Tue. Oct 30, 2018

Room1

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

[SY-C3] Symposium C-3

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

[SY-C3] Quantifying the effect of hydrogen on dislocation dynamics in microcrystals: A three-dimensional discrete dislocation dynamics study

Yejun Gu, ○Jaafar A. El-Awady (Johns Hopkins University, United States of America)

[SY-C3] Discrete dislocation plasticity modelling of hydrogen dislocation interactions in micro-cantilevers

○Haiyang Yu[1], Alan Cocks[2], Ed Tarleton[1] (1.Dept. of Materials, Univ. of Oxford, UK, 2.Dept. of Engineering, Univ. of Oxford, UK)

[SY-C3] Dislocation climb models from atomistic scheme to dislocation dynamics

○Yang Xiang[1], Xiaohua Niu[2] (1.Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong, 2.Department of Mathematics, Jimei University, China)

[SY-C3] Investigation of the Hall-Petch Effect with DD Simulation

○Maoyuan Jiang[1,2], Benoit Devincre[2], Ghiath Monnet[1] (1.EDF - R&D, Les Renardieres, France, 2.Laboratoire d'Etude des Microstructures, CNRS/ONERA, France)

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

[SY-C4] Symposium C-4

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

[SY-C4] **Hydrogen consequences on cyclic behaviour of <001> nickel single crystals : a multi-scale approach.**

○xavier Feaugas, Guillaume Hachet, Arnaud Metsue, abdelali Oudriss (université de la rochelle, France)

[SY-C4] **Atomistic and continuum approaches to analyse precipitation hardening in metallic alloys**

Gustavo Esteban-Manzanares[1,2,3], Rodrigo Santos[1,2], Anxin Ma[1], Ioannis Papadimitriou[1], Enrique Martínez[3], Laurent Capolungo[3], Javier Segurado[1,2], ○Javier LLorca[1,2] (1.IMDEA Materials Institute, Spain, 2.Polytechnic University of Madrid, Spain, 3.Los Alamos National Laboratory, United States of America)

[SY-C4] Dislocation-precipitate interaction in Al-Mg-Si alloys

○Inga Gudem Ringdalen[1], Sigurd Wenner[1], Jaime Marian[2] (1.Dept. of Materials and Nanotechnology, SINTEF, Norway, 2.Dept. of Material Science and Engineering, UCLA, United States of America)

Room2

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E3] Symposium E-3

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

[SY-E3] 3D mesoscopic study of the stability of three-dimensional short cracks in FCC metals using the Discrete-Continuous Model

Laurent Korzeczek[1], Riccardo Gatti[1], Arjen Roos[2], ○Benoit Devincre[1] (1.LEM, CNRS-ONERA, France, 2.Safran Tech, France)

[SY-E3] Role of cracks, voids and interfaces in hot spot formation and initiation of energetic materials

Michael Sakano[1], Chunyu Li[1], Nicolo Grilli[2], Brenden Hamilton[1], Camilo Duarte[2], Marisol Koslowski[2], ○Alejandro Strachan[1] (1.School of Materials Engineering, Purdue University, United States of America, 2.School of Mechanical Engineering, Purdue University, United States of America)

[SY-E3] Precipitation hardening effects on extension twinning in magnesium

○Haidong Fan[1], Jaafar El-Awady[2], Dierk Raabe[3] (1.Sichuan University, China, 2.The Johns Hopkins University, United States of America, 3.Max-Planck-Institut für Eisenforschung GmbH, Germany)

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E4] Symposium E-4

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

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

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

[SY-E4] Catalyst design for ammonia synthesis of ammonia

○Chenghua Sun （Swinburne University of Technology, Australia）

[SY-E4] A solid-solution structure model for multi-component alloys

○Xingyu Gao[1,2], Fuyang Tian[3], Yafan Zhao[2], Deye Lin[2], Haifeng Song[1,2] （1.Institute of Applied Physics and Computational Mathematics, China, 2.CAEP Software Center for High Performance Numerical Simulation, China, 3.University of Science and Technology, China）

[SY-E4] First-princples prediction of plastic deformation modes in alloys

○Song Lu, Levente Vitos （KTH Royal Institute of Technology, Sweden）

[SY-E4] The local-orbital construction of strongly correlated electrons based on the PAW method

○Yu Liu[1,2], Xingyu Gao[1,2], Jianzhou Zhao[3], Haifeng Song[1,2] （1.Institute of Applied Physics and Computational Mathematics, China, 2.CAEP Software Center for High Performance Numerical Simulation, China, 3.Southwest University of Science and Technology, China）

Room3

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

[SY-F3] Symposium F-3

Chair: Carl Krill(Institute of Micro and Nanomaterials, Ulm University, Germany)
9:45 AM - 11:00 AM Room3

[SY-F3] Biomineralization in molluscan shells: From ideal to hierarchical grain growth

○Dana Zoellner, Igor Zlotnikov （B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany）

[SY-F3] **Mesoscale modeling of cement: texture, mechanics and durability**

○Katerina Ioannidou[1,2,3], Emanuela Del Gado[4], Franz J. Ulm[1], Roland J.-M. Pellenq[1,2,3] （1.Dept. of Civil and Enviromental Engineering, Massachusetts Institute of Technology, United States of America, 2.MultiScale Material Science for Energy and Environment, Massachusetts Institute of Technology-CNRS/MIT/AMU Joint Lab. at MIT, United States of America, 3.MIT Energy Initiative, United States of America, 4.Dept. of Physics and Institute for Soft Matter Synthesis and Metrology, Georgetown Univ., United States of America）

[SY-F3] **Actuation in Metal-Polymer Nanocomposites: Chemoelectromechanical Coupling on Interfaces**

○Jana Wilmers, Swantje Bargmann （Chair of Solid Mechanics, University of Wuppertal , Germany）

[SY-F3] Mechanics of Cilia Beating - A Relationship Between Metachronal Wavelength and Fluid Flow Rate

○Jon Hall, Nigel Clarke （The University of Sheffield, UK）

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

[SY-F4] Symposium F-4

Chair: Dana Zoellner(B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany)
11:15 AM - 12:30 PM Room3

[SY-F4] Showdown! Pitting computer simulations against time-resolved experimental measurements of grain growth in 3D

