompatibility between a curved, stiff membrane and an (initially flat) liquid substrate. We observe several types of instabilities, including a wrinkle-to-fold transition from periodic sinusoidal solutions to morphologies that combine sinusoidal wrinkles and folds; a transition from dimples (geometric inversions) to periodic sinusoidal solutions; and a transition from flat bands with zero Gaussian curvature, to dimpled periodic patterns. We show that the wrinkling patterns can be described via an effective theory of liquid crystalline smectics at intermediate length scales. This insight allows better understanding of the wrinkling patterns seen in such systems, with which we explain pattern breaking into domains, the properties of domain walls and wrinkle undulation. We compare our predictions with numerical simulations and experimental observations. We investigate how the global geometry of the curved shells and their elastic properties control the transitions between the various morphologies. Last, we discuss various new strategies for creating and controlling patterns in thin elastic shells with natural curvature.

 (Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room6)

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

[○]Ryuichiro Oguma¹, Long-Qing Chen², Syo Matsumura³ (1.Fukuoka Univ., Japan, 2.The Pennsylvania State Univ., United States of America, 3.Kyushu Univ., Japan)

Domain structures consisting of multiple off-phase variants are generally formed in ordering process in binary alloy systems. The $L1_0$ type order is formed in AB type alloys on the basis of an *fcc* lattice. The crystal structure is tetragonal. Therefore three orientational variants can be formed depending on which of $\langle 100 \rangle$ directions corresponds to c-axis and two translational variants are possible for each of them; six distinct crystallographic variants exist in this type of order. The present authors previously developed a phase-field formulation for ordering process of $L1_0$ type in binary alloys, taking into account the symmetry of the crystal structure. In the $L1_0$ structure the *fcc* lattice is divided into four simple cubic sublattices. The atomic occupation probabilities on the sublattices are represented by three independent order parameters and a composition parameter. If the state of order of atomic arrangement is represented by a point in the three dimensional Euclidean space spanned by the three order parameters, the six equivalent variants are defined by the six tips of a regular octahedron centered on the origin for the disordered state. A mean-field free energy is defined in a form of Landau type expansion with the order parameters and the composition parameter. In this presentation we further consider the effect of the lattice distortion. An elastic energy is introduced with eigen strains according to Khachatrian's method. The interface energy automatically reflects the direction of c-axis and satisfies symmetries of cubic, tetragonal and orthorhombic structures. Kinetic equations for time-evolution of the order parameters and the concentration are derived from the Ginzburg-

Landau type thermodynamical potential. Formation of domain structures was simulated by treating the kinetic equations numerically in a three-dimensional cell scheme. The microstructures obtained are compared with experimental results of TEM observation.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room6)

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

[○]Inge Bellemans¹, Nico Vervliet², Lieven De Lathauwer^{2,3}, Nele Moelans⁴, Kim Verbeken¹ (1.Department of Materials, Textiles and Chemical Engineering, Ghent University, Belgium, 2.Department of Electrical Engineering, KU Leuven, Belgium, 3.Group Science, Engineering and Technology, KU Leuven - Kulak, Belgium, 4.Department of Materials Engineering, KU Leuven, Belgium)

An important focus in creating more realistic phase field models is the incorporation of the thermodynamic driving forces in multicomponent multiphase-field models by coupling to thermodynamic databases. This coupling, which aims at retrieving Gibbs energies and chemical potentials, becomes increasingly intricate as the number of components/chemical elements in the system increases. This is caused by the fact that the number of elements in a tensor increases exponentially with the number of dimensions, and so do the computational and memory requirements. The exponential dependency (and the problems that are caused by it) is called the curse of dimensionality.

Alternatives need to be investigated for the storage and handling of the thermodynamic data required for the phase field simulations. A possible solution for this might be the use of a canonical polyadic decomposition on the tensors containing the thermodynamic data. In this way, the huge tensors are approximated well by compact multilinear models or decompositions. Tensor decompositions are more versatile tools than the linear models resulting from traditional matrix approaches.

This solution promises to be suitable for this challenge and has been applied to a quaternary and quinary metal-oxide system in a multicomponent multiphase-field model which incorporates faceted and dendritic growth and can also treat the boundaries as an open boundary where the melt is locally in equilibrium with the atmosphere at a certain partial oxygen pressure. The results and improvements in computational requirements are compared for various methods to couple to a thermodynamic database.

(Wed. Oct 31, 2018 4:00 PM - 5:30 PM Room6)

[SY-A8] A Sharp Phase Field Method

Invited

[○]Alphonse FINEL¹, Yasunori YAMADA², Yann LE BOUAR¹, Benoît DABAS¹, Benoît APPOLAIRE¹, Tetsuo MOHRI² (1.Laboratoire d'Etude des Microstructures, CNRS, ONERA, France, 2.Institute for Materials Research, Tohoku University, Japan)

Phase field modelling offers an extremely general framework to predict microstructural evolutions in complex systems. However, its computational implementation requires a discretisation scheme with a grid spacing

small enough to preserve the diffuse character of the theory. We present a new formulation in which the interfaces are resolved with essentially one grid point with no pinning on the grid and an accurate rotational invariance, allowing to multiply the accessible linear dimensions by an order of magnitude or, conversely, to reduce the computational time by almost three orders of magnitude. We show that this Sharp Phase Field Method (S-PFM) reproduces interfacial kinetic properties with a very high accuracy. Then, we apply the model to a situation where conserved and non-conserved fields are coupled. Finally, to couple S-PFM to elastic fields, we propose a new elastic solver that efficiently treats strong elastic heterogeneities and that is mathematically stable.

[SY-I5] Symposium I-5

Chairs: Stephen M Foiles(Sandia National Laboratories, United States of America), Mitra L Taheri(Drexel University, United States of America)

Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room7

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

○Nicolas Combe^{1,2}, Frederic Momprou¹, Marc Legros¹ (1.CEMES Toulouse, France, 2.Univ. Toulouse, UPS, France)

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

○Chaozhen Wei^{1,2}, Luchan Zhang⁵, Yang Xiang², Jian Han⁴, Spencer Thomas⁴, kongtao Chen⁴, David J. Srolovitz^{3,1} (1.HKUST Jockey Club Institute for Advanced Study, Hong Kong University of Science and Technology, Hong Kong, 2.Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong, 3.Materials Science and Engineering, Mechanical Engineering and Applied Mechanics, Computer and Information Science, University of Pennsylvania, United States of America, 4.Materials Science and Engineering, University of Pennsylvania, United States of America, 5.Department of Mathematics, National University of Singapore, Singapore)

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

○Bob Svendsen^{1,2}, Jaber Rezaei Mianroodi², Juan Li³, Christoph Kirchlechner³, Gerhard Dehm³ (1.Material Mechanics, RWTH Aachen University, Germany, 2.Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Germany, 3.Structure and Nano-/Micromechanics of Materials, Max-Planck-Institut für Eisenforschung GmbH, Germany)

 (Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room7)

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

Invited

○Nicolas Combe^{1,2}, Frederic Momprou¹, Marc Legros¹ (1.CEMES Toulouse, France, 2.Univ. Toulouse, UPS, France)

In specific conditions, grain boundary (GB) migration occurs in polycrystalline materials as an alternative vector of plasticity compared to the usual dislocation activity. The shear-coupled GB migration, the expected most efficient GB based mechanism, couples the GB motion to an applied shear stress. The migration of the GB occurs through the nucleation and motion of disconnections.

We report a detailed theoretical study of the elementary mechanisms occurring during heterogeneous disconnections nucleation. Using molecular simulations, the absorption of a $\frac{1}{2}[110]$ edge bulk dislocation in a symmetric $\Sigma(17)(410)[001]$ tilt GB generates an immobile disconnection in the GB. We show that the shearing of this GB induces its migration and reveals a new GB migration mechanism through the nucleation of a mobile disconnection from the immobile one. Energy barriers and yield stress for the GB migrations are evaluated and compared to the migration of a perfect GB. As expected, the migration of imperfect GB is easier than the one of perfect GB. An immobile disconnection in a BG can thus operate as a source of disconnections driving the GB migration.

 (Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room7)

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

○Chaozhen Wei^{1,2}, Luchan Zhang⁵, Yang Xiang², Jian Han⁴, Spencer Thomas⁴, kongtao Chen⁴, David J. Srolovitz^{3,1} (1.HKUST Jockey Club Institute for Advanced Study, Hong Kong University of Science and Technology, Hong Kong, 2.Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong, 3.Materials Science and Engineering, Mechanical Engineering and Applied Mechanics, Computer and Information Science, University of Pennsylvania, United States of America, 4.Materials Science and Engineering, University of Pennsylvania, United States of America, 5.Department of Mathematics, National University of Singapore, Singapore)

We propose a novel approach to simulate the evolution of polycrystalline microstructures based upon a disconnection model for grain boundary (GB) kinetics. The model incorporates surface tension, applied stress, and jumps in chemical potential across GBs. The model also includes disconnection nucleation and mobility. Disconnections are line defects that lie solely with GB and are characterized by both a Burgers vector and a step height, as set by the GB bicrystallography. We first derive a continuum equation of motion for individual GBs and then for GB triple junctions (TJ) within a polycrystalline microstructure that rigorously accounts for conservation of disconnection Burgers vectors and step heights and couples the GBs meeting at the TJ. We then implement this model in a continuum simulation of GB dynamics without TJs, with TJs and in a polycrystalline microstructure. The resultant simulations provide clear demonstrations of the importance of including a crystallography-respecting microscopic model of microstructure evolution and the intrinsic coupling between stress, capillarity, and microstructure connectivity in microstructure evolution.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room7)

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

Invited

○Bob Svendsen^{1,2}, Jaber Rezaei Mianroodi², Juan Li³, Christoph Kirchlechner³, Gerhard Dehm³ (1.Material Mechanics, RWTH Aachen University, Germany, 2.Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Germany, 3.Structure and Nano-/Micromechanics of Materials, Max-Planck-Institut für Eisenforschung GmbH, Germany)

In the current work, mechanisms for dislocation-mediated motion of and deformation at coherent boundaries in fcc materials is investigated along with the resulting mechanical behavior.

On the modeling side, molecular dynamics (MD) simulations are carried out on bulk single and bi-crystal Cu, the latter containing two $\Sigma 3(111)$ boundaries. These are subject to loading conditions varying between shear loading parallel to the boundaries and perpendicular uniaxial loading. In the case of pure shear loading, MD results demonstrate that $\langle 112 \rangle$ shearing on $\Sigma 3(111)$ results in monotonic flow depending on the shear sign, whereas $\langle 110 \rangle$ shearing leads to oscillatory flow. As it turns out, this difference in behavior can be related to corresponding changes in the coincidence site lattice (CSL). In particular, in the case of $\langle 112 \rangle$ shearing, new potential boundary positions in the CSL occur every three atomic layers. Depending on the shear sign, however, one of these positions is closer to the current boundary position than the other. Since less energy is required for the boundary to shift to the closer position, the boundary moves to this position. In contrast, $\langle 110 \rangle$ shearing results in new potential boundary positions in the CSL having the same distance to the current boundary. Consequently, none of these is favored energetically, resulting in oscillatory motion of the boundary between these.

On the experimental side, nano-indentation experiments with 2μm sized spherical indenter tips are used to study the impact of coherent $\Sigma 3(111)$ boundaries on the yield strength distribution in copper. The indents are performed either inside a grain or close to a coherent $\Sigma 3(111)$ boundary aligned normal to the sample surface. The force-displacement curves show elastic loading following Hertz's predictions until a sudden displacement burst - a "pop-in" - is observed. The maximum shear stress beneath the indenter tip at the pop-in force is interpreted as yield stress. The statistical behavior of the yield stress is analyzed via cumulative probability (CP) plots. The CP plots show a significantly lower average yield stress at the boundary with respect to the single grains and an extremely narrow distribution at the boundary. The later finding suggests that the mechanism responsible for dislocation source activation is omnipresent at the boundaries.

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

[SY-I6] Symposium I-6

Chairs: Garritt Tucker(Colorado School of Mines, United States of America), Chuang Deng(University of Manitoba, Canada)

Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room7

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

○Sherri Hadian¹, Blazej Grabowski¹, Mike W Finnis², Jörg Neugebauer¹ (1.Max-Planck-Institut fuer Eisenforschung, Germany, 2.Imperial College London, UK)

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

○Shuyang Dai¹, Yang Xiang², David Joseph Srolovitz³ (1.Wuhan University, China, 2.Hong Kong University of Science and Technology, Hong Kong, 3.University of Pennsylvania, United States of America)

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

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

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room7)

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

Invited

[○]Sherri Hadian¹, Blazej Grabowski¹, Mike W Finnis², Jörg Neugebauer¹ (1.Max-Planck-Institut fuer Eisenforschung, Germany, 2.Imperial College London, UK)

We report molecular dynamics simulations and their analysis for grain boundaries vicinal to the Sigma 7 symmetric tilt boundary of the type {1 2 3} in aluminium. When minimized in energy at 0K a grain boundary of this type exhibits nano-facets that contain kinks. We observe that at higher temperatures of migration simulations, given extended annealing times, it is energetically favorable for these nano-facets to coalesce into a large terrace-facet structure. Therefore we initiate the simulations from such a structure and study as a function of applied driving force and temperature how the boundary migrates. We find the migration of a faceted boundary can be described in terms of the flow of steps. The migration is dominated at lower driving force by the collective motion of the steps incorporated in the facet, and at higher driving forces by the step detachment from the terrace-facet junction and propagation of steps across the terraces. The velocity of steps on terraces is faster than their velocity when incorporated in the facet, and very much faster than the velocity of the facet profile itself, which is almost stationary. A simple kinetic Monte Carlo model matches the broad kinematic features revealed by the molecular dynamics. Since the mechanisms seem likely to be very general on kinked grain boundary planes, the step flow description is a promising approach to more quantitative modeling of general grain boundaries.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room7)

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

[○]Shuyang Dai¹, Yang Xiang², David Joseph Srolovitz³ (1.Wuhan University, China, 2.Hong Kong University of Science and Technology, Hong Kong, 3.University of Pennsylvania, United States of America)

We present a multiscale model to describe the structure and the energetics for various grain boundaries. The model incorporates both the anisotropy elasticity in each grain and the first-principle calculation informed interaction between two grains across the grain boundary, i.e., the generalized stacking-fault energy based upon the disregistry. The force balance between these two contributions determines the structure. We apply this approach to determine the structure and energetics of several twist grain boundaries and tilt grain boundaries in FCC metals such as Cu, Al and Ni.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room7)

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

Invited

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

It is now widely accepted that stress plays important roles on the kinetics of grain boundaries. Past studies on grain boundary kinetics by atomistic simulation mainly focused on those under shear deformation by recognizing that shear coupling is one of the most fundamental modes of grain boundary motion. However, grain boundaries in polycrystalline materials under realistic loading conditions rarely experience pure shear deformation and stresses with both shear and normal components are more common. In this work, we used molecular dynamics simulations to investigate (1) how normal stress would influence the ground state structures of a few types of special CSL grain boundaries and (2) how such structural change would further influence the modes and energy barrier for migration in those grain boundaries.

We found that while both constant and cyclic normal stresses can facilitate the transition in grain boundary structure among its metastable states, the influences of tension and compression are not the same and vary among different types of grain boundaries. It is also found that the macroscopic strain caused in the materials due to the structural transformation in grain boundaries under cyclic stress can be well described by Coble creep, which implies a possible new mechanism of Coble creep that has been overlooked before. Furthermore, the grain boundary structural transformation can either lower or raise the energy barrier for grain boundary migration depending on the grain boundary type, which can be explained by the relative easiness of atomic shuffling in each grain boundary based on their DSC lattice.

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

[SY-I7] Symposium I-7

Chairs: Nicolas Combe(CEMES Toulouse, France), Brandon Runnels(University of Colorado Colorado Springs, United States of America)

Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room7

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

○Chris P Race (University of Manchester, UK)

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

○Ali Al-Hadi I. Kobaissy¹, Georges Ayoub², Mu'Tasem Shehadeh¹ (1.Department of Mechanical Engineering, American University of Beirut, Lebanon, 2.Department of Industrial and Manufacturing Systems Engineering, University of Michigan-Dearborn, United States of America)

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

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

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

○Saryu Fensin¹, Timothy Frolov² (1.Los Alamos National Lab, United States of America, 2.Lawrence Livermore National Laboratory, United States of America)

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room7)

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

Invited

○Chris P Race (University of Manchester, UK)

A critical process in the development of a desirable microstructure in polycrystalline metals is that of recrystallisation, in which new grains of defect-free material nucleate and grow within the defect-laden microstructure of deformed material.

Thus, recrystallisation involves the creation and migration of grain boundaries between pristine and highly defective crystal. The structure and properties of these grain boundaries will be strongly affected by the plastic deformation in the defective grain. Furthermore, the driving force for their migration will be the elimination of the deformation defects. This force will be larger in magnitude and different in character to the driving forces present in other cases of grain boundary migration, such as grain growth. Grain boundary properties under these conditions have, however, received comparatively little attention.

Here we present insights from atomistic models of grain boundaries between cold-worked and defect-free grains which begin to uncover trends in their static and dynamic properties under conditions of recrystallisation.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room7)

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

○Ali Al-Hadi I. Kobaissy¹, Georges Ayoub², Mu'Tasem Shehadeh¹ (1.Department of Mechanical Engineering, American University of Beirut, Lebanon, 2.Department of Industrial and Manufacturing Systems Engineering, University of Michigan-Dearborn, United States of America)

In this work, the mechanical response as well as the microstructural features of face-centered cubic (fcc) metals subjected to severe plastic deformation (SPD) are investigated. A multi-scale framework that couples crystal plasticity (CP) scheme with continuum dislocation dynamics (CDD) model is proposed to mimic the loading conditions during Equal Channel Angular Pressing (ECAP) processes. Several aspects of the deformation process have been considered including texture evolution, the evolution of statistically stored dislocations (SSDs) and geometrically necessary dislocations (GNDs), and the fragmentation of the grains and its effect on the overall mechanical response. The framework is applied to a reference volume element (RVE) in which the grains are distributed and assigned a position. Within the model, each grain is allowed to split into 1024 new smaller grains which subsequently lead to strain hardening and grain refinement. The latter is modeled by accounting for the grain-grain interaction, for which the concept of the GNDs is incorporated into the mean free path of the dislocations. GNDs are assumed to be induced by grain boundaries that restrict the free deformation of a grain and result in an increase of stresses leading to the grain size reduction. The grain refinement procedure is triggered when the misorientation threshold between subgrains is exceeded. The calibration of the model parameters is performed using torsion test of pure copper material. The simulations results of generated texture and grain size reduction are in very good agreement with experimental data available in the literature.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room7)

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

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

Stress-assisted grain boundary motion is a prominent phenomenon in crystalline materials. On the other hand, crack/voids are common features in physical materials, thus the interaction of a moving grain boundary mediated by stress with such features are important to study the microstructural evolution of crystalline materials under severe plastic deformation. In this work three major behaviors are studied using atomistic simulations when a stress-mediated moving grain boundary interacts with crack, i.e., crack healing, crack propagation and sub-grain formation. The underlying macromechanism is described using atomistic configurations for each case and the effect of loading type, i.e., monotonic or cyclic is described. It is shown that metastable phases are the main reason for crack heal-ability of grain boundaries. The effect of material type which is in terms of stacking fault energy is also explored.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room7)

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

Invited

○Saryu Fensin¹, Timothy Frolov² (1.Los Alamos National Lab, United States of America, 2.Lawrence Livermore National Laboratory, United States of America)

Grain boundaries (GBs) can play an important role in governing the mechanical behavior and damage evolution of a material during both quasistatic and dynamic loading. However, the general consensus of the shock physics community has been that minute details about the GB structure should not affect the response of a material to dynamic loading. In this paper, we present results of molecular-dynamics simulations investigating whether or not small changes in boundary structure are 'recognized' by the shock wave and can in turn affect the spall strength of a material. As a test case, we will study grain boundaries in both Copper and Tungsten with similar orientation relationships but varying local structures. Specifically, we propose to use grand-canonically optimized structures for grain boundaries that retain their ordered structure even at elevated temperatures.

[SY-I8] Symposium I-8

Chair: Srikanth Patala(North Carolina State University, United States of America)

Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room7

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

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

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

○Alexandre Dimanov¹, Jean Raphanel¹, Michel Bornert², Eva Héripé³, Mathieu Bourcier¹, Ababacar Gaye², Alexandre El Sabbagh¹, Wolfgang Ludwig⁴, Andrew King⁵ (1.LMS, CNRS-UMR7649, Ecole Polytechnique, France, 2.Laboratoire Navier, CNRS-UMR8205, Ecole des Ponts, France, 3.MSSMAT, CNRS-UMR8579, Centrale-Supélec, France, 4.MATEIS, UMR5510, INSA-Lyon, France, 5.SOLEIL Synchrotron, Beam line Psiché, France)

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

○Nikhil Chandra Admal¹, Javier Segurado^{2,1}, Jaime Marian¹ (1.University of California Los Angeles, United States of America, 2.IMDEA, Spain)

 (Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room7)

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

Invited

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

Engineering interest in nanocrystalline (NC) materials has been founded on the potential to improve mechanical properties such as increased strength/hardness, while scientific interest stems from the alternative fundamental mechanisms that are operative. Compared to their coarser-grained counterparts, the influence of interfaces (i.e., grain boundaries (GB)) becomes more significant in NC materials. Current simulation techniques for understanding NC mechanics rely on non-physical microstructures, first-order grain boundary descriptors that poorly capture the complexity of interfacial structure-property relationships, and a lack of quantitative approaches that can accurately capture the specific contribution of different deformation mechanisms. In this study, we propose utilizing higher-order GB descriptors to improve interfacial understanding, while determining polycrystalline behavior through networks connecting bulk and boundary behaviors. We perform atomistic modeling (e.g., Molecular Dynamics) studies of both favored CSL and general high-angle GBs for analyzing empirical and structural descriptors from atomic-scale behavior at the interfaces. These descriptors then aid in our GB network modeling to understand larger-scale polycrystalline behavior by unraveling the complexity surrounding the competition/cooperation between different deformation mechanisms. The importance of choosing physically-based atomistic microstructures and proper equilibration techniques in such simulations are also discussed. Finally, by utilizing continuum-based kinematic metrics, which can resolve the individual contribution of various deformation mechanisms such as GB and dislocation-mediated deformation to the total strain in the material, we help to further unravel the complex microstructural deformation behavior in NC metals.

 (Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room7)

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

 ○Alexandre Dimanov¹, Jean Raphanel¹, Michel Bornert², Eva Héripré³, Mathieu Bourcier¹, Ababacar Gaye², Alexandre El Sabbagh¹, Wolfgang Ludwig⁴, Andrew King⁵ (1.LMS, CNRS-UMR7649, Ecole Polytechnique, France, 2.Laboratoire Navier, CNRS-UMR8205, Ecole des Ponts, France, 3.MSSMAT, CNRS-UMR8579, Centrale-Supélec, France, 4.MATEIS, UMR5510, INSA-Lyon, France, 5.SOLEIL Synchrotron, Beam line Psiché, France)

Viscoplastic deformation of polycrystalline materials conditions many aspects of our everyday life from industrial hot forming of metallic items and durability of engineered structures, to glacier flow or plate tectonics powered by convection of Earth's mantle rocks. Usually, polycrystalline viscoplastic deformation is largely based on crystal slip plasticity (CSP). However, grain boundary sliding (GBS) may become a dominant mechanism at high temperatures, small grain sizes and low strain rates. Both mechanisms are often considered to act in parallel and to contribute independently to the global behaviour. We considered different classes of polycrystalline materials, such as Silicates, NaCl and Aluminium, combining high temperature rheological investigations and micromechanical testing with *in situ* SEM multi-scale

observations. In the latter case, we performed full field strain measurements, based on digital image correlation (DIC). For NaCl we could perform micromechanical tests *in situ* synchrotron X-ray microtomography and obtain both 2D and 3D strain fields. We show that for all of the considered materials CSP and GBS are not independent, but co-operative. Depending on microstructure and loading conditions, each one may be either the dominant strain cumulative mechanism, or a secondary mechanism, allowing for accommodation of the local strain incompatibilities related to the previous one. Both are necessary to ensure macroscopically homogeneous flow. We show examples of minor but crucial contribution of GBS to ductile localization phenomena and strain propagation throughout the microstructure.

(Wed. Oct 31, 2018 4:00 PM - 5:00 PM Room7)

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

○Nikhil Chandra Admal¹, Javier Segurado^{2,1}, Jaime Marian¹ (1.University of California Los Angeles, United States of America, 2.IMDEA, Spain)

At high temperatures, grain boundaries are not static entities but can migrate in response to thermo-mechanical forces brought about by temperature, external stresses, and internal microstructure. This gives rise to a wide array of dynamic behavior, including recovery, recrystallization, grain growth, etc.

In this talk, we present a recently developed three-dimensional polycrystal plasticity model driven by a single energy functional that captures both grain boundary (GB) energy and bulk elastic energy in response to plastic deformation. The model represents any arbitrary grain boundary using geometrically necessary dislocations (GNDs), and the GB energy is constructed as a function of the GNDs. Moreover, in contrast to previous phase-field approaches for grain boundary evolution, our model's energy functional is described on the entire five-dimensional grain boundary space allowing the consideration of both misorientation and inclination in the grain boundary energy.

The model is parameterized using grain boundary energy data from atomistic simulations, after which it is used to simulate the microstructure evolution of polycrystalline samples. The framework is used first to simulate the recrystallization process in a three dimensional polycrystal without external loads. Finally, the deformation of polycrystals under external loads is simulated for a few selected cases.

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

[SY-G1] Symposium G-1

Chairs: Byeongchan Lee(KyungHee Univ., Korea), Keonwook Kang(Yonsei University, Korea)

Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room8

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

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

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

○Hyunggyu Lee¹, Byeongchan Lee², Keonwook Kang¹ (1.yonsei university, Korea, 2.kyung hee university, Korea)

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

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

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

○Jean-Michel Scherer^{1,2}, Samuel Forest², Jacques Besson², Benoit Tanguy¹, Jérémy Hure¹
(1.DEN-Service d'Etudes des Matériaux Irradiés, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette cedex, France, France, 2.MINES ParisTech, PSL-Research University, Centre des matériaux, CNRS UMR 7633, 63-65 rue Henri Auguste DesbruèresBP 87 91003 Evry Cedex, France, France)

 (Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room8)

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

Invited

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

Molecular dynamics (MD) calculation is an important computational method for materials science and engineering. To obtain meaningful results from MD simulations for harsh environments, one has to prepare a quality potential model that works appropriately not only in equilibrium states but also in non-equilibrium states. We have recently developed a systematic method to construct (i) two-body potentials [T. Oda, W.J. Weber, H. Tanigawa, *Comp. Mater. Sci.* 111 (2016) 53] and (ii) embedded-atom method (EAM) potentials [T. Oda, submitted]. In this method, potential functions are expanded with cosine/sine series in reference to energies, forces and stresses evaluated by first-principles calculations. In the present study, using this method, we aim to construct potential models of a metal (bcc-Fe) and a metal oxide (Li_2O) for radiation environments. For this aim, results of first-principles molecular dynamics calculations of several atomic collision events are included in the reference data. MD simulation results with the constructed potential models show a reasonable agreement with available experimental data on fundamental material properties and threshold displacement energies. It is indicated that the method can effectively construct a potential model for MD simulations of harsh environments.