Mingyan Wang[1], Nan Wang[2], Jules Dake[1], Søren Schmidt[3], ○Carl Krill[1] （1.Institute of Micro and Nanomaterials, Ulm University, Germany, 2.Dept. of Physics, McGill University, Canada, 3.Dept. of Physics, Technical University of Denmark, Denmark）

[SY-F4] Coarsening and grain-growth in an SOFC-anode under surface and grain boundary self-diffusion: A Multiphase-field approach

○Paul Hoffrogge[1], Daniel Schneider[1,2], Britta Nestler[1,2], Patricia Haremski[2,3], Matthias Wieler[3], Piero Lupetin[3] （1.Karlsruhe University of Applied Sciences, Germany, 2.Karlsruhe Institute of Technology, Germany, 3.Robert Bosch GmbH, Germany）

[SY-F4] Solidification Simulation in Additive Manufacturing Process of Ti-Alloy by ICME approach

○Yusuke SHIMONO, Mototeru Oba, Sukeharu Nomoto （Itochu Techno-Solutions Corp., Japan）

[SY-F4] **Phase Field Model of Microstructural Evolution in Metal Alloy for Designing Mechanical Property**

Wooju Lee, ○Dongchoul Kim （Dept. of Mechanical Engineering, Sogang Univ., Korea）

Room4

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

[SY-M3] Symposium M-3

Chair: Thomas Franosch(University of Innsbruck, Austria)
9:45 AM - 11:00 AM Room4

[SY-M3] Heterogeneous thermal properties in a glass from molecular dynamics calculations

○Jean-Louis BARRAT （Univ. Grenoble Alpes, France）

[SY-M3] Structural-dynamical phase transition in the phase space of histories of a polydisperse hard sphere liquid

○Matteo Campo[1,2], Thomas Speck[1] （1.Johannes Gutenberg University Mainz, Germany, Germany, 2.Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany, Germany）

[SY-M3] Time- and History-dependent Structure and Morphology of van-der-Waals Liquids forming Physical Gels and Porous Glasses

○Magdaleno Medina-Noyola, Leticia Lopez-Flores, Jose Manuel Olais-Govea, Benigno Zepeda-Lopez （Instituto de Fisica (Laboratorio Nacional de Ingenieria de la Materia Fuera de Equilibrio), Universidad Autonoma de San Luis Potosi, Mexico）

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

[SY-M4] Symposium M-4

Chair: Leticia Lopez Flores(University of San Luis Potosi, Mexiko)
11:15 AM - 12:30 PM Room4

[SY-M4] Mechanical behavior and emerging morphologies in active matter

○Ignacio Pagonabarraga （CECAM, EPFL, Switzerland）

[SY-M4] Time dependent interaction between intruders in granular media

○Hisao Hayakawa [1], Takahiro Tanabe[2] （1.Yukawa Institute for Theoretical Physics, Kyoto Univeristy, Japan, 2.Graduate School of Advanced Mathematical Sciences, Meiji University, Japan）

[SY-M4] Hystory-dependent shear jamming of granular materials under oscillatory shear

○Michio Otsuki[1], Hisao Hayakawa[2] （1.Graduate School of Engineering Science, Osaka Univ., Japan, 2.Yukawa Institute for Theoretical Physics, Kyoto Univ., Japan）

[SY-M4] Structural predictor for nonlinear sheared dynamics in simple glass-forming liquids

○Trond S. Ingebrigtsen, Hajime Tanaka （University of Tokyo, Japan）

Room5

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

[SY-O3] Symposium O-3

Chairs: Momoji Kubo(Tohoku University, Japan), Michael Moseler(Fraunhofer Institute for Mechanics of Materials IWM, Germany)
9:45 AM - 11:00 AM Room5

[SY-O3] Scale Dependence of Friction: How Elasticity Destroys Superlubricity

Joseph Monti[1], Lars Pastewka[2], ○Mark Owen Robbins[1] （1.Dept. of Physics and Astronomy, Johns Hopkins University, United States of America, 2.University of Freiburg, Germany）

[SY-O3] Coarse-Grain Simulations of Polymer Solutions with Hydrodynamics and Long-range Interactions

○Hitoshi Washizu[1,2], Hiroaki Yoshida[3], Soma Usui[1], Taiki Kawate[1] （1.Univ. Hyogo, Japan, 2.Kyoto Univ., Japan, 3.Toyota Central R&D Labs., Inc., Japan）

[SY-O3] **A Multi-Scale Approach for the Design of Novel Lubricants**

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

[SY-O3] Impact of ionic liquid ordering on their triborheological properties

○Konstantinos Gkagkas[1], Andras Vernes[2,3] （1.Advanced Material Research Division, Toyota Motor Europe NV/SA, Belgium, 2.AC2T research GmbH, Austria, 3.Institute of Applied Physics, TU Wien, Austria）

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

[SY-O4] Symposium O-4

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

[SY-O4] Molecular simulation to better understand soot-detergent interactions in engine oils

○Sophie LOEHLE[1], Elias Gebremedhn[2], Michael Mazarin[1], Stephan Steinman[2], Carine Michel[2] （1.Total M&S, France, 2.ENS Lyon, France）

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

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

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

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

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

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

Room6

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A3] Symposium A-3

Chair: Katsuyo Thornton(University of Michigan, Ann Arbor, United States of America)
9:45 AM - 11:00 AM Room6

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

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

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

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

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

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

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

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

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A4] Symposium A-4

Chair: David L McDowell(Woodruff School of Mechanical Engineering, Georgia Institute of Technology, United States of America)
11:15 AM - 12:30 PM Room6

[SY-A4] Effective Transport Properties of Polycrystalline Materials

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

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

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

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

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

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

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

Room7

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

[SY-I3] Symposium I-3

Chair: Peter Voorhees(Northwestern University, United States of America)
9:45 AM - 11:00 AM Room7

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

and continuum

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

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

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

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

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

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

[SY-I4] Symposium I-4

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

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

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

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

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

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

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

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

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

Room8

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

[SY-L3] Symposium L-3

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

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

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

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

○Lasse Laurson （Aalto University, Finland）

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

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

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

[SY-L4] Symposium L-4

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

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

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

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

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

[SY-L4] **Temporal and spatial plastic instability of**

micrometer-scaled materials

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

Room9

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

[SY-H1] Symposium H-1

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

[SY-H1] **Multiscale modeling of electro-responsive gels**

○Masao Doi （Beihang University, China）

[SY-H1] Non-monotonic particle size effect on the glass transition in polymer-particle blends and its application to shape memory polymers

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

[SY-H1] **Thermomechanical behavior of shape-memory polyurethane copolymer : A coarse-grained molecular dynamics simulation**

○SUNGWOO PARK, JUNGHWAN MOON, BYUNGJO KIM, MAENGHYO CHO （Seoul National University, South Korea, Korea）

[SY-H1] **Investigation of photo-mechanical behavior of azobenzene-based polymer: A coarse-grained molecular dynamics study**

○Junghwan Moon[1], Byungjo Kim[1], Joonmyung Choi[2], Maenghyo Cho[1,3] （1.Divison of Multiscale Mechanical Design, School of Mechanical and Aerospace Engineering, Seoul National University, Korea, 2.Mechatronics R&D center, SAMSUNG ELECTRONICS CO., LTD, Korea, 3.Institute of Advanced Machines and Design, Seoul National University, Korea）

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

[SY-H2] Symposium H-2

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

[SY-H2] **Hydrogels with Dynamic Sacrificial Bonds - From Toughness to Adhesion to Composites -**

○Jian Ping Gong[1,2] （1.Faculty of Advanced Life Science, Hokkaido University, Japan, 2.Soft Matter GI-CoRE, Hokkaido University, Japan）

[SY-H2] Elastic properties and effective interactions of *in silico* realistic microgels

○Lorenzo Rovigatti[1,2], Nicoletta Gnan[1,2], Emanuela Zaccarelli[1,2] （1.Institute for Complex Systems, Uos Sapienza - CNR, Italy, 2.Dipartimento di Fisica, Sapienza Università di Roma, Italy）

[SY-H2] Controlling the mechanics of a synthetic hydrogel with motor-like internal contractility

Marcos Fernandez-Castano Romera[1], Rint P Sijbesma[1], ○Cornelis Storm[1] （1.Theory of Polymers and Soft Matter, Technische Universiteit Eindhoven, The Netherlands）

[SY-H2] **Study on viscoelastic behavior of natural rubber with multiscale approach**

○Byungjo Kim, Junghwan Moon, Maenghyo Cho （Seoul National University, Korea）

Room10

Symposium | J. Multiscale Modeling of Heterogeneous Layered Media

[SY-J3] Symposium J-3

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

[SY-J3] Fundamentals of Generalized Particle (GP) Multiscale Methods with Applications to Analyses of Alternatively-Arranged Soft and Hard Layers

○Jinghong Fan （Kazuo Inamori School of Engineering, Alfred University, United States of America）

[SY-J3] **The effect of layer thickness ratio on the plastic deformation mechanisms of nonoindented Ti/TiN nanolayered composite: A molecular dynamics study**

○Georges Y Ayoub[1], Wei yang[2], Iman Salehinia[3], Bilal Mansoor[2], Hussein Zbib[4] （1.Dept. of Industrial and manufacturing system Engineering, Univ. of Michigan, United States of America, 2.Dept. of Mechanical Engineering, Texas A&M Univ., United States of America, 3.Dept. of Mechanical Engineering, Northern Illinois Univ., United States of America, 4.School of Mechanical and Materials Engineering, Washington State Univ., United States of America）

[SY-J3] The attenuation of stress wave propagation in multilayer structure

○Fengyuan Yang, Zhanli Liu （Tsinghua University,

China）

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

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

Symposium | J. Multiscale Modeling of Heterogeneous Layered Media

[SY-J4] Symposium J-4

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

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

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

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

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

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

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

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

[SY-C3] Symposium C-3

Chair: Francois Willaime(DEN-Departement des Materiaux pour le Nucleaire, CEA, Universite Paris-Saclay, France)

Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room1

[SY-C3] Quantifying the effect of hydrogen on dislocation dynamics in microcrystals: A three-dimensional discrete dislocation dynamics study

Yejun Gu, ○Jaafar A. El-Awady （Johns Hopkins University, United States of America）

[SY-C3] Discrete dislocation plasticity modelling of hydrogen dislocation interactions in micro-cantilevers

○Haiyang Yu[1], Alan Cocks[2], Ed Tarleton[1] （1.Dept. of Materials, Univ. of Oxford, UK, 2.Dept. of Engineering, Univ. of Oxford, UK）

[SY-C3] Dislocation climb models from atomistic scheme to dislocation dynamics

○Yang Xiang[1], Xiaohua Niu[2] （1.Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong, 2.Department of Mathematics, Jimei University, China）

[SY-C3] Investigation of the Hall-Petch Effect with DD Simulation

○Maoyuan Jiang[1,2], Benoit Devincre[2], Ghiath Monnet[1] （1.EDF - R&D, Les Renardieres, France, 2.Laboratoire d'Etude des Microstructures, CNRS/ONERA, France）

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room1)

[SY-C3] Quantifying the effect of hydrogen on dislocation dynamics in microcrystals: A three-dimensional discrete dislocation dynamics study

Invited

Yejun Gu, ○Jaafar A. El-Awady (Johns Hopkins University, United States of America)

We present a new framework to quantify the effect of hydrogen on dislocation plasticity using large scale three-dimensional (3D) discrete dislocation dynamics (DDD) simulations. In this model, the first order elastic interaction energy associated with the hydrogen-induced volume change is accounted for. The three-dimensional stress tensor induced by hydrogen concentration, which is in equilibrium with respect to the dislocation stress field, is derived using the Eshelby inclusion model, while the hydrogen bulk diffusion is treated as a continuum process. This newly developed framework is utilized to quantify the effect of hydrogen on the different aspects of dislocation-mediated plasticity in Ni single crystal microcrystals. The combined effect of hydrogen concentration, crystal size, and dislocation density is quantified. Finally, the effects of pipe diffusion is also rationalized from comparisons with experimental results.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room1)

[SY-C3] Discrete dislocation plasticity modelling of hydrogen dislocation interactions in micro-cantilevers

○Haiyang Yu[1], Alan Cocks[2], Ed Tarleton[1] (1.Dept. of Materials, Univ. of Oxford, UK, 2.Dept. of Engineering, Univ. of Oxford, UK)