 (Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room8)

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

○Hyunggyu Lee¹, Byeongchan Lee², Keonwook Kang¹ (1.yonsei university, Korea, 2.kyung hee university, Korea)

Tungsten is widely used as a facing material, because it has a high thermal conductivity and low sputtering yield. However, under the neutron irradiation, pure tungsten transmutes into the Re and Os. This causes degradation of material properties due to the formation of defect clusters, such as precipitates, that caused by irradiation. Therefore, it is important to understand the formation mechanism of defect clusters for preventing the degradation of material properties. In this study, for knowing the formation mechanism of defect clusters, we conducted irradiation simulation of bulk W-Re alloy using molecular dynamics simulation. To describe the neutron irradiation, we choose the certain atom that is hit by neutron, which is called PKA (Primary Knock-on Atom) and shot the PKA with certain kinetic energy. We analyze the defects formation of bulk system as changing the initial energy of PKA.

Acknowledgement

This research was supported by Nuclear Fusion Research Program through the National Research Foundation of Korea(NRF) (2017M1A7A1A01016221)

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room8)

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

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

W has been considered as a potential core element for plasma facing material of fusion reactors for ITER thanks to its outstanding high-temperature properties. However, studies so far on W and W-based binary alloys show precipitation and defect clustering under neutron irradiation. In this talk, we report the first principles calculations of the defect energetics in ternary W alloys. W-Ta-Re systems are chosen for extensive calculations on interstitial defect structures around solute atoms.

Overall, as in pure W or W binary alloys such as W-Re, the most preferable defect type is found to be the bridge interstitial, followed by $\langle 111 \rangle$ interstitials. With negative solute-solute binding energy, Ta and Re atoms prefer to make a solute pair in the system and the solute pair strongly attracts W self-interstitial atom, forming a solute-interstitial complex. The binding between a Ta-Re solute pair and a W self-interstitial atom can be stronger in this ternary alloy than in binary systems, and plays a role in slowing down the W interstitial diffusion as a primary dissociation barrier. The defect energetics in the alloys can be understood as the combined results of both strain-relief effect and electronic effect, but the former, which is related with atomic size of elements and local pressure felt by each atom in lattice, seems dominant.

To summarize, the defect complexes in W-Ta-Re alloys are expected to trap W self-interstitial atoms, preventing self-interstitial atoms from escaping to the surface or grain boundary. The reduction in the number of disappearing self-interstitial atoms increases the odds for Frenkel defects to annihilate, reducing residual void concentration and hence void formation. It is also expected that, at elevated temperature, the rise in configuration entropy increases the interaction energy between solute pair and self-interstitial atom, and hence further slows interstitial migration.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room8)

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

○Jean-Michel Scherer^{1,2}, Samuel Forest², Jacques Besson², Benoit Tanguy¹, Jérémy Hure¹ (1.DEN-Service d'Etudes des Matériaux Irradiés, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette cedex, France, France, 2.MINES ParisTech, PSL-Research University, Centre des matériaux, CNRS UMR 7633, 63-65 rue Henri Auguste Desbruères BP 87 91003 Evry Cedex, France, France)

Stainless steels are widely used as structural materials for nuclear core internals. Due to their proximity with the nuclear fuel, these materials are subjected to high level of irradiation doses. In the last decades, irradiation effects on structural materials' mechanical properties have been heavily investigated in order to ensure structures' reliability over nuclear plant lifetime. Irradiation induced defects - such as Frank dislocation loops and nanocavities - can lead to significant mechanical properties changes, as for example a significant hardening due to pinning of dislocations on defects. Under mechanical loading, gliding dislocations may incorporate sessile defects lying in their gliding plane, leaving behind a reduced defect density path. These zones, typically bands or channels of 10-100 nm width, being therefore softened by the "defects cleaning", may localize strain and lead to highly heterogeneous deformation at the grain scale. This process is called dislocation channelling. A peculiar fracture mode called channel fracture is observed in

austenitic stainless steels irradiated at high temperature to high doses, leading to transgranular facets on fracture surfaces. It has been hypothesized [1] that channel fracture is due to nanovoids coalescence in dislocation channels. Channel fracture is therefore assessed numerically in this study using a strain gradient crystal plasticity model that has been developed in order to take into account irradiation defect densities in the hardening/softening behaviour of the material and that has been implemented in a Finite Element solver [2]. Such model allows to regularize strain localization, and is used to model dislocation channelling. Single crystal porous unit-cells are subjected to simple shear, and the effect of void sizes and dislocation channels widths are systematically investigated. Numerical results are finally used to assess the hypothesis proposed in [1] regarding channel fracture in irradiated stainless steels.

[1] Margolin B. et al. (2016) The radiation swelling effect on fracture properties and fracture mechanisms of irradiated austenitic steels. *Journal of Nuclear Materials*

[2] Ling C. et al. (2017) Void growth and coalescence in triaxial stress fields in irradiated fcc single crystals. *Journal of Nuclear Materials*

[SY-G2] Symposium G-2

Chairs: Seunghwa Ryu(Korea Advanced Institute of Science and Technology, Korea), Keonwook Kang(Yonsei University, Korea)

Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8

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

○Han Henri ZHAO¹, Bing Hou² (1.Ecole Normale Paris-Saclay, France, 2.School of aeronautics, NWPU, , China)

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

○Janghyuk Moon¹, Kyeongjae Cho², Maenghyo Cho³ (1.School of Energy System Engineering, Chung-Ang Univ., Korea, 2.Department of Materials Science and Engineering, University of Texas at Dallas, United States of America, 3.School of Mechanical &Aerospace Engineering, Seoul National University, Korea)

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

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

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

○Hussein M Zbib¹, Mehdi Hamid¹, Rahul Panat², Sadeq Saleh² (1.Washington State university, United States of America, 2.Carnegie Mellon University, United States of America)

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

○Mihkel Veske¹, Andreas Kyritsakis¹, Kyrre Ness Sjobak², Vahur Zadin³, Flyura Djurabekova¹ (1.Helsinki Institute of Physics, University of Helsinki, Finland, 2.Department of Physics, University of Oslo, Norway, 3.Institute of Technology, University of Tartu, Estonia)

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8)

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

○Han Henri ZHAO¹, Bing Hou² (1.Ecole Normale Paris-Saclay, France, 2.School of aeronautics, NWPU, , China)

Aluminum honeycombs are widely used as sandwich cores in the protective component in transport industry. For example, they are involved in the bird strike shielding as well as in the crashworthiness design, etc. Under impact loading, testing results showed a significant enhancement of the out-of-plane crushing strength of honeycombs with respect to the quasi-static case, which cannot be explained by the rate sensitivity of aluminum alloy.

This paper firstly presents the quasi-static and impact testing results for a series of aluminium honeycombs of different cell sizes (3003 and 5052 alloys). A significantly different strength enhancement of 3003 honeycombs is found from the 5052 ones. In order to understand and model this strength enhancement, a comprehensive numerical investigation with rate insensitive constitutive laws is performed to reproduce the experimental results for different cell size/wall thickness/base materials. In fact, due to the lateral inertia effect under impact buckling, larger strain under impact loading than quasi-static case in the element nears intersectional line is observed. Different ratios of the strain hardening stress over the yield stress of the 3003 alloy from the 5052 alloy lead to the different honeycomb strength enhancements. Finally, aluminum 5052 and 3003 honeycombs are studied under combined shear-compression loading. It was focused on the interaction between the additional shear loading and the lateral inertia effect under the impact loading. It was found that the expansion of the crush envelopes from the quasi-static loading to the dynamic loading was almost homogeneous for the two honeycombs.

Hou B., Zhao H., Pattofatto S., Liu J.G., Li Y.L., 2012, Inertia effects on the progressive crushing of aluminium honeycombs under impact loading, *Int. J. Solids & Struct.*, 49 (19-20), 2754-2762.

Hou B., Pattofatto S., Li Y. L., Zhao H., 2011, Impact behavior of honeycombs under combined shear-compression, Part II Analysis, *Int. J. Solids & Struct.* 48, 698-705

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8)

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

○Janghyuk Moon¹, Kyeongjae Cho², Maenghyo Cho³ (1.School of Energy System Engineering, Chung-Ang Univ., Korea, 2.Department of Materials Science and Engineering, University of Texas at Dallas, United States of America, 3.School of Mechanical & Aerospace Engineering, Seoul National University, Korea)

The mechanical issues on high capacity electrode materials, such as silicon, tin, and silicon oxide, prevents their usage for lithium ion batteries. So, the oxides (i.e. silicon dioxide) are the prevalent materials used for a high-expected capacity and strong mechanical stability during cycles. Although tremendous efforts have devoted to the study of the electro-chemo-mechanical behaviors of high-capacity electrode materials, the mechanical behavior of amorphous SiO₂ during electro-chemical reaction remains largely unknown. Here we

systematically investigate the inelastic stress evolution, the electronic structure and the mechanical deformation of lithiated silicon dioxide through first-principles computation and finite element method. The structural and thermodynamics analysis was performed to predict electrochemistry characteristics Si and Si-O system. The mechanical strength and brittle behavior of SiO₂ due to strong Si-O bonds are also compared with Si. Although both Si and SiO₂ experience mechanical softening during lithiation, the clearly distinguishable relaxation kinetic of SiO₂ inducing deviatoric inelastic strains due to mechanical constraints is found by density functional theory calculation. These results would provide fundamental perspectives on the chemo-mechanical behavior of silicon and silicon oxide electrode for the practical use.

ACKNOWLEDGMENT

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(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8)

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

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

Coatings suffer dramatic deterioration and premature damage in the deep-sea environment, in sharp contrast to the good protective performance in typical marine environments. Hydrostatic pressure (HP), which varies with ocean depth, has pronounced impact on coating performance when compared with other factors, such as oxygen level and pH value. The idea that loss of wet adhesion is the first step towards coating failure seems to be raising some controversy, with some researchers suggesting that the loss of adhesion results from the pressure relief process in the experiment rather than from hydrostatic pressure itself. AHP decreased the protective properties of coatings more rapidly than HP via a “push-and-pull” effect, which promotes bubbles formation at the interface between coatings and base metal.

Compared to other simulation methods, the finite element method (FEM) is capable of providing a multi-physical field to solve complex engineering problems more effectively. The interface is most susceptible to corrosion and the coating failure can be affirmed when the corrosion products are visible on there.

In this study, we attempt to develop a model of the growth of a bubble and the change of the stress distribution at the coating/substrate interface under AHP by means of FEM. The results show that the impacts of alternating hydrostatic pressure and hydrostatic pressure on the interface were compared with a precondition of bubbles inducing the coating failure.

1. Hydrostatic pressure cannot mechanically destroy the coating/metal interface because it acts as a compressive stress on the dry bubbles. If the bubbles turn into wet, the pressure loaded on the bubble will disappear.
2. Alternating hydrostatic pressure can provide tensile stress on the wet bubbles during every immersion period, so it accelerates disbonding of the coating.

3. The maximum stress on the bottom of wet bubbles is able to be minimized to less than the stable adhesion value if the lag time is large enough. In this case, alternating hydrostatic pressure cannot accelerate disbonding any more. The lag time will be different if the period of alternating pressure is changed. Thus, the lag time of a coating should be considered when it is designed to serve under alternating hydrostatic pressure.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8)

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

○Hussein M Zbib¹, Mehdi Hamid¹, Rahul Panat², Sadeq Saleh² (1.Washington State university, United States of America, 2.Carnegie Mellon University, United States of America)

Designing high energy-efficiency structural materials with superior mechanical properties is a key challenge for scientists and engineer. Among these properties, strength versus mass density and strength versus ductility are amongst the most important factors that affect component design, and thus structure weight. Ideal structural materials are the ones that may retain high strength with low mass density and excellent ductility. However, current state-of-the-art materials have a drastic tradeoff between these properties. In this work, a multiscale modeling approach is developed and used to design a new class of high-strength-ductility material system. It is shown that by integrating the effects of nanoparticle, nanolaminate and gradient structure on strength and ductility, it is possible to design and manufacture 3D-architected lightweight metamaterial systems. The system is made of interconnected microscale metallic ligaments reinforced by nanolaminate metallic layers and have superior mechanical properties (strength-density, strength-ductility) compared to their bulk counterparts.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room8)

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

○Mihkel Veske¹, Andreas Kyritsakis¹, Kyrre Ness Sjobak², Vahur Zadin³, Flyura Djurabekova¹ (1.Helsinki Institute of Physics, University of Helsinki, Finland, 2.Department of Physics, University of Oslo, Norway, 3.Institute of Technology, University of Tartu, Estonia)

We propose a method for efficiently coupling the finite element method with atomistic simulations like molecular dynamics or kinetic Monte Carlo. Our method enables to dynamically build an unstructured mesh with optimized density that follows the geometry defined by atomistic data. On this mesh, multiphysics problems can be solved to obtain distribution of physical quantities of interest, which can then be fed back to the atomistic system. The simulation flow is optimized to maximize computational efficiency while maintaining good accuracy.

We use this method to simulate the evolution of nanostructures under high electric field. By solving Poisson equation, we obtain the 3D distribution of electric field around the nanostructure. Using the field, we calculate electron emission currents, surface and space charge and electrostatic forces for surface atoms. By

taking Joule and Nottingham heating into account and solving 3D heat equation, we also obtain atomistic velocity perturbation.

Our method has shown remarkable overlapping with an analytical solution and has proved to be efficient and robust enough to simulate large-scale thermal runaway processes. Using those simulations, we demonstrated for the first time the disintegration of Cu nanotip in extreme field conditions. This process is widely believed to lead to the formation of plasma and cause vacuum arcing in high gradient structures.