One of the most widely accepted theories for hydrogen embrittlement is the hydrogen enhanced localized plasticity (HELP) mechanism which claims hydrogen enhances dislocation activity locally. Experimental evidence for this mechanism has been reported across different scales. Simulations however are mainly limited to the atomistic scale, and continuum scale. Direct simulation of hydrogen dislocation interactions in micromechanical tests is rarely simulated, due to the fact that this scale is beyond the computational capacity of most atomistic calculations and beyond the resolution of most continuum approaches. Discrete dislocation plasticity (DDP) is an ideal technique to bridge the gap in multiscale modelling of hydrogen embrittlement. Recently, a framework which incorporates hydrogen effects in a discrete dislocation simulation was derived by Gu and El-Awady [1] enabling direct investigation of hydrogen dislocation interactions at the microscale. We have implemented this formulation in a new code called *EasyDD,* a GPU accelerated version of *DDLab* coupled with FEM, and performed virtual micromechanical tests with mixed boundary conditions. We have simulated the behaviour of hydrogen charged micro-cantilevers and included the hydrogen induced tractions on the free surfaces. Hydrogen is observed to shield dislocation mutual interactions and to enhance dislocation generation, the combination of these effects leads to global softening and local stress concentrations promoting failure; consistent with the HELP mechanism. To the best of our knowledge, this work is the first to reveal hydrogen dislocation interactions at the discrete dislocation scale in finite volumes, acting as an essential bridge in multiscale modelling.

[1] Gu, Y., &El-Awady, J. A. (2018). Journal of the Mechanics and Physics of Solids, 112, 491-507.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room1)

[SY-C3] Dislocation climb models from atomistic scheme to dislocation dynamics

○Yang Xiang[1], Xiaohua Niu[2] （1.Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong, 2.Department of Mathematics, Jimei University, China）

We develop a mesoscopic dislocation dynamics model for vacancy-assisted dislocation climb by upscalings from a stochastic model on the atomistic scale. Our models incorporate microscopic mechanisms of (i) bulk diffusion of vacancies, (ii) vacancy exchange dynamics between bulk and dislocation core, (iii) vacancy pipe diffusion along the dislocation core, and (iv) vacancy attachment-detachment kinetics at jogs leading to the motion of jogs. Our mesoscopic model consists of the vacancy bulk diffusion equation and a dislocation climb velocity formula. The effects of these microscopic mechanisms are incorporated by a Robin boundary condition near the dislocations for the bulk diffusion equation and a new contribution in the dislocation climb velocity due to vacancy pipe diffusion driven by the stress variation along the dislocation. Our climb formulation is able to quantitatively describe the self-climb of prismatic loops at low temperatures when the bulk diffusion is negligible. Simulations performed show evolution, translation, coalescence of prismatic loops by self-climb that agree with the experimental observations.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room1)

[SY-C3] Investigation of the Hall-Petch Effect with DD Simulation

○Maoyuan Jiang[1,2], Benoit Devincre[2], Ghiath Monnet[1] （1.EDF - R&D, Les Renardieres, France, 2.Laboratoire d'Etude des Microstructures, CNRS/ONERA, France）

Dislocation Dynamics (DD) simulation is used to identify the elementary mechanisms controlling the Hall-Petch (HP) effect on the dislocation scale. The influence of grain size is explored by considering simple periodic polycrystalline aggregates made of grains with cube, plate or needle shapes. We show that the HP effect is globally well reproduced with DD simulations. The HP constant is found to be a function of the grain orientations and shapes. A model is proposed to quantify the influence of the grain morphology. The simulated HP effect is justified by the existence of a backstress inside the grains that emerges from strain incompatibility between grains in a deformed polycrystal. As theoretically expected, Geometrically Necessary Dislocations (GND) are found to accumulate at grain boundaries to accommodate the distortion field discontinuities. By virtue of the Nye’ s tensor, the above property can be directly tested and quantified in DD simulations. For the simplest simulation geometry, the calculated backstress is compared with theoretical predictions. Those results suggest a new strategy for the prediction of the grain size effect in crystal plasticity models.

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

[SY-C4] Symposium C-4

Chair: Dan Mordehai(Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel, Israel)
Tue. Oct 30, 2018 11:15 AM - 12:15 PM Room1

[SY-C4] Hydrogen consequences on cyclic behaviour of <001> nickel single crystals : a multi-scale approach.

○xavier Feaugas, Guillaume Hachet, Arnaud Metsue, abdelali Oudriss （université de la rochelle, France）

[SY-C4] Atomistic and continuum approaches to analyse precipitation hardening in metallic alloys

Gustavo Esteban-Manzanares[1,2,3], Rodrigo Santos[1,2], Anxin Ma[1], Ioannis Papadimitriou[1], Enrique Martínez[3], Laurent Capolungo[3], Javier Segurado[1,2], ○Javier LLorca[1,2] （1.IMDEA Materials Institute, Spain, 2.Polytechnic University of Madrid, Spain, 3.Los Alamos National Laboratory, United States of America）

[SY-C4] Dislocation-precipitate interaction in Al-Mg-Si alloys

○Inga Gudem Ringdalen[1], Sigurd Wenner[1], Jaime Marian[2] （1.Dept. of Materials and Nanotechnology, SINTEF, Norway, 2.Dept. of Material Science and Engineering, UCLA, United States of America）

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

[SY-C4] Hydrogen consequences on cyclic behaviour of <001> nickel single crystals : a multi-scale approach.

Invited

○xavier Feaugas, Guillaume Hachet, Arnaud Metsue, abdelali Oudriss （université de la rochelle, France）

A multi-scale study on the influence of hydrogen on cyclically strained <001> oriented nickel single crystals is conducted in order to understand the impact of the solute on the microstructure and the fatigue properties of nickel single crystal. At macroscopic scale, uniaxial cyclic tests are performed to evaluate the impact of pre-charged hydrogen on the work hardening of the material. Then, at microscopic scale, a mechanical database is provided and associated with the dislocation features, which are explored by transmission electronic microscopy (TEM) observations and correlated with the mechanical behaviour of nickel single crystal with hydrogen. In addition, at atomistic scale, molecular dynamics simulations are carried out to quantify the influence of hydrogen on the dipole sizes and the dislocation organisations, which are partially connected to the elastic properties of nickel. Therefore, we have finally performed a comprehensive study on the impact of hydrogen on the elastic properties of nickel single crystal using a theoretical formalism based on Density Functional Theory and uniaxial tensile tests on <001> oriented nickel single crystals with different concentrations of hydrogen.

This multi-scale approach allows to question the main effect of hydrogen on cyclic plasticity mechanisms. The impact of hydrogen on cyclic stress-strain curves highlights a softening behaviour for <001> multi slips orientation in a similar way as previously related for single slip orientation. This result is firstly discussed in term of dislocation organisations, dipole sizes and distribution but also internal stresses states. Hydrogen impacts the density and the distribution of dislocations and consequently, modifies the internal stress state. Moreover, according to TEM observations, hydrogen ingress promotes the formation of vacancy clusters, in agreement with the super-abundant vacancies (SAV) model. The main consequence of this result is a decrease of the elastic properties of the material, which depends mainly on the formation of the defect induced by the incorporation of hydrogen than a direct effect of the solute itself.

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

[SY-C4] Atomistic and continuum approaches to analyse precipitation hardening in metallic alloys

Gustavo Esteban-Manzanares[1,2,3], Rodrigo Santos[1,2], Anxin Ma[1], Ioannis Papadimitriou[1], Enrique Martínez[3], Laurent Capolungo[3], Javier Segurado[1,2], ○Javier LLorca[1,2] （1.IMDEA Materials Institute, Spain, 2.Polytechnic University of Madrid, Spain, 3.Los Alamos National Laboratory, United States of America）

Precipitation hardening is one of the most efficient mechanisms to increase the yield strength of metallic alloys but accurate quantitative models for this phenomenon are still lacking. Two different approaches, based on atomistic simulations and discrete dislocation dynamics, are presented to address this problem.

Atomistic simulations, in combination with the transition state theory, were used to determine the interaction between Guinier-Preston zones and dislocations in an Al-Cu alloy and between $Mg_{17}Al_{12}$ precipitates and basal dislocations in an Mg-Al alloy. The rate at which dislocations sheared the precipitates (determined by means of molecular dynamics) was controlled by the activation Gibbs free energy, in agreement with the

postulates of the transition state theory. However, harmonic TST does not hold for this interaction. In addition, the activation enthalpy energy and the activation volume were determined and an estimation of the initial shear flow stress as a function of temperature was carried out from the thermodynamic data provided by the atomistic simulations.

In the case of large precipitates that cannot be sheared by dislocations (such as q’ precipitates in Al-Cu alloy), the dislocations overcome the precipitates by the formation of an Orowan loop. The mechanisms of dislocation/precipitate interaction were studied by means of discrete dislocation dynamics using the discrete-continuous method in combination with a fast Fourier transform solver to compute the mechanical fields. Simulations took into account the effect of precipitate shape, orientation and volume fraction as well the elastic mismatch between the matrix and the precipitate, the stress-free transformation strain around the precipitate and the dislocation character as well as dislocation cross-slip. It was found that the influence of the precipitate aspect ratio and orientation were reasonably well captured by the simple Orowan model in the absence of the stress-free transformation strain. Nevertheless, the introduction of the stress-free transformation strain led to dramatic changes in the dislocation/precipitate interaction and in the critical resolved shear stress to overcome the precipitate, particularly in the case of precipitates with small aspect ratio.

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

[SY-C4] Dislocation-precipitate interaction in Al-Mg-Si alloys

○Inga Gudem Ringdalen[1], Sigurd Wenner[1], Jaime Marian[2] （1.Dept. of Materials and Nanotechnology, SINTEF, Norway, 2.Dept. of Material Science and Engineering, UCLA, United States of America）

Partial ageing of commercial Al-Mg-Si aluminum results in microstructures characterized by needle-shaped Si/Mg-rich precipitates. These precipitates belong to the non-equilibrium β" phase and are coherent with the fcc Al lattice, despite of which they can cause considerable hardening. We have investigated the interaction between these β" precipitates and dislocations using a unique combination of modeling and experimental feedback. Dislocation-precipitate interactions including precipitate stress fields are simulated using discrete dislocation dynamics. The displacement fields due to the precipitates are captured by expressions that satisfy elastic equilibrium and are fitted to high-resolution electron microscopy measurements. The stress fields are derived from the displacements assuming isotropic elasticity, and used to study the strength of individual precipitates to dislocation glide as a function of precipitate size, orientation, and dislocation character and length. The dislocation dynamics results are then used to parameterize a probabilistic analysis model to study the difference between the bulk material and the precipitate free zones along the grain boundaries of these alloys.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E3] Symposium E-3

Chairs: Benoit Devincre(LEM, CNRS-ONERA, France), Alejandro Strachan(Purdue University, United States of America)

Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room2

[SY-E3] 3D mesoscopic study of the stability of three-dimensional short cracks in FCC metals using the Discrete-Continuous Model

Laurent Korzeczek[1], Riccardo Gatti[1], Arjen Roos[2], ○Benoit Devincre[1] （1.LEM, CNRS-ONERA, France, 2.Safran Tech, France）

[SY-E3] Role of cracks, voids and interfaces in hot spot formation and initiation of energetic materials

Michael Sakano[1], Chunyu Li[1], Nicolo Grilli[2], Brenden Hamilton[1], Camilo Duarte[2], Marisol Koslowski[2], ○Alejandro Strachan[1] （1.School of Materials Engineering, Purdue University, United States of America, 2.School of Mechanical Engineering, Purdue University, United States of America）

[SY-E3] Precipitation hardening effects on extension twinning in magnesium

○Haidong Fan[1], Jaafar El-Awady[2], Dierk Raabe[3] （1.Sichuan University, China, 2.The Johns Hopkins University, United States of America, 3.Max-Planck-Institut für Eisenforschung GmbH, Germany）

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room2)

[SY-E3] 3D mesoscopic study of the stability of three-dimensional short cracks in FCC metals using the Discrete-Continuous Model

Invited

Laurent Korzeczek[1], Riccardo Gatti[1], Arjen Roos[2], ○Benoit Devincre[1] （1.LEM, CNRS-ONERA, France, 2.Safran Tech, France）