[SY-G3] Symposium G-3

Chairs: Seunghwa Ryu(Korea Advanced Institute of Science and Technology, Korea), Keonwook Kang(Yonsei University, Korea)

Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8

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

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

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

Jae-Wan Lee¹, Jimin Choi¹, Keonwook Kang¹, Soonho Song¹, ○Won-Suk Ohm¹, Jung Su Park²
(1.Yonsei University, Korea, 2.Agency for Defense Development, Korea)

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

○Jimin Choi¹, Sanghyuk Yoo¹, Soonho Song¹, Jung Su Park², Keonwook Kang¹ (1.Yonsei Univ., Korea, 2.Agency for Defense Development, Korea)

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

○Roman Kositski¹, Dominik Steinberger², Stefan Sandfeld², Dan Mordehai¹ (1.Department of Mechanical Engineering, Technion - Israel Institute of Technology, 32000 Haifa, Israel, 2.Chair of Micromechanical Materials Modelling (MiMM), Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, 09599 Freiberg, Germany)

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

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

 (Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8)

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

Invited

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

Some special numerical techniques are desired when simulating the behavior of matters in extreme conditions, and in particular, the chemical-thermal energy release from the combustion of explosives and propellants must be carefully addressed when capturing the high strain rate deformation of metals and polymeric binders interacting with the energetic elements of the system. In this talk, selective research accomplishments associated with modeling of both energetic and inert matters exposed to high pressure conditions are discussed. Models are developed for addressing the problems of shock-induced ignition and multi-scale hot spot initiation of metalized energetic components from the shock compression system. To do so, one needs to adapt a stable interface tracking algorithm for severely transient fluid-structure interaction problems. We have developed a multi-material hydrodynamic shock physics code with a hybrid particle level set method for simulating the shock induced chemical reaction of energetic materials and volumetric deformation of metals. The experimental measurements are obtained to validate the simulated results presented in this talk.

 (Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8)

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

 Jae-Wan Lee¹, Jimin Choi¹, Keonwook Kang¹, Soonho Song¹, ○Won-Suk Ohm¹, Jung Su Park² (1.Yonsei University, Korea, 2.Agency for Defense Development, Korea)

Shock compression is an effective means of probing the mechanical and thermodynamic properties of solids. The majority of shock compression studies to date have reported principal Hugoniot curves, for which the material ahead of the shock is conveniently chosen to be in the quiescent state ($P = 0$ and $u = 0$). However, studies of branched Hugoniot (that emanate from non-quiescent states) are relatively rare, although branched Hugoniot are equally important for accurate description of shock wave physics involving interaction. In this talk, we discuss a sophisticated modeling scheme for shock hydrodynamics, accompanied by a full deck of principal and branched Hugoniot obtained with molecular dynamics computations. The system is a single-crystalline aluminum impacted at velocities ranging from 0.1 to 3.0 km/s, as described in the companion paper. Simulations show that branched Hugoniot should be used for accuracy in predictions, especially when there are material boundaries causing reflection and interaction of shocks.

 (Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8)

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

○Jimin Choi¹, Sanghyuk Yoo¹, Soonho Song¹, Jung Su Park², Keonwook Kang¹ (1.Yonsei Univ., Korea, 2.Agency for Defense Development, Korea)

Two different embedded-atom method(EAM) potentials were used in single crystalline FCC Al : WKG (J.M. Winey, Alison Kubota, and Y.M. Gupta), and FWYD (Qin-Na Fan, Chong-Yu Wang, Tao Yu, Jun-Ping Du). A 300k single crystalline Al system is inflicted planar shock at an adiabatic condition of 0.1 to 3.0 km/s. Pressure, volume and temperature profiles are obtained after shock as impact velocity. We extract the principle Hugoniot curve in averaged value of profiles. Branch points are selected on the principle Hugoniot curve. We made an isentropic equilibrium system that approximates branch points. The isentropic equilibrium system is inflicted planar shock to impact at an adiabatic condition of 0.1 to 3.0 km/s to obtain the branched Hugoniot curve. It is observed that either stacking fault formation or phase transformation from FCC to HCP or FCC to BCC occurs depending on the potential model. This study shows how the branched Hugoniot curve of single crystalline aluminum differs from the principle Hugoniot curve in strong shock. In addition, by analyzing the differences according to potential models, we show that the potential model must be carefully selected in the strong shock simulation.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8)

[SY-G3] Shear relaxation behind the shock front in $\langle 110 \rangle$ molybdenum

○Roman Kositski¹, Dominik Steinberger², Stefan Sandfeld², Dan Mordehai¹ (1.Department of Mechanical Engineering, Technion - Israel Institute of Technology, 32000 Haifa, Israel, 2.Chair of Micromechanical Materials Modelling (MiMM), Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, 09599 Freiberg, Germany)

In this work we study shock-induced plasticity in Mo single crystals, using a method to relate information of dislocations from the atomic to the continuum scale [1]. We use molecular dynamics (MD) simulations to simulate the shock propagation along the $\langle 110 \rangle$ crystal orientation. Shock waves with compressive axial stresses of about 120 GPa are simulated. These stresses induce homogeneous nucleation of dislocations but barely lead to a phase transition. Using the Dislocation Extraction Algorithm (DXA) and the newly developed Discrete to Continuum (D2C) technique, the atomistic information is turned into continuous dislocation fields. In conjunction, we extract from the MD simulations thermo-dynamical macroscopic quantities such as macroscopic strain, density, temperature and stress tensor during the propagation of the shock wave. Correlating the stress evolution and the evolution of the continuous dislocation fields, we analyze the attenuation of the sharp elastic jump at the front of the shock wave and the plastic deformation behind it. Analyzing the MD simulations, we show that the initially an elastic precursor wave overshoots the dislocation nucleation stress, after which dislocations on a specific group of slip planes (which we denote as out-of-plane) are nucleated, slightly lagging behind the elastic front. As dislocations are nucleated in the out-of-plane direction, the resolved shear stress on these planes is relaxed, but the principal lateral stresses increase. This leads to an increase in the shear stresses on a plane parallel to the shock wave (denoted as in-plane), resulting in an additional retarded front of dislocation nucleation on planes parallel to the shock front. Finally, the two-stage process of plasticity results in close to isotropic stress state. Interestingly, the DXA-D2C analysis shows that non-zero contributions in the Kroener-Nye tensor appear only in the first stage of plasticity, right behind the shock front. The MD simulation results are employed to calculate the dislocation densities on specific slip planes and the plastic deformation behind the shock, bridging the gap between the information on the atomic scale and the continuum level.

[1] Kositski, et al. Computational Materials Science 149 (2018): 125-133.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room8)

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

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

Graphene and other 2D materials with superior mechanical properties have been widely proposed as effective reinforcement for stronger and tougher nanocomposites [1] to realize structures capable to sustain extreme mechanical conditions, such impact loads. However current studies are limited to constitutive properties in the quasi-static regime [1] or to the impact properties of stand-alone 2D materials armors [2] without considering the behavior of the resulting nanocomposite under real hypervelocity shock conditions, where second order effect occur, such as elastic-plastic shock wave propagation or induced phase transformation. We present a molecular dynamics (MD) simulation study on shock behavior of graphene-reinforced single crystal copper (Cu), investigating the role of graphitic inclusion on the shock Hugoniot of such nanocomposites. Our results give insights of the failure behavior of graphene-metal nanocomposite under hypervelocity shock load and the consequent implications to their engineering applications.

References

- [1] Y. Kim, J. Lee, M. Yeom, J. Shin, H. Kim, Y. Cui, J.W. Kysar, J. Hone, Y. Jung, S. Jeon, S. Han. Strengthening effect of single-atomic-layer graphene in metal-graphene nanolayered composites. *Nature Communications* 4:2114, 2013.
- [2] S. Signetti, S. Taioli, N.M. Pugno. 2D Materials Armors Showing Superior Impact Strength of Few Layers. *ACS Applied Materials & Interfaces* 8:40820-40830, 2017.

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

[SY-G4] Symposium G-4

Chairs: Keonwook Kang(Yonsei University, Korea), Byeongchan Lee(KyungHee Univ., Korea)

Wed. Oct 31, 2018 4:00 PM - 4:45 PM Room8

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

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

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

[○]Junyoung Park¹, Jaehee Lyu¹, Shibutani Yoji² (1.Dept. of Mechanical Design Engineering, Kumoh National Institute of Technology, Korea, 2.Dept. of Mechanical Engineering, Osaka University, Japan)

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

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

(Wed. Oct 31, 2018 4:00 PM - 4:45 PM Room8)

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

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

Despite the significance of surface effects on the deformation behaviors of small-scale metallic glasses, systematic investigations on surface states are lacking. In this work, by employing atomistic simulations, we characterize the distributions of local inhomogeneity near surfaces created by casting and cutting, along with internal distributions in pristine and irradiated bulk specimens, and investigate the effects of inhomogeneity on the mechanical properties. The cast surface shows enhanced yield strength and degrees of shear localization, while the cut surface shows the opposite effects, although the fraction of vibrational soft spots, known to indicate low-energy barriers for local rearrangement, is high near both surfaces. Correspondingly, plastic deformation is initiated near the cut surface, but far from the cast surface. We reveal that improved local orientational symmetry promotes strengthening in cast surfaces and originates from the effectively lower quenching rate due to faster diffusion near the surface. However, a significant correlation among vibrational soft spots, local symmetries, and the degree of shear localization is found for the pristine and irradiated bulk materials. Our findings reveal the sensitivity of the surface state to the surface preparation methods, and indicate that particular care must be taken when studying metallic glasses containing free surfaces.

(Wed. Oct 31, 2018 4:00 PM - 4:45 PM Room8)

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

[○]Junyoung Park¹, Jaehee Lyu¹, Shibutani Yoji² (1.Dept. of Mechanical Design Engineering, Kumoh National Institute of Technology, Korea, 2.Dept. of Mechanical Engineering, Osaka University, Japan)

Voronoi tessellation technique, or also called as Voronoi analysis, has been quite widely adopted to describe the internal structure of materials from molecular level such as short-range order of icosahedra on metallic glasses to centimeter-order powder level such as occupied volume on powder packing. Especially, Voronoi tessellation technique is applied to the investigations by molecular dynamics or discrete element method. In the ordinary Voronoi tessellation technique, a face is placed halfway between equal-sized atoms or particles. However, as the size of particles or atoms in single material are not same, bisection cannot depict the exact plane to represent a convex polyhedron including an atom or a particle. Moreover, packed particles in an vessel usually has a Gaussian particle size distribution for natural powders and a Rosin-Rammler particle size distribution for pulverized powders. It is not just a problem for size distribution. It makes a huge difference on estimation of occupied volume and number of faces by atoms or particles. Therefore, we suggest an alternative way, Radical Plane Method, to solve these problems in this paper. It shows that the error of results could reach up to 60% differences.

(Wed. Oct 31, 2018 4:00 PM - 4:45 PM Room8)

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

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

The hydrated cement paste has complex microstructures. The pore and solid phase distribution characteristics within microstructures affect the material responses significantly. Material microstructure and its responses have been correlated with porosity [1]. However, porosity might not be sufficient to describe the complex microstructures. In this study, the relation between microstructure characteristics and material properties is investigated using a statistical method. To extract the microstructural characteristics of cement paste, micro-CT images are used. Pore and solid phase are separated from micro-CT images using the Powers' model. A lineal-path function [2], one of the low-order probability functions, is selected for estimating the microstructure characteristics. Particularly, the area of lineal-path function [3] is used as a quantitative parameter related to the material property in this study. Virtual specimens obtained from synchrotron micro-CT are used to evaluate material mechanical properties. The phase field fracture model is applied to evaluate stiffness and strength of cement paste with complex microstructures. From this study, it is concluded that the area of lineal-path function has a potential to be an alternative parameter for correlating material characteristics and properties.

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- [2] B. Lu, S. Torquato, Lineal-path function for random heterogeneous materials, *Phys. Rev. A* 45 (1992) 922-929.
- [3] T. S. Han, X. Zhang, J. S. Kim, S. Y. Chung, J. H. Lim, C. Linder, Area of lineal-path function for describing the pore microstructures of cement paste and their relations to the mechanical properties simulated from μ -CT microstructures. *Cem. Concr. Compos.* 89 (2018) 1-17.

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

[SY-H3] Symposium H-3

Chair: Hansohl Cho (Los Alamos National Laboratory, United States of America)

Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room9

[SY-H3] Polydomain liquid crystal elastomers¹

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

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

[○]William Goncalves¹, Takuya Mabuchi², Takashi Tokumasu¹ (1.Institute of Fluid Science, Tohoku University, Sendai, Miyagi 980-8577, Japan, 2.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Sendai, Miyagi 980-8577, Japan)

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

[○]Emanuele Locatelli¹, Daniele Parisi^{2,3}, Maria Merola², Domenico Truzzolillo⁴, Mario Gauthier⁵, Christos N. Likos¹, Dimitris Vlassopoulos^{2,3} (1.Faculty of Physics, University of Vienna, Austria, 2.Institute of Electronic Structure and Laser, FORTH, Greece, 3.Department of Materials Science and Technology, University of Crete, Greece, 4.Laboratoire Charles Coulomb, UMR 5221 CNRS - Université de Montpellier, France, 5.Faculty of Science, University of Waterloo, Canada)

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room9)

[SY-H3] Polydomain liquid crystal elastomers¹

Invited

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

Liquid crystal elastomers are rubbery solids with liquid crystal mesogens incorporated into their main chains. They display an isotropic to nematic phase transformation accompanied by a large spontaneous deformation. Depending on how these liquid crystal elastomers are synthesized, they can either be a mono domain (uniform liquid crystal order) or polydomain (nonuniform liquid crystal order). This talk will describe various phenomena and modeling questions related to the effective behavior of polydomain liquid crystal elastomers¹

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room9)

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

[○]William Goncalves¹, Takuya Mabuchi², Takashi Tokumasu¹ (1.Institute of Fluid Science, Tohoku University, Sendai, Miyagi 980-8577, Japan, 2.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Sendai, Miyagi 980-8577, Japan)

Because of their emissions free of carbon dioxide, polymer electrolyte fuel cells (PEFCs) are of great interest for energy production respectful of the environment. The transport of charges between the electrodes of the fuel cell is insured by a hydrated polymer membrane such as perfluorosulfonic acid (PFSA) membrane. The durability of the fuel cell is still limited by the chemical and mechanical degradation of the polymer membrane after cycles of utilization. This work focuses on the study of the mechanical behavior of PFSA membrane at nanoscale. The understanding of the relation between structure and mechanical properties is the key point to improve the resistance of the membrane against mechanical degradation.