The erratic behaviour of short cracks propagation under low cyclic loading in ductile metals is commonly attributed to a complex interplay between stabilisation mechanisms that occur at the mescopic scale. Among these mechanisms, the interaction with the existing dislocation microstructure play a major role. The dislocation microstructure is source of plastic deformation and heat transfer that reduce the specimen stored elastic energy, screen the crack field due to its self generated stress field or change the crack geometry through blunting mechanisms. For the first time, these mechanisms are investigated with 3D-DD simulations using the Discrete- Continuous Model, modelling three different crack orientations under monotonic traction loading promoting mode I crack opening. Surprisingly, screening and blunting effects do not seem to have a key role on mode I crack stabilisation. Rather, the capability of the specimen to deform plastically without strong forest hardening is found to be the leading mechanism. Additional investigations of two different size effects confirm those results and show the minor contribution of a polarised dislocations density and the associated kinematic hardening on crack stabilisation.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room2)

[SY-E3] Role of cracks, voids and interfaces in hot spot formation and initiation of energetic materials

Invited

Michael Sakano[1], Chunyu Li[1], Nicolo Grilli[2], Brenden Hamilton[1], Camilo Duarte[2], Marisol Koslowski[2], ○Alejandro Strachan[1] （1.School of Materials Engineering, Purdue University, United States of America, 2.School of Mechanical Engineering, Purdue University, United States of America）

The chemical initiation of high-energy (HE) materials following mechanical insults requires the excitation of chemical bonds with lengths of a few angstroms and sub-picosecond vibrational periods. This would be a nearly impossible task were it not for: i) the materials' microstructure that localizes the input energy into hotspots, and ii) the equilibration of inter- and intra-molecular degrees of freedom that transfers input energy to the high-frequency bond vibrations responsible for chemistry. Thus, a predictive understanding of the response of HE to strong mechanical insults requires identifying, characterizing and modeling coupled processes at the microstructural level (interfacial friction, cracks, void collapse), crystal level (dislocations and shear bands) and the molecular/electronic level (inter- and intra-molecular energy transfer and chemical reactions).

While our large-scale molecular dynamics (MD) simulations recently provided an atomic picture of the formation of a steady deflagration wave following shock loading of a defective HE crystal, such simulations cannot capture the complex microstructure of the materials of interest nor the size of the hot spots of interest in real applications. Thus, we developed a multiscale model that combines large-scale reactive and non-reactive MD simulations with a continuum model capable of describing dynamical loading, plastic deformation, fracture and friction, together with thermal transport and chemistry. The MD simulations

provide insight and parameters to characterize energy localization as shock waves interact with several pre-existing defects, including cracks and voids as well as interfaces. In addition, reactive MD simulations are used to characterize thermal transport and develop chemical kinetics models. These results inform the continuum model that is used to predict energy localization in microstructurally complex systems of plastic bonded energetic formulations. These simulations enable us to characterize the relative potency of various microstructural features to general hot spots that can result in sustained chemistry. Both the atomistic and continuum simulations are validated against experiments capable of capturing the physics of interest at scales matching those of the simulations.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room2)

[SY-E3] Precipitation hardening effects on extension twinning in magnesium

○Haidong Fan[1], Jaafar El-Awady[2], Dierk Raabe[3] （1.Sichuan University, China, 2.The Johns Hopkins University, United States of America, 3.Max-Planck-Institut für Eisenforschung GmbH, Germany）

Precipitation is an efficient method to strengthen metallic materials. While precipitation hardening effects on dislocation slip have been studied extensively in the past, the influence of precipitates on twinning mediated plasticity and the development of corresponding hardening models that account for twin-precipitate interactions have received less attention. The interaction of {10-12} extension twin boundaries (TBs) in pure magnesium with precipitates of plate-, sphere- and rod-like shapes is studied using molecular dynamics (MD) simulations. We find that TBs that engulf precipitates are absorbed by the precipitate-matrix interfaces, and the precipitates are neither twinned nor sheared but deform elastically leading to their rotation. TBs can pass small precipitates (length ≈20 nm) and remain intact. In contrast when TBs are interacting with large precipitates (length ≈50 nm), basal dislocations or stacking faults nucleate from the interfaces, causing local plastic relaxation. The stress field around a plate-like precipitate as calculated in the MD simulations suggests that a strong back-stress is imposed on the TBs. We then coarse grain these mechanisms into an analytical mean field model of precipitation hardening on twinning in magnesium alloys, which is based on the energy conservation during the TB-precipitate interaction. The model is in good agreement with the current MD simulations and published experimental observations. The hardening model shows that spherical precipitates have the strongest hardening effect on twinning, basal and prismatic plate-like precipitates have a medium effect while rod-like precipitates exert the weakest influence. We also find that most types of precipitates show a stronger hardening effect on twinning mediated plasticity than on basal dislocation slip. Finally, prismatic plate-like precipitates are predicted to have reasonable hardening effects on both twinning and basal slip. These results can help guiding the development of magnesium alloys with enhanced strength and ductility.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E4] Symposium E-4

Chairs: Haifeng Song(Institute of Applied Physics and Computational Mathematics, China), Chenghua Sun(Swinburne University of Technology, Australia)

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

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

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

[SY-E4] Catalyst design for ammonia synthesis of ammonia

○Chenghua Sun （Swinburne University of Technology, Australia）

[SY-E4] A solid-solution structure model for multi-component alloys

○Xingyu Gao[1,2], Fuyang Tian[3], Yafan Zhao[2], Deye Lin[2], Haifeng Song[1,2] （1.Institute of Applied Physics and Computational Mathematics, China, 2.CAEP Software Center for High Performance Numerical Simulation, China, 3.University of Science and Technology, China）

[SY-E4] First-princples prediction of plastic deformation modes in alloys

○Song Lu, Levente Vitos （KTH Royal Institute of Technology, Sweden）

[SY-E4] The local-orbital construction of strongly correlated electrons based on the PAW method

○Yu Liu[1,2], Xingyu Gao[1,2], Jianzhou Zhao[3], Haifeng Song[1,2] （1.Institute of Applied Physics and Computational Mathematics, China, 2.CAEP Software Center for High Performance Numerical Simulation, China, 3.Southwest University of Science and Technology, China）

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

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

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

With the development of high-performance computer, first-principles calculation becomes to be a feasible way in many nuclear material research fields. In this talk, we will give two examples to demonstrate it. Firstly, we develop two high-performance oriented methods for wave functions in solving the Kohn-Sham equations: a more parallel scalable FFT and optimal extrapolation order for the initial guess at next time step. Armed with adaptive time stepping, we estimate the threshold displacement energy of zirconium by large-scale first-principles calculations. We utilize CESSP to realize the calculations of about 100 tasks on the Tianhe-2 supercomputer in 3 months, where each task is the first-principles molecular dynamic simulation of 9600 valence electrons and 1 picosecond. Compared to classical molecular dynamic simulations, we arrive at the results closest to most recent experiment. Secondly, we have combined a novel crystal structure search method based on the basin hopping algorithm into our first-principles code. Several improvements were implemented, including a symmetry structure generation algorithm based on the crystal space groups, a structure adjustment method based on a virtual spring-force to adjust unreasonably structures. The method is also highly paralleled to make full use of the computing resources. We have applied the method into the structure searching of Zr hydrides (ZrHx, x= 0.5, 1.0, 1.5, 2.0). All experimentally observed Zr hydrides are reproduced, and several new structures were found. The dynamic and thermodynamic stability of these Zr hydrides will also be discussed.