Molecular Dynamics (MD) simulations are performed using a Coarse-Grained model to generate samples of PFSA membranes. The results obtained from structural characterization are compared with data from previous atomistic models and experiments. After validation of the nanostructures, mechanical tests are performed on the hydrated polymer membrane. With an increasing level of hydration, the results for elastic properties are in good agreement with experimental values and a similar trend as experiments is observed for early plastic behavior. The computation of the local mechanical properties of the samples allows to discuss the void nucleation and the influence of water content on the rupture behavior.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room9)

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

[○]Emanuele Locatelli¹, Daniele Parisi^{2,3}, Maria Merola², Domenico Truzzolillo⁴, Mario Gauthier⁵, Christos N. Likos¹, Dimitris Vlassopoulos^{2,3} (1.Faculty of Physics, University of Vienna, Austria, 2.Institute of Electronic Structure and Laser, FORTH, Greece, 3.Department of Materials Science and Technology, University of Crete,

Greece, 4.Laboratoire Charles Coulomb, UMR 5221 CNRS - Université de Montpellier, France, 5.Faculty of Science, University of Waterloo, Canada)

We employ a novel coarse-graining approach[6], to study star-chain mixtures[1-4], in the limit of long chains. The coarse-grained approach is based on the calculation of the effective interaction between a star polymer and a short chain of length $N_c = 10$ at infinite dilution. A multi-blob-like approach is then employed to coarse-grain chains of arbitrary length N_c . We study mixtures of star polymer and linear chains in the protein limit, i.e. when $q = R_h^c/R_h^s > 1$. We find that the addition of linear chains makes the star fluid more structured, confirming experimental observation obtained through rheological measurements.

[1] E. Stiakakis, et al. Physical Review Letters, (2002).

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[3] M. Camargo and C.N. Likos. Physical Review Letters, (2010).

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

[SY-H4] Symposium H-4

Chair: Meredith Silberstein (Cornell University, United States of America)

Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room9

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

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

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

○Chrystelle A. Bernard¹, Tiana Deplancke⁴, Olivier Lame⁴, Kazuhiro Ogawa³, Jean-Yves Cavallé²

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Japan, 4.Materials Engineering and Science (MATEIS), CNRS, INSA-Lyon, UMR5510 Univ. de Lyon,

France)

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

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

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

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

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room9)

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

Invited

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

Liquid-crystalline elastomers (LCEs) are soft stimuli-responsive materials that exhibit remarkable mechanical and optical properties. LCEs consist of stiff mesogens, bound in a network of flexible polymer chains, which can self-organize into crystalline order while retaining liquid-like properties. The directional ordering of the mesogens changes in response to external stimuli and the director coupling between the mesogens and network chains brings about unusual behaviors. These include large reversible actuation in response to temperature or light and soft-elasticity. LCEs also exhibit enhanced dissipation behaviors, including a high $\tan \delta$ 0.5-1.0 for wide range of frequencies and temperatures, spanning the glass and nematic transition temperatures, and large hysteresis in the stress response that increases with the strain rate [1]. We hypothesize that the enhanced dissipation behavior arises from the relative motions of the mesogens within the network and set out to measure the effect of mesogen ordering and network orientation on the enhanced dissipation behavior of LCEs. Experiments were performed to measure the rate-dependent hysteresis and frequency dependent dynamic properties for main-chain LCEs in the nematic state with different network structures, including an unoriented and macroscopically isotropic polydomain as well as monodomains with different degrees of mesogens and chain alignment. Oriented monodomains with an aligned or unaligned network can be synthesized by applying a second-stage crosslinking or exchangeable bond reaction to a stretched LCE sample. In this presentation, I will briefly describe the experimental methods, then compare the dissipative behavior of the different network structures, and discuss how the results will be applied to develop a rate-dependent constitutive model for the main-chain LCE networks.

[1] A. Azoug, V. Vasconcellos, J. Dooling, M. Saed, C. M. Yakacki and T. D. Nguyen (2016) *Polymer* 98:165-171.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room9)

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

○Chrystelle A. Bernard¹, Tiana Deplancke⁴, Olivier Lame⁴, Kazuhiro Ogawa³, Jean-Yves Cavaillé² (1.Frontier Research Institute for Interdisciplinary Sciences (FRIS), Tohoku Univ., Japan, 2.Engineering Science Lyon Tohoku joint lab for Materials under Extreme Conditions (ELyTMaX) UMI3757, Tohoku Univ., Japan, 3.Fracture and Reliability Research Institute (FRI), Tohoku Univ., Japan, 4.Materials Engineering and Science (MATEIS), CNRS, INSA-Lyon, UMR5510 Univ. de Lyon, France)

Polymers are largely used in everyday life; however, their large strain behavior is still not well understood because of the complexity of the mechanisms involved in their deformation. To improve the current knowledge on these materials, extensive experimental and theoretical researches have been performed leading to development of constitutive numerical models to predict their large strain behavior. Most of models based on polymer physics have been developed for amorphous polymers. The few ones predicting the mechanical behavior of semi-crystalline polymers do not consider the important evolution of microstructure occurring during the plasticity. This is especially true for ultra-high molecular weight semi-crystalline (UHMWSC) polymers. Because their microstructure exhibits very long macromolecular chains, one

chain belongs at the same time at the crystal network and macromolecular network. During the plastic deformation of the polymers, fibrillation process occurs leading to the progressive collapse of the crystalline network and inducing strong variations in the material mechanical properties. Thus, to accurately predict the mechanical behavior of UHMWSC polymers, the mechanical coupling between crystallites and fibrils and its evolution during the deformation has to be taken into account. From the expression of the mechanical coupling for the elastic modulus given by Humbert et al. [1] (non-parallel/non-series configuration), Deplancke et al. [2] developed a one-dimensional model for the prediction of the mechanical behavior of Ultra High Molecular Weight PolyEthylene (UHMWPE). However, to extend its possible range of applications, transformation into a three-dimensional model is needed. Therefore, we have developed a 3D model which take into account the evolutive mechanical coupling, between crystals and fibrils, as a function of the deformation. The model is based on series configuration with consideration of the crystal ratio in the definition of the deformation gradients. Good agreement is found between the experimental results and 3D numerical predictions during loading and unloading.

[1] Humbert et al., *Polymer* **52** (2011) 4899-4909

[2] Deplancke et al., on going

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room9)

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

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

Matrix-free polymer-grafted nanocrystals, called assembled hairy nanoparticles (aHNPs), can significantly enhance the thermomechanical performance of nanocomposites by overcoming nanoparticle dispersion challenges and achieving stronger interfacial interactions through grafted polymer chains. However, effective strategies to improve both the mechanical stiffness and toughness of aHNPs is lacking given the general conflicting nature of these two properties and the large number of molecular parameters involved in design of aHNPs. Here, we propose a computational framework that combines multi-response Gaussian process metamodeling and coarse-grained molecular dynamics simulations to establish design strategies for achieving optimal mechanical properties of aHNPs within a parametric space. Taking poly(methyl methacrylate) grafted to high-aspect ratio cellulose nanocrystals as a model nanocomposite, our multi-objective design optimization framework reveals that the polymer chain length and grafting density are the main influencing factors governing the mechanical properties of aHNPs, in comparison to the nanoparticle size and the polymer-nanoparticle interfacial interactions. In particular, the Pareto frontier marking the upper-bound of mechanical properties within the design parameter space can be achieved when the weight percentage of nanoparticle is above around 60% and the grafted chains exceed the critical length scale governing transition into the semi-dilute brush regime. We show that theoretical scaling relationships derived from the Daoud-Cotton model capture the dependence of the critical length scale on graft density and nanoparticle size. Our established modeling framework provides valuable insights into the mechanical behavior of these hairy nanoparticle assemblies at the molecular level and allows us to establish guidelines for nanocomposite design.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room9)

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

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

Extrusion in fused filament fabrication is typically fast enough to produce significant chain alignment that may change the weld strength of 3D printed objects in several ways. Some studies suggest that alignment may enhance interdiffusion because of the entropic force driving chains towards unaligned conformations or by reducing entanglement density. Alignment of strong backbone bonds along the interface may also change the mechanical properties of material near the joint. As part of a multiscale study of 3D printing, we have used molecular dynamics simulations of a generic polymer model to examine the effect of alignment on the dynamics of welding and evolution of weld strength. Entropy drives chain retraction in the tube, but this does not speed interdiffusion since the tubes are aligned along the interface. There is also no indication of accelerated interdiffusion due to entanglement loss. The ambiguities in recent real space methods for identifying entanglements will be discussed. Alignment does reduce the strength of bulk material adjacent to the weld. At intermediate times this greatly enhances weld strength by moving failure away from the interface. The dependence of the bulk strength on alignment is presented for different thermal histories.

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

[SY-H5] Symposium H-5

Chair: Alexey Lyulin (Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands)

Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room9

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

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

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

○Ryota Osawa¹, Yoshiteru Aoyagi² (1.Dept. of Mechanical Engineering, Tohoku Univ., Japan, 2.Tohoku Univ., Japan)

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

○Sumit Basu (Indian Institute of Technology Kanpur, India)

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

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

 (Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room9)

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

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

Polymeric foams materials can have various applications in engineering. We consider in this work the effect of the foam microstructure in the homogenized response of a random 3D structural polymeric foam under high dynamic mechanical loading conditions (shock). In the analysis, the microstructure of the foam is extracted from 3D computed micro-tomography. The mechanical response of the solid part of the foam is described in terms of deviatoric and pressure response. Using Direct Numerical Simulations (DNS), Finite Element Method (FEM) and the concepts of Micromechanics the average foam response to shock is determined. The results are compared with the 1D-shock equations for the homogenized case to determine the effect of fluctuating fields of physical quantities due to the randomness of the foam microstructure.

LA-UR-18-22612

 (Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room9)

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

○Ryota Osawa¹, Yoshiteru Aoyagi² (1.Dept. of Mechanical Engineering, Tohoku Univ., Japan, 2.Tohoku Univ., Japan)

Crystalline thermoplastic polymers have a complicated hierarchical structure consisting of lamellae of amorphous phases with a random coil structure and crystalline phases in which molecular chains are regularly arranged. The lamellae grow radially repetition of secondary nucleation on a surface of growing lamellae and spherulite structures are generated. Peculiar mechanical characteristics of the crystalline thermoplastic polymers, such as nonlinear elasticity, strain softening after yielding, propagation of necking, and orientation rehardening cannot be seen in the case of metals. Mechanical properties of crystalline thermoplastic polymers depend on the complicated microstructures, and the microstructures varies depending on molding conditions. A theoretical model predicting the microstructure and reproducing the mechanical properties are expected in the field of industrial CAE to enhance formability and reliability of the crystalline thermoplastic polymers. Phenomenological models on macroscopic crystallinity or crystallization rate are popular in terms of industrial availability. Such models cannot investigate effects of sizes, shapes, and distribution of spherulites. In this study, we construct a model expressing generation of spherulite structures for prediction of microstructures of crystalline thermoplastic polymers depending on thermal conditions. A spherulite growth are represented by initial nucleation in an amorphous phase and secondary nucleation on surfaces of spherulites. Rates of the both nucleation are identified by experimental observations of spherulites growth under different thermal conditions. Monte Carlo simulations are performed using the constructed method to reproduce the generation and growth of spherulites in an amorphous phase. In addition, we evaluate effects of crystallization temperature on the nucleation rate and the growth rate by comparison of experiment and analysis results.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room9)

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

○Sumit Basu (Indian Institute of Technology Kanpur, India)

Polymers, by virtue of being synthetic, microscopically tailorable and light materials, are finding uses in challenging new technological situations. These new applications, involving high temperatures, harsh environments, impact, sustained dead loading and others, often demand changes in the macromolecular architecture. The ability to predict the effects of an architectural alteration on the ultimate mechanical behaviour of a bulk polymer is therefore, useful. Coarse grained molecular dynamics provide a route to conducting large and long simulations to establish structure property relationships in these materials. However, a wide variety of coarse graining methodologies exist and their suitability for obtaining mechanical properties needs to be systematically established before they can become effective predictive tools. In this talk, we will focus on our experience with coarse grained molecular dynamics simulations on long chained and crosslinked polymers. In particular, we will discuss, coarse graining strategies that rely on Boltzmann inversion based techniques for calibrating bonded interactions, and a variety of heuristic techniques targetting specific physical properties for the non-bonded. We will highlight the problems associated with simultaneously targetting multiple end properties like density, total energy and atomic virial. Moreover, the mismatch in time scales between detailed atomistic and coarse grained simulations and their influence on the rate dependent behaviour of properties like the glass transition temperature and uniaxial stress-strain response will also be discussed. Finally, we will demonstrate a few case studies on polystyrene and a group of crosslinked polyimides to show that coarse grained molecular dynamics simulations of polymers have good predictive capability and sometimes can provide useful insights into material behaviour.