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

[SY-E4] Catalyst design for ammonia synthesis of ammonia

○Chenghua Sun (Swinburne University of Technology, Australia)

Ammonia (NH3) is a critical chemical widely used in modern agriculture and chemical engineering. Currently, it is based on the Haber-Bosch process at high temperature and high pressure. This computational work is to design novel catalysts to achieve ammonia synthesis at room temperature. Single-atom catalyst and defects of low-dimensional materials will be particularly considered. As revealed by first pricinple calculations, Mo-based various catalysts are promising for this applications.

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

[SY-E4] A solid-solution structure model for multi-component alloys

○Xingyu Gao[1,2], Fuyang Tian[3], Yafan Zhao[2], Deye Lin[2], Haifeng Song[1,2] (1.Institute of Applied Physics and Computational Mathematics, China, 2.CAEP Software Center for High Performance Numerical Simulation, China, 3.University of Science and Technology, China)

First-principles calculations have been widely used to predict and design the properties of metallic alloys. However, it is still a challenge to generate *ab initio* suitable structure for multi-component random alloys in a

finite supercell. In this talk, we propose a novel solid-solution structure model to mimic the similar local atomic environment (SLAE) of the random alloys. In the SLAE model, local solid-solution environment such as the random disorder, partial disorder, and short-range order can be calibrated via the standard deviation of the pair distribution function and three-body correlation function. Taking the typical high-entropy alloy CoCrFeMnNi, medium-entropy alloy CoCrNi, and continued solid-solution binary alloy TaW as test cases, we evalueate the SLAE models by comparing between the *ab initio* predicted phase stability and some available experiments.

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

[SY-E4] First-princples prediction of plastic deformation modes in alloys

○Song Lu, Levente Vitos （KTH Royal Institute of Technology, Sweden）

First-principles alloy theory is used to establish the gamma-surface of alloys. Then we put forward a transparent model solely based on first principles simulations for mapping the deformation modes in alloys. The model bridges intrinsic energy barriers and different deformation mechanisms and resolves the complexity of the observed orientation-dependent deformation mechanisms in alloys. Examples of studies are given in austenitic stainless steels and polysynthetic twinned gamma-TiAl alloys.

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

[SY-E4] The local-orbital construction of strongly correlated electrons based on the PAW method

○Yu Liu[1,2], Xingyu Gao[1,2], Jianzhou Zhao[3], Haifeng Song[1,2] （1.Institute of Applied Physics and Computational Mathematics, China, 2.CAEP Software Center for High Performance Numerical Simulation, China, 3.Southwest University of Science and Technology, China）

The effects of electron strong correlation, spin-orbit coupling and multi-configuration bring out challenges in the first principle studies of some nuclear materials and rare-earth materials. Density functional theory (DFT), however, cannot properly describe their electronic structures. For this reason, people have developed Hubbard model based post-DFT method (DFT+X) to correct the strong correlation effect. The coupler that connects the DFT and X still requires more intensive research. In this report, we will present the most recent progress on the DFT+X coupler and its realization in the projector augmented wave (PAW) method under the infrastructure of CESSP code. Firstly, there are three major schemes, namely P0, P1 and P2, to construct the local orbitals of the strong correlated electrons. Prof. Haule from Rutgers University demonstrate the advantages of P2 scheme under the linear augmented plane wave (LAPW) method. However, we are going to show that under the PAW method, P2 is more appropriate for systems with d electrons while P1 is more appropriate for systems with f electrons. Secondly, we realize the correction of spin-orbit coupling and crystal field splitting to the local orbitals, which improves the convergence and accuracy of the DFT+X calculations. We further test our code in the typical strong correlated materials $SrVO_3$ and Ce.

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

[SY-F3] Symposium F-3

Chair: Carl Krill(Institute of Micro and Nanomaterials, Ulm University, Germany)

Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room3

[SY-F3] Biomineralization in molluscan shells: From ideal to hierarchical grain growth

○Dana Zoellner, Igor Zlotnikov （B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany）

[SY-F3] Mesoscale modeling of cement: texture, mechanics and durability

○Katerina Ioannidou[1,2,3], Emanuela Del Gado[4], Franz J. Ulm[1], Roland J.-M. Pellenq[1,2,3] （1.Dept. of Civil and Enviromental Engineering, Massachusetts Institute of Technology, United States of America, 2.MultiScale Material Science for Energy and Environment, Massachusetts Institute of Technology-CNRS/MIT/AMU Joint Lab. at MIT, United States of America, 3.MIT Energy Initiative, United States of America, 4.Dept. of Physics and Institute for Soft Matter Synthesis and Metrology, Georgetown Univ., United States of America）

[SY-F3] Actuation in Metal-Polymer Nanocomposites: Chemoelectromechanical Coupling on Interfaces

○Jana Wilmers, Swantje Bargmann （Chair of Solid Mechanics, University of Wuppertal , Germany）

[SY-F3] Mechanics of Cilia Beating - A Relationship Between Metachronal Wavelength and Fluid Flow Rate

○Jon Hall, Nigel Clarke （The University of Sheffield, UK）

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room3)

[SY-F3] Biomineralization in molluscan shells: From ideal to hierarchical grain growth

Invited

○Dana Zoellner, Igor Zlotnikov （B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany）

The microstructure of grain networks as they can be found in many polycrystalline materials like metals, alloys, and bionic composite structures have an immense impact on their physical properties. Any change in the structure in terms of the size and shape of the grains leads to a change in the properties. Hence, understanding structural changes is of enormous importance for materials development, processing, and application.