(Wed. Oct 31, 2018 2:00 PM - 3:30 PM Room9)

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

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

Non-covalent cross-linking interactions such as metal ligands can be used to tailor stiffness and structure of linear polymers while enabling interesting features like self-healing, energy dissipation, and extended stretching capability. Here we present a novel system of copper(II) carboxylate bonds used to crosslink a low T_g acrylic backbone. These crosslinks behave in a covalent manner to form novel materials with increased stiffness, strength, and dissolution resistance, and decreased ductility. It was found that substitution of the copper cation with different ligands imparts a dynamic nature to the crosslinks, thereby enabling dissolution and regeneration of the initial linear polymer. These ligands also strongly influence behavior in the solid-state polymer, increasing ductility with minimal stiffness and strength reduction, and enabling self-healing behavior. The polymer was characterized under monotonic uniaxial tensile loading at different temperatures and strain rates. This experimentally observed mechanical behavior is then considered in the context of topological and mechanochemical elastomer models. The mechanochemical model highlights how modulation of the dynamic cross-link strength within an otherwise linear elastomer can modulate bulk mechanical behavior.

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

[SY-H6] Symposium H-6

Chair: Alexey Lyulin (Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands)

Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9

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

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

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

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

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

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

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

○Yaguang Sun¹, Hua Yang², Yafang Guo¹ (1. Dept. of Mechanics, Beijing Jiaotong Univ., China, 2. State Key Lab. for Geomechanics and Deep Underground Engineering, China Univ. of Mining and Tech., China)

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

Arjan E. Boerema¹, Patrick R. Onck¹, ○Erik Van der Giessen¹, Stefanos Papanikolaou² (1. Univ. of Groningen, Netherlands, 2. West Virginia Univ., United States of America)

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9)

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

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

Filler morphology, radius, and strength of the filler-polymer interaction impact the physical properties of filled rubber. It is crucial to understand relationships between them so as to improve tire performances. Four large-scale coarse-grained molecular dynamics models were created. The first model is a reference model in which filler particles are distributed in a lattice pattern. The second model is an aggregated model including a non-homogenous filler distribution. The third model is a small particle size model in which small particles are distributed with identical morphology and volume fraction with the reference model. The forth model is a weak interaction model. The polymer-filler interaction is weaker than the reference model, even though the morphology and the particle size match the reference model.

Comparing stress-strain curves, we confirmed that effects of them which are observed in experimental results; filler aggregates, small particles, and strong interaction make modulus and hysteresis greater, were reproduced qualitatively. Measuring a polymer density distribution and a change of polymer chains bridging fillers, it was found that an increase of polymer density around fillers induced by the polymer-filler attractive interaction grows the modulus of the polymer phase and irreversible changes of polymer chains cause hysteresis. We determined that these changes observed in all models are fundamental mechanisms of filled rubber. Comparing the stress-strain curves of the reference model and the aggregated model, we found that the differences are attributed to filler stress. Fillers are to be contacted with another filler particle during deformation and filler stress grows when fillers are aggregated. Comparing the reference model and the weak interaction model, we found that the number and force per a bond of extended chains in the reference model, which are main sources of polymer stress, are greater than the weak interaction model, even though length of the extended chains are much the same. These differences of polymer stress make modulus and hysteresis greater.

Last, a significant increase of the number of extended chains grows polymer stress, when fillers are small and the volume fraction of filler is identical with the reference model. Thus the modulus and hysteresis become greater.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9)

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

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

Rubbers are frequently used in vibration isolation, e.g. as the material for engine mounts or tram wheel suspension segments. These parts are subjected to periodical mechanical loading and to the effects of the environment, such as temperature or chemical reactions. Depending on the nature of the structure changes induced by the environment, physical or chemical ageing may be distinguished (see e.g. [1]). Chemical ageing is governed by the consumption of oxygen, which in turn depends on its transport by diffusion.

Both damage and ageing lead to changes in mechanical properties, each of the phenomena, however, takes

place at a different length scale. This contribution is focused on the influence of fatigue damage on the diffusion of oxygen. The central assumption is that the formation and growth of microcracks influence the paths of the gas molecules, which manifest itself as the coefficient of diffusivity on the macroscopic scale. We present various examples of crack geometries and the resulting oxygen flux and concentration computed by the finite element method (FEM). These results will be further used to derive a phenomenological model of coupled fatigue damage and diffusion-limited oxidation (DLO). This model will be an extension of an existing model [2], in which, however, no explicit relation for the coupling between fatigue damage and diffusivity is considered.

[1] Herzig, A. , Johlitz, M. and Lion, A. Consumption and diffusion of oxygen during the thermoxidative ageing process of elastomers. *Mat.-wiss. u. Werkstofftech*, 47: 376-387, 2016.

[2] Heczko, J., Kottner, R. Modelling of ageing and fatigue under large strains. In *Computational Mechanics - EXTENDED ABSTRACTS*, 2017.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9)

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

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

A molecular dynamics approach to calculate general tensile properties of real rubber is developed to alleviate lengthy experimental procedures for the determination of the strain energy function of the rubber material. In this presentation, first, the general framework for the calculation of tensile properties of rubber using molecular dynamics simulation will be illustrated. The overview on the molecular modeling for the real rubber is followed and some pilot calculations are performed to obtain the tensile properties for carbon black filled styrene-butadiene rubbers.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9)

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

○Yaguang Sun¹, Hua Yang², Yafang Guo¹ (1.Dept. of Mechanics, Beijing Jiaotong Univ., China, 2.State Key Lab. for Geomechanics and Deep Underground Engineering, China Univ. of Mining and Tech., China)

Thermosets have outstanding mechanical strength and solvent resistance due to their permanently cross-linked networks. They cannot flow upon heating and cannot be reshaped and recycled. The recently developed reversible networks provide opportunities to recycle thermoset polymers. For example, the covalent adaptable networks (CANs; also known as vitrimers) can rearrange their network topology through reversible bond exchange reactions (BERs). It was recently reported that CANs can be dissolved in solvents. At high temperature, small solvent molecules can break long polymer chains into short segments via BERs. In this study, molecular dynamics simulations are used to investigate the dissolution of an epoxy CAN in alcohol solvents due to the transesterification type BER. The diffusion of solvent molecules and the decomposition of epoxy networks are analyzed. It is found that the dissolution proceeds in a surface erosion mode, which is consistent with experimental observations.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room9)

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

Arjan E. Boerma¹, Patrick R. Onck¹, [○]Erik Van der Giessen¹, Stefanos Papanikolaou² (1.Univ. of Groningen, Netherlands, 2.West Virginia Univ., United States of America)

The static elastic behaviour of biophysical networks comprising cross-linked semi-flexible filaments is well characterised due to extensive theoretical, computational and experimental studies of in-vitro materials. The dynamic response of these networks, however, still holds several mysteries, including the peculiar variation of the loss modulus with frequency, $G''(\omega)$. For example, entropic effects can explain the increase of G'' with frequency at high frequencies, but not the minimum in $G''(\omega)$ at intermediate frequencies. The latter feature has been suggested to be governed by the cross-linker dynamics, but the experimental trends are yet to be predicted by theory in a phenomenologically consistent manner. Here, we present a minimal micromechanical description, consisting of two semi-flexible filaments coupled by cross-linkers, whose dynamics is described through a Grand Canonical Monte Carlo scheme.

[SY-B1] Symposium B-1

Chair: Lorenzo Malerba(CIEMAT, Energy, Environment and Technology Research Centre, Spain)

Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10

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

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

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

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

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

○Marcin Roland Zemla¹, Jan Stanislaw Wrobel¹, Marek Muzyk¹, Tomasz Wejrzanowski¹, Duc Nguyen-Manh², Sergei L. Dudarev², Luca Messina³, Par Olsson³, Christophe Domain⁴ (1.Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland, 2.CCFE, Culham Centre for Fusion Energy, Abingdon, Oxon OX14 3DB, UK, 3.KTH Royal Institute of Technology, Nuclear Engineering, 106 91 Stockholm, Sweden, 4.Département Matériaux et Mécanique des Composants, EDF-R&D, Les Renardières, F-77250 Moret sur Loing, France)

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

○Jesper Byggmatar¹, Fredric Granberg¹, Andrea E Sand¹, Kai Nordlund¹ (1. Department of Physics, University of Helsinki, Finland)

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

○Fredric Granberg¹, Haixuan Xu², Kai Nordlund¹ (1.Department of Physics, University of Helsinki, Finland, 2.Department of Materials Science and Engineering, University of Tennessee, United States of America)

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10)

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

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

Many industrially important alloys and steels are intentionally processed and explored, as metastable microstructures comprising a supersaturation of crystal defects in various forms of aggregation. Even though it is well understood that this microstructural complexity governs the material performance, the defects composition, thermal stability, how they are distributed and in which concentrations are not yet resolved experimentally. Hardened ferritic steels are important example where the lattice defects play deterministic role in their deformation behavior..

While it is long-known that carbon atoms dispersed in the matrix of iron and steels have an influence on the type of defects produced, it is only recently that atomistic simulations have clearly and quantitatively revealed that carbon atoms bind very strongly to vacancies, giving rise to the formation of a whole fauna of carbon-vacancy (mCnV) complexes. These complexes may act as traps for other defects, which suggests that hardening in iron and its alloys will be the consequence of the interaction of dislocations with complex defects formed by not only point defects but also carbon atoms. In this context, the formation of mCnV clusters is the triggering mechanisms for the growth of other complex defects.

In this study, the focus is given on the examination of relaxation processes which occur in the internal friction spectra of a variety of iron alloys and steels with different carbon concentrations, and out-of-equilibrium vacancy concentrations, achieved either by fast cooling (quenching) or plastic deformation. The relaxation peaks are analyzed on the basis of the Debye relaxation model and their activation energies and integrated intensities are determined. By comparing the results with theoretical calculation, positron annihilation spectroscopy results, and magnetic after effect measurements, the observed relaxation processes are assigned to the dissolution of carbon-vacancy (mCnV) clusters [1]. Dissolution energies and relaxation strengths (concentrations) of various mCnV clusters are found to be in the correct energy range according to density functional calculations.

[1] M. J. Konstantinović and L. Malerba, Phys. Rev. Mat. **1**, 053602 (2017).

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10)

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

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

Phosphorus(P) causes Grain-boundary(GB) embrittlement that is considered as one factor of ductile-brittle transition in reactor pressure vessel steels. While the prediction of GB P segregation is desired, the detailed process of P segregation to GB is still unclear. We studied the process of P segregation to GB by simulating the migration of a mixed interstitial dumbbell, an octahedral interstitial P atom and a P-vacancy complex using a molecular dynamics method. As a result, it was found that the P atom of them becomes a substitutional atom before they reach the GB. The self-interstitial atom (SIA) or vacancy of them was absorbed by the GB. This phenomenon was also confirmed partially by first-principles calculations. In

addition, it was found that the P atom left behind approaches the GB by successively interacting with an SIA or a vacancy coming to its nearest neighbor site. We think that the conventional understanding of GB P segregation should be revised.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10)

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

[○]Marcin Roland Zemla¹, Jan Stanislaw Wrobel¹, Marek Muzyk¹, Tomasz Wejrzanowski¹, Duc Nguyen-Manh², Sergei L. Dudarev², Luca Messina³, Par Olsson³, Christophe Domain⁴ (1.Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland, 2.CCFE, Culham Centre for Fusion Energy, Abingdon, Oxon OX14 3DB, UK, 3.KTH Royal Institute of Technology, Nuclear Engineering, 106 91 Stockholm, Sweden, 4.Département Matériaux et Mécanique des Composants, EDF-R&D, Les Renardières, F-77250 Moret sur Loing, France)

Point defects, for example self-interstitials and vacancies, play an important part in controlling properties of materials and their kinetic evolution. As a consequence, proper understanding and modelling of materials properties require precise knowledge of point defect behaviour and their characteristics, in particular their formation and migration energies. In magnetic alloys such as FeCr, the investigation of point defects is complicated, because their properties strongly depend on various parameters such as Cr composition, alloy short-range ordering and the defect local environment [1-3].

In this work, we have investigated properties of dumbbell-type defects in FeCr with a large dataset of density functional theory calculations, for Cr concentrations ranging from low to approx. 35%. Analysis shows that properties of self-interstitial and interstitial (IA) defects in concentrated bcc FeCr alloys fluctuate significantly as functions of the above parameters. These fluctuations are observed to a lesser or greater extent for the lattice parameter, chemical potentials, bulk moduli, relaxation volumes, magnetic moments, and migration energies of dumbbells. We conclude that the formation energy of dumbbells depends on the Cr content and also on the number of Cr atoms in the local environment of a defect. For each chemical composition the average migration energies of Cr IA defects (Cr-Cr, Cr-Fe dumbbells) moving to the first nearest-neighbour (1NN) position, are significantly smaller than those of Fe-Fe exchanging with the 1NN Fe atom. The relaxation volumes of dumbbells increase in the ordered structure and decrease in the disordered one with the increase of number of Cr atoms in the local environment of a defect. The trends exhibited by the mean values of the various properties have been observed and analysed, and the most stable directions of Fe-Fe, Fe-Cr and Cr-Cr dumbbells have been determined. Moreover, the energy of elastic interaction between such defects are quantitatively estimated using the suitably parametrized dipole tensors of the defects.

[1] D. Costa, G. Adjanor, C.S. Becquart, et al., J. Nucl. Mater. 452 (2014) 425-433

[2] D. Nguyen-Manh, M.Y. Lavrentiev, S.L. Dudarev, C. R. Physique 9 (2008) 379-388

[3] D. Nguyen-Manh, M.Y. Lavrentiev, M. Muzyk et al., J Mater Sci (2012) 47: 7385

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10)

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

○Jesper Byggmestar¹, Fredric Granberg¹, Andrea E Sand¹, Kai Nordlund¹ (1. Department of Physics, University of Helsinki, Finland)

During the lifetime of a typical reactor, the radiation damage in the wall materials will reach high damage doses. Collision cascades initiated by subsequent irradiation will therefore become increasingly likely to overlap with pre-existing atomistic damage, such as dislocation loops, voids, and other defect structures. We have therefore carried out a large number of molecular dynamics simulations using well-established interatomic potentials, to build a database for the defect production in collision cascades overlapping with pre-existing defect clusters in both iron and tungsten. We primarily study cascades overlapping with dislocation loops of different size. Cascade overlap on other defect clusters leads to similar results. We find that cascades overlapping with pre-existing interstitial clusters result in a significant reduction in the number of new point defects. The overlap effect on vacancy clusters is weaker. By running cascades on different-sized clusters, with different cascade energies and at different temperatures, we obtain a database that can be used to fit a simple analytical model for the defect production bias due to the overlap effects. The data and the fitted analytical model can be transferred to larger-scale simulation methods, such as Monte Carlo techniques, to model the radiation damage accumulation at longer length and time scales.

(Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room10)

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

○Fredric Granberg¹, Haixuan Xu², Kai Nordlund¹ (1. Department of Physics, University of Helsinki, Finland, 2. Department of Materials Science and Engineering, University of Tennessee, United States of America)

In order to predict the behaviour of materials used in places where radiation is present, many aspects must be considered. The macroscopic effects like swelling and cracking, are a product of defect evolution starting at atomistic level. The energetic ion will, on the atomic level, transmit energy to lattice atoms, which will start collision cascades in the material. To be able to predict what the irradiation will do to the material, we must start on this level. The problem arises from that there is no single method that can accurately simulate everything from single atoms or electrons up to macroscopic parts that builds up the construction. To tackle this problem, a combination of two or more methods can be used consecutively, to be able to extend the time and/or length scale of the simulation. In this study, we focus on extending the time scale, to be able to predict the evolution of irradiation induced defects.

To study the irradiation effect in Fe and Fe-based alloys we utilize Molecular Dynamics (MD), to simulate the primary damage production on an atomistic level. The simulations are carried out by giving a recoil energy to a random atom in the simulation box. These simulations are very accurate to study the movement of all atoms, but are limited to nanoscale simulation boxes and times on the pico- or nanosecond time scale. The length scale is sufficient to accurately simulate the defect production, however the time scale is not sufficient for a long term evolution of the system. This long term evolution is needed to obtain comparable results with experiments and to compare with materials in use in these kinds of environments. To remedy the time scale problem, we utilize Kinetic Monte Carlo (KMC), to obtain longer time scales. A special version of KMC, Self-Evolving Atomistic KMC (SEAKMC), is used as no predefined and pre-calculated barriers are needed. This on-

the-fly method is perfect for cases where the defects produced can have many different complicated structures. In these cases, it would be impossible to predict their structure beforehand and calculate all the barriers. A combination of MD and SEAKMC is used to both accurately predict the produced primary damage (with MD) as well as its evolution (with SEAKMC), before a second cascade will hit the same region, as in experimental cases where intensive irradiation is present.

[SY-B2] Symposium B-2

Chair: Davide Pizzocri(Politecnico di Milano, Italy)

Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room10

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

○Emeric Bourasseau, Marjorie Bertolus, Michel Freyss, Gérald Jomard, Ibrahim Cheik Njifon, Martin-Stéphane Talla Noutack, Cyrille Takoukam Takoundjou (CEA/DEN/DEC, Centre CEA de Cadarache, France)

[SY-B2] Influence of vibrational entropy on the concentrations of uranium vacancies in UO_2

○Jean-Paul Crocombette¹, Fabien Bruneval¹, Aurélien Soulié¹, Mihai-Cosmin Marinica¹, Samuel Murphy² (1.CEA Saclay, France, 2.Lancaster University, UK)

[SY-B2] Modelling of defect and rare gas transport properties in UO_2 from the atomic to the grain scale

○Marjorie Bertolus, Michel Freyss, Emerson Vathonne, Emeric Bourasseau, Serge Maillard, Gérald Jomard (CEA, DEN, Département d'Etude des Combustibles, Centre de Cadarache, 13108 Saint-Paul-lez-Durance, France)

[SY-B2] Intragranular bubble impact on nuclear fuel thermomechanical properties

Fabienne Ribeiro¹, Mehdi Colbert¹, ○Jack Arayro¹, Guy Trégliat² (1.Institut de Radioprotection et de Sûreté Nucléaire/PSN-RES/SEMIA/LPTM, France, France, 2.Centre Interdisciplinaire de Nanoscience de Marseille, CNRS, France, France)

 (Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room10)

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

Invited

[○]Emeric Bourasseau, Marjorie Bertolus, Michel Freyss, Gérald Jomard, Ibrahim Cheik Njifon, Martin-Stéphane Talla Noutack, Cyrille Takoukam Takoundjou (CEA/DEN/DEC, Centre CEA de Cadarache, France)

Until recently, simulations of the fuel behavior during normal or accidental operation in nuclear reactor were based on rather empirical laws built from numerous experimental observations. Nowadays, simulation codes try to render the underlying physics, and are used to understand the measurements performed during irradiations or post-irradiation experiments. Thus, the fuel modelling and the laws used to predict its behavior must be improved by fundamental researches and feed by results from separate effects experiments. In support to these experiments, multi-scale modelling is an important tool, which aim is to understand the phenomena occurring at the microscopic scale to improve the modelling of the material at the macroscopic scale.

In this presentation, we will show our recent works concerning atomic scale simulations used to improve the knowledge of nuclear fuel properties before and during irradiation. Three points will be emphasized. First, we will present ab initio calculations of point defects in MOX fuels, and how they can be used to determine the elementary mechanisms of atomic diffusion in the irradiated fuel. Then, we will show a study of the energetic and structural properties of grain boundaries in UO_2 using classical molecular dynamics. In particular, an interesting correlation observed between cleavage energy and disorientation angle will be shown. And finally, we will present the results of the determination of thermodynamic properties of $(\text{U,Pu})\text{O}_2$ through molecular Monte Carlo method. This method appears to be particularly relevant to explore the various cationic configurations available in mixed oxide.

For each examples, we will try to underline the link with experimental works, and to show how our results are included in simulations at higher scales.

 (Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room10)

[SY-B2] Influence of vibrational entropy on the concentrations of uranium vacancies in UO_2

[○]Jean-Paul Crocombette¹, Fabien Bruneval¹, Aurélien Soulié¹, Mihai-Cosmin Marinica¹, Samuel Murphy²
(1.CEA Saclay, France, 2.Lancaster University, UK)

The wide deviations of the composition of UO_2 around its nominal composition are accommodated by point defects or clusters of oxygen interstitials. The formation energies of these defects have been the subject of many studies DFT calculations. In the high temperature understoichiometric regime, atomistic calculations and experiment agree on the fact that oxygen vacancies are the dominant defect. At the opposite for the overstoichiometric material the formation energies predict uranium vacancies to dominate over oxygen interstitials. This contradicts experimental facts which show that oxygen interstitials, either isolated or clustered are accommodating the overstoichiometry in UO_{2+x} . This so-called “uranium vacancy problem” has been noticed for many years [1] and has resisted the various calculations improvements, either methodological (e.g. use of DFT+U) or numerical (e.g. calculations made on bigger boxes).

Considering the vibrational entropy of the defects enables to solve this problem. We have combined ab initio formation energies of point defects and oxygen clusters in UO_2 [2] with harmonic entropies calculated with a many body empirical potential with charge equilibration [3]. Including the vibrational contribution to the free energy of defects de-stabilizes the uranium vacancies compared to the oxygen defects. The latter are then predicted to be dominant at high temperatures or large overstoichiometry in agreement with experiments. However our calculations exhibit a composition and temperature domain where uranium vacancies may in fact be the majority defect in UO_{2+x} . Some experimental observations (dilatometry, positron annihilation spectroscopy and uranium diffusion measurements) tend to confirm this prediction.

[1] J.P. Crocombette, *et al.*, Phys. Rev. B **64**, 104107 (2001).

[2] F. Bruneval, *et al.*, Phys. Rev. Materials **2**, 023801 (2018).

[3] A. Soulié, *et al.*, Acta Mater. **150**, 248 (2018).

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room10)

[SY-B2] Modelling of defect and rare gas transport properties in UO_2 from the atomic to the grain scale

[○]Marjorie Bertolus, Michel Freyss, Emerson Vathonne, Emeric Bourasseau, Serge Maillard, Gérald Jomard (CEA, DEN, Département d'Etude des Combustibles, Centre de Cadarache, 13108 Saint-Paul-lez-Durance, France)

One of the challenges for the next generation of nuclear reactors is to increase significantly the efficiency in designing and qualifying innovative fuels. One way of doing this is to develop a more physically-based description of nuclear fuels to enhance the predictive capability of fuel behaviour simulation. This should enable a better selection of promising fuel systems and a reduction of the effort necessary for the design of new fuels. Basic research approaches combining multiscale modelling and separate effect experiments can bring significant insight into key phenomena involved in the evolution of nuclear fuels during their reactor life.

We will describe the multiscale modelling approach developed from the atomic to the mesoscopic scale to investigate the transport properties of defects and rare gases in nuclear fuels. We will show examples of the results obtained at atomic scale on uranium dioxide concerning the data necessary for the mesoscale models and for the interpretation of separate experiments on fuels. We will also present the application of mesoscale models, in particular cluster dynamics.

(Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room10)

[SY-B2] Intragranular bubble impact on nuclear fuel thermomechanical properties

Fabienne Ribeiro¹, Mehdi Colbert¹, [○]Jack Arayro¹, Guy Trégliat² (1.Institut de Radioprotection et de Sûreté Nucléaire/PSN-RES/SEMIA/LPTM, France, France, 2.Centre Interdisciplinaire de Nanoscience de Marseille, CNRS, France, France)

UO₂ is used as a standard fuel in pressurized water reactors. During fission reactions bubbles of xenon are generated. The presence of these bubbles modifies the thermo-mechanical properties of the fuel. The need to characterize these effects led to an extensive work both from experimental and theoretical points of view. Our contribution belongs to the later type.

First, the variation of the thermomechanical properties of UO₂ versus porosity is studied through atomistic simulations with semi-empirical potentials. A good agreement is found between the elastic properties calculated in the present simulations, and those coming from micro-mechanical modelling and experimental ones. Concerning thermal properties, an analytical model taking into account the nanoporosities is derived. This study emphasizes the importance of bubble surface effects of intragranular bubbles on the thermomechanical behavior of the matrix.

Second, to clarify this effect, we study simplified systems of xenon on UO₂ surfaces. We first determine the surface relative stability according to their orientations and then to their polarities, by combining thermostistical relaxation and analytic formulations within a simple electrostatic model. The main result is that, whereas the (111) surface appears stable with only minor reorganization, the polar (100) one is only stabilized through drastic rearrangement of the surface region. Xenon adsorption on these relaxed surfaces is then realized through Grand Canonical Monte Carlo simulation.

Finally, the pressure inside the Xenon and in the UO₂ matrix is investigated. For the Xenon, we show that whatever its cristallographic structure, the pressure increases with the density, but not with the temperature for a fixed density. In the latter case, we present stress profiles through the UO₂ matrix before and after xenon adsorption. The next step will be to introduce these results in a micromechanical model in order to derive a thermomechanical behavior law for the porous UO₂.

[SY-B3] Symposium B-3

Chair: Kazuto Arakawa(Shimane University, Japan)

Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10

[SY-B3] **Formation of radiation-induced Re and Os precipitation in W and its effects on mechanical properties**

○Guang-Hong Lu, Yu-Hao Li, Hong-Bo Zhou (Beihang University, China)

[SY-B3] **Elastic fields and interaction between self-interstitial atom defects in bcc metals.**

○Sergei L Dudarev, Pui-Wai Ma (UK Atomic Energy Authority, UK)

[SY-B3] **Molecular dynamics simulation study of the interaction of Re with interstitial defects in tungsten bulk**

Yangchun Chen¹, Jingzhong Fang¹, Ning Gao², Hong-Bo Zhou³, Wangyu Hu⁴, Fei Gao^{4,5}, ○Huiqiu Deng^{1,4} (1.School of Physics and Electronics, Hunan University, China, 2.Institute of Modern Physics, Chinese Academy of Sciences, China, 3.Department of Physics, Beihang University, China, 4.College of Materials Science and Engineering, Hunan University, China, 5.Department of Nuclear Engineering and Radiological Science, University of Michigan, United States of America)

[SY-B3] **Hydrogen super-saturated layers in plasma loaded tungsten: a global model combining Density Functional Theory data, Thermodynamic and Kinetic models**

○Yves Ferro, Etienne Hodille (Aix-Marseille University, France)

[SY-B3] **Mobility of small vacancy and interstitial prismatic dislocation loops in BCC tungsten**

○Jan Fikar¹, Roman Gröger¹, Robin Schäublin² (1.Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic, Switzerland, 2.Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, Switzerland)

 (Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10)

[SY-B3] Formation of radiation-induced Re and Os precipitation in W and its effects on mechanical properties

Invited

[○]Guang-Hong Lu, Yu-Hao Li, Hong-Bo Zhou (Beihang University, China)

Tungsten (W) is one of the most promising candidates for plasma facing materials in future fusion reactors. Rhenium (Re) and Osmium (Os) are not only the typical alloying elements but also the main productions of transmutation in W. More importantly, Re and Os will aggregate and precipitate under high energy radiation, which substantially enhance the radiation hardening and embrittlement, leading to the great concerns for the life-limiting of W. So far, the formation mechanism of Re/Os-rich clusters in W as well as its influences on the mechanical properties remains to be fully elucidated.

We have investigated the interaction between Re/Os and defects in W using a first-principles method in combination with thermodynamic models in order to explore the precipitating mechanism of Re/Os under irradiation. It is found that the presence of defects can significantly reduce the total nucleation free energy change of Re/Os, and thus facilitate the nucleation of Re/Os in W. Kinetically, self-interstitial atom is shown to be easily trapped by substitutional Re/Os, and form W-Re/Os mixed dumbbell. Such W-Re/Os dumbbell combining with the substitutional Re/Os atom will transfer to high stable Re/Os-Re/Os dumbbell, which can serve as a trapping centre for subsequent W-Re/Os dumbbells, leading to the growth of Re/Os-rich clusters. Consequently, an interstitial-mediated migration and aggregation mechanism for Re and Os precipitation has been proposed.

To shed light on the effects of transmutation elements on the mechanical properties, we further have investigated the influences of Re on the motion of $1/2$ screw dislocation in W. It is found that the influence of Re on the dislocation motion is directly related to the distribution of Re in W. For the state of Re dispersed distribution, the addition of Re will reduce the generalized stacking fault energy (GSFE) for both $1/2\{112\}$ and $1/2\{110\}$, and improve the ductility. However, the influence of Re clusters (for the state of Re aggregation) on the dislocation motion is significantly different from that of dispersed Re. The presence of Re clusters will substantially increase the Peierls stress and energy, inhibiting the dislocation mobility. This will significantly exacerbate the irradiation hardening, and thus degrade the mechanical properties of W.

 (Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10)

[SY-B3] Elastic fields and interaction between self-interstitial atom defects in bcc metals.

[○]Sergei L Dudarev, Pui-Wai Ma (UK Atomic Energy Authority, UK)

Strongly anisotropic self-interstitial defect configurations form spontaneously in body-centred cubic metals, like sodium or tungsten, if an extra atom is inserted in the crystal lattice and the resulting structure is relaxed into the lowest energy configuration. The equilibrium structure and modes of Brownian motion of individual SIA defects in body-centred transition metals are now well established. Yet, there is still no regular approach to modelling evolution of ensembles of such defects that would include the treatment of elastic interaction between them. The difficulty appears fundamental, illustrating the lack of a suitable mathematical formalism, linking the discrete atomistic representation of nano-scale defects with continuum elasticity. We derive an analytical expression for the dipole tensor of a dislocation loop, valid in the isotropic and anisotropic

elasticity approximations, and explore it in the limit of infinitely small loop size. We discover that the prediction for the dipole tensor of a point defect that does not agree with numerical calculations even for defects in tungsten, a material that is well described by isotropic elasticity theory. We then derive an analytical formula for the dipole tensor of a defect using a two-parameter tensor form, which shows that in addition to a pure prismatic dislocation loop character, the elastic field of a SIA defect contains a significant dilatation component. We evaluate the energy of interaction between SIA defects, and between a SIA defect and a dilatation centre, e.g. a vacancy cluster. To illustrate applications of the new formalism, we compute the energy of interaction between SIA defects ordered as a periodic simple cubic super-lattice, encountered in a DFT calculation. Surprisingly, we find that the energy minimum of such a periodic configuration corresponds to the orientation of the directional unit vector of the defect collinear with a 111 direction.

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(Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10)

[SY-B3] Molecular dynamics simulation study of the interaction of Re with interstitial defects in tungsten bulk

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Tungsten (W) and W-based alloys have been considered as promising candidates for plasma-facing materials (PFMs) in future fusion reactors. However, the neutrons generated in fusion reactions result in not only the cascade damage but also the transmutation products (mainly Re and Os) in W bulk. The irradiation defects and transmutation products will have a serious effect on the service behaviors of W PFMs under the condition of fusion irradiation. With molecular dynamics simulations and W-Re potentials developed recently in our group, we have systematically investigated the interaction between Re atom/cluster and interstitial defects in W bulk. It is found that: (1) the self-interstitial atoms (SIAs) and interstitial Re atoms are energetically favorable to align along $\langle 111 \rangle$ direction in the form of W-W and Re-W dumbbell/crowdion, respectively; (2) the SIA clusters and $1/2\langle 111 \rangle$ interstitial dislocation loops can undergo fast migration along $\langle 111 \rangle$ direction and their migration barriers (< 0.1 eV) are nearly independent of defect size; (3) Re atoms inhibit the migration and growth of SIA clusters, due to their strong attractions; (4) newly formed Re-Re dumbbells and Re-W mixed dumbbell clusters are thermally stable and immobile, which can serve as the trapping center for subsequent Re-W mixed dumbbell, leading to the growth of Re clusters in W. The present work is helpful for understanding the interaction of Re with interstitial defects and dislocation loops and the initial nucleation mechanism of Re atoms in bulk W, and the results can also be used to supply more accurate inputs for larger-scale simulations such as object kinetic Monte Carlo simulations.

(Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10)

[SY-B3] Hydrogen super-saturated layers in plasma loaded tungsten: a global model combining Density Functional Theory data, Thermodynamic and Kinetic models

Yves Ferro, Etienne Hodille (Aix-Marseille University, France)

In this work, we combined Density Functional Theory data, a Thermodynamic and a kinetic model to build a global model enabling to determine the total concentration of hydrogen implanted in the sub-surface of tungsten exposed to a hydrogen flux. This is achieved given a flux of hydrogen, a temperature of implantation, and the energy of the incoming hydrogen ions. This model is built step by step; an equilibrium with a molecular hydrogen gas phase is first considered and the resulting solubility is compared with experimental results. A kinetic model is subsequently used to determine a chemical potential for hydrogen in the sub-surface of tungsten. Combining both these models, two regimes are then established in which hydrogen is trapped at interstitial sites or in vacancies. The existence of these two regimes are driven by the temperature of implantation; above a temperature of implantation is the *interstitial* regime, below is the *vacancy* regime in which super-saturated layers are formed. A simple analytical and easy to use expression is work-out for the transition temperature, which allows to plot a diagram of existence of the super-saturated layer depending on the implantation temperature, the incident energy and the flux of the hydrogen ions.

(Wed. Oct 31, 2018 2:00 PM - 3:15 PM Room10)

[SY-B3] Mobility of small vacancy and interstitial prismatic dislocation loops in BCC tungsten

Jan Fikar¹, Roman Gröger¹, Robin Schäublin² (1.Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic, Switzerland, 2.Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, Switzerland)

Vacancies and self interstitials produced in collision cascades often form clusters, which can further collapse into prismatic dislocation loops. In BCC metals dislocation loops with Burgers vectors $1/2$ and are observed and they can be either vacancy or interstitial type. These dislocation loops usually move easily in the direction of the Burgers vector. The mobility of prismatic dislocation loops is studied by molecular dynamics. The small dislocation loops under 100 defects seem to behave more like point defect clusters and the mobility of vacancy loops is substantially lower than the one of interstitial loops. Similar effect is observed in formation energies, where the small vacancy loops have higher formation energies than the corresponding interstitial loops. At larger sizes the dislocation loops seem to behave as perfect dislocations and there is no difference between vacancy and interstitials loops mobilities and formation energies.

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

[SY-B4] Symposium B-4

Chair: Gary S Was (University of Michigan, United States of America)

Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room10

[SY-B4] Kinetics of Precipitation in Fe-Cr and Fe-Cr-C alloys under Irradiation

○ Frederic Soisson (CEA Saclay, France)

[SY-B4] The complex problem of the experimental validation of atomistic and microstructural evolution models

○ Lorenzo Malerba (CIEMAT, Energy, Environment and Technology Research Centre, Spain)

[SY-B4] Physically based prediction of radiation hardening: application to steels and model alloys

○ Ghiath Monnet (EDF - R&D, MMC, France)

[SY-B4] Oxygen diffusion in bcc Fe under the influence of foreign atoms and vacancies

○ Xiaoshuang Wang, Matthias Posselt, Jürgen Faßbender (Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany)

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room10)

[SY-B4] Kinetics of Precipitation in Fe-Cr and Fe-Cr-C alloys under Irradiation

Invited

○Frederic Soisson (CEA Saclay, France)

In ferritic steels, the precipitation of the Cr-rich α' phase leads to a degradation of mechanical properties. Below 400°C, the precipitation is usually too slow to be a real concern, but it can be significantly accelerated by irradiation, due to an increase in point defect concentrations. Irradiation also produces a ballistic mixing between Fe and Cr atoms, and therefore prevent the nucleation of α' precipitates or the dissolution of existing ones.

We present a multiscale approach which models these contradictory effects by taking into account the different mechanisms of atomic transport taking place under irradiation: the creation of vacancies and self-interstitials and the ballistic mixing within displacement cascades, the thermally activated diffusion of point defects, and their elimination at sinks or by mutual recombination. The method combines DFT calculations (which provide the fundamental information on thermodynamics and point defects properties), atomistic Kinetic Monte Carlo Simulations (to model the diffusion of point defects and the α' precipitation), and Cluster Dynamics (to model the evolution of the sink density under irradiation). The simulations show that the acceleration of the α' precipitation occurs under irradiation at low or moderate dose rates, but that ballistic dissolution becomes dominant under ion irradiation at high dose rates -- due to a large density of sinks that limits the point defect supersaturation.

The results of the simulations are compared with recent experimental studies. The same multiscale approach is used to model the diffusion of carbon atoms in Fe-Cr alloys and their strong interaction with point defects. We will consider their possible effect on Fe and Cr diffusion, and on the kinetics of α' precipitation under irradiation.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room10)

[SY-B4] The complex problem of the experimental validation of atomistic and microstructural evolution models

○Lorenzo Malerba (CIEMAT, Energy, Environment and Technology Research Centre, Spain)

The development of physical models for the description of the behaviour of materials under certain conditions goes hands-in-hands with the use of advanced experimental characterization techniques. The experiments provide data and reveal phenomena that the models are expected to predict and explain. The exchange of information between models and experiments is therefore continuous and goes in two directions: models may predict results that need to be verified experimentally and experiments observe processes that the models are expected to reproduce and explain in terms of physical laws and mechanisms. This continuous interplay is often denoted as "experimental validation" of models. While this definition is somewhat restrictive, the validation of models is a discipline in itself that requires first of all the performance of experiments that may be long and expensive, and need to be carefully designed. In addition, the comparison between the results of the models, in particular computer simulations, and the observations from characterization techniques is not always straightforward, because both the experimental and the simulation

outcomes need to be properly treated.

In this presentation these problems will be discussed taking the example of the comparison between models that describe the microstructural evolution of iron alloys under irradiation and the results of microstructural characterization techniques such as positron annihilation, small angle neutron scattering, atom probe and transmission electron microscopy.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room10)

[SY-B4] Physically based prediction of radiation hardening: application to steels and model alloys

○Ghiath Monnet (EDF - R&D, MMC, France)

Based on a multiscale modeling framework, it is shown that radiation hardening can be rationalized in several industrial materials and model alloys. Microstructure features of the as-received materials are first considered for the assessment of the yield stress prior to irradiation. The later can be decomposed into two contributions: short-range stresses induced by local obstacles (such as forest dislocations, precipitates, etc.) and long-range stresses resulting from sub-grain dislocation walls and grain boundaries. Introducing radiation defects as local obstacles, the same methodology can be employed to predict the yield stress of the irradiated materials. The considered radiation defects are solute clusters (SCs) and Dislocations Loops (DLs). SCs are assumed to be spherical coherent precipitates that can be sheared by dislocations with a given shear resistance, computed from atomistic simulations. This resistance is used in Dislocations Dynamics (DD) simulations to compute hardening induced by SCs. The sizes and densities implemented in DD simulations are those given by experiment (TEM, APT, SANS etc.). The contribution of DLs is computed from DD simulations. Upon interaction with mobile dislocations, small DLs are absorbed leading to strong pinning and high hardening level, while large DLs experience classical dislocation-dislocation interactions (junction, annihilation, etc.). The yield stress of the irradiated materials is predicted using the constitutive equations of radiation hardening induced by SCs and DLs.

Several FeCr, FeMnNi model alloys and some RPV steels are considered for the validation of the model. It is shown that local obstacles (present before irradiation) may have a significant effect on radiation effects on the mechanical properties: radiation hardening is not independent of the initial yield stress. With almost no adjustable parameters, the predicted increase in the yield stress is found in close agreement with experiment.

(Wed. Oct 31, 2018 4:00 PM - 5:15 PM Room10)

[SY-B4] Oxygen diffusion in bcc Fe under the influence of foreign atoms and vacancies

○Xiaoshuang Wang, Matthias Posselt, Jürgen Faßbender (Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany)

A multiscale approach including Density Functional Theory (DFT) and Atomistic Kinetic Monte Carlo (AKMC) simulations is applied to investigate the diffusion of oxygen in bcc Fe under the influence of substitutional

foreign atoms or solutes (Al, Si, P, S, Ti, Cr, Mn, Ni, Y, Mo, W) and vacancies. The solutes can be assumed to be immobile since their diffusion coefficient is much smaller than that of oxygen. On the other hand, the vacancy mobility must be considered in the calculations because it is comparable to that of oxygen. The most stable state of oxygen in pure bcc Fe is the octahedral interstitial configuration. Recently, jumps of oxygen in pure bcc Fe, between first-, second-, and third-neighbor octahedral interstitial sites were investigated by DFT. It was found that the first-neighbor jump is most relevant. The second-neighbor jump consists of two consecutive first-neighbor jumps whereas the barrier of the third-neighbor jump is too high to be significant for the diffusion process. In this work DFT is used to determine the modified migration barriers in the presence of solutes. It is found that Si, P, Ni, Mo and W have some effect on the migration barriers of oxygen and their interaction with O is mainly repulsive. Al, Cr and Mn have a significant influence on the barriers and they exhibit strong attractive interactions with O. The most important modification of the barriers is found for S, Ti, and Y where deep attractive states exist. The barriers for oxygen jumps near a vacancy and barriers for vacancy jumps in the environment of oxygen are also calculated by DFT. Based on the migration barriers obtained by DFT, AKMC simulations on a rigid lattice are employed to determine the diffusion coefficient of oxygen in a dilute iron alloy containing different substitutional foreign atoms. It is found that Si, P, Ni, Mo, and W have almost no influence on the diffusivity of O. The presence of Al, Cr, Mn, S, Ti, and Y causes a significant reduction of the mobility of oxygen. Another version of the AKMC code is applied to investigate the mutual influence of oxygen and vacancy diffusion as well as the migration of the oxygen-vacancy pair.