In the present work, we investigate the evolution of the prismatic ultrastructures in molluscan shells in form of a comparative study bringing together large numerical and experimental data sets of molluscan shells from different families. To that aim, a framework has been developed for a quantitative study of the process of shell morphogenesis. The method is based on Monte Carlo Potts model simulations of grain boundary motion that, classically, were developed to study coarsening of polycrystalline metals. By employing this approach, we fully reconstruct the growth process of the different molluscan shells: While the prismatic ultrastructure of *Atrina vexillum* is an archetype of ideal grain growth fulfilling the classical growth theories, shells like *Atrina rigida* and *Pinna nobilis* show retarded growth comparable with triple junction controlled grain growth in nanocrystalline metals, and, finally, the mollusc *Pinctada nigra* is characterized by a two-level hierarchical prismatic microstructure, which can be represented in the Potts model by introducing sub-grain boundaries.
The proposed framework is a fundamental approach to study the structural regulation during biomineralization.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room3)

[SY-F3] Mesoscale modeling of cement: texture, mechanics and durability

○Katerina Ioannidou[1,2,3], Emanuela Del Gado[4], Franz J. Ulm[1], Roland J.-M. Pellenq[1,2,3] （1.Dept. of Civil and Enviromental Engineering, Massachusetts Institute of Technology, United States of America, 2.MultiScale Material Science for Energy and Environment, Massachusetts Institute of Technology-CNRS/MIT/AMU Joint Lab. at MIT, United States of America, 3.MIT Energy Initiative, United States of America, 4.Dept. of Physics and Institute for Soft Matter Synthesis and Metrology, Georgetown Univ., United States of America）

Cement is a multiscale porous material, widely produced, more than any other synthetic material on Earth. In this talk, I will present a multiscale bottom-up approach for cement and specifically for calcium-silicate hydrate (C-S-H) that is the most abundant phase of cement. During cement hydration C-S-H nano-scale particles precipitate in the pore solution and form a cohesive gel that is the main binding agent in cement and concrete, crucial for the strength and the long-term evolution of the material. Even more than the molecular structure of C-S-H particles, the C-S-H mesoscale texture over hundreds of nanometers plays a crucial role for material properties. We use a statistical physics framework for aggregating nanoparticles and numerical simulations to obtain a first, to our knowledge, quantitative model for such a complex amorphous material. Our approach is based on precipitation of colloidal particles interacting with effective potentials

associated to the chemical environment. The effective potential can be calculated from atomistic models of C-S-H and are corroborated by experiments. This multiscale informed modelling approach generates realistic micron scale textures in terms of pore size distributions and solid volume fractions and allows to calculate mechanical properties. The extensive comparison with experiments ranging from small-angle neutron scattering, EM imaging, adsorption/desorption of N_2, and water to nano-indentation provides new fundamental insights into the microscopic origin of the cement properties measured. Our results provide a quantitative insight into how the heterogeneities developed during the early stages of hydration persist in the structure of C-S-H and impact the mechanical performance of the hardened cement paste. Moreover, this approach allowed to address durability issues on cement such as freeze-thaw and alkali-silica reaction damage leading to the formation of cracks and fractures.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room3)

[SY-F3] Actuation in Metal-Polymer Nanocomposites: Chemoelectromechanical Coupling on Interfaces

○Jana Wilmers, Swantje Bargmann （Chair of Solid Mechanics, University of Wuppertal , Germany）

Nanoporous metals have recently garnered interest as actuator materials because of their unique microstructure. The characteristic interconnected pore network and resulting high interface-to-volume ratio allows them to react sensitively to electric signals. By coating the metal backbone with ionically-activated polymers, increased actuation strains are achieved while still retaining the metal’s superior mechanical properties.

In understanding and modelling the chemoelectromechanically coupled behaviour of such nanocomposite actuators, one has to account for charge carrier transport and coupled effects in the polymer as well as effects arising from build-up of charges in and at the metal-electrolyte interface. We present an interface-extended continuum model that couples large deformations with electrostatics and charge carrier transport for the bulk and the interface. The developed framework utilises the concept of interface stresses to model the different coupling mechanisms occurring on the interface, that is, interface charging and electroadsorption, in addition to the coupled behaviour in the bulk material arising from mass transport in the pore space. This allows to study the different phenomena and their interaction with each other, giving insight into the underlying physical mechanisms. Simulations reveal that both, the nanocomposite’s structure and the ions’ mobilities, strongly affect the actuator’s response, providing the means to tailor the actuator’s behaviour to specialised applications.

References

[1] Wilmers, McBride, Bargmann, Interface Elasticity Effects in Polymer-Filled Nanoporous Metals, JMPS, 163-177, 2017.
[2] Wilmers, Bargmann, Functionalisation of Metal-Polymer-Nanocomposites: Chemoelectromechanical Coupling and Charge Carrier Transport, EML, accepted, 2018
[3] McBride, Javili, Steinmann, Bargmann, Geometrically nonlinear continuum thermomechanics with surface energies coupled to diffusion, JMPS 59, 2116-2133, 2011
[4] Soyarslan, Bargmann, Pradas, Weissmüller, 3d stochastic bicontinuous microstructures: generation, topology and elasticity, Acta Mater., 326-340, 2018
[5] Bargmann et al., Generation of 3d representative volume elements (RVEs) for heterogeneous materials: a

review, Prog. Mater. Sci., accepted, 2018

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room3)

[SY-F3] Mechanics of Cilia Beating - A Relationship Between Metachronal Wavelength and Fluid Flow Rate

○Jon Hall, Nigel Clarke (The University of Sheffield, UK)

Cilia driven fluid flow is a complex fluid mechanical system that is dependent on several physical parameters, including mucus rheology, cilia density, and beat coordination. We have developed a computational model of an array of beating cilia using a hybrid immersed boundary lattice Boltzmann algorithm in order to study the how the flow behaviour is affected by these key parameters. Our main focus is on quantifying the relationship between metachronal wavelength and the rate of fluid flow which we find exhibits two maxima at particular wavelengths. We attempt to rationalise this observation by considering how the metachronal wavelength relates to the volume of fluid that is accelerated by each cilium during an active stroke, and thus the momentum of the fluid region as a whole. We also observe that the rate of fluid flow decreases significantly when cilia in close proximity are synchronised, and that this behaviour becomes more dominant as cilia density increases.

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

[SY-F4] Symposium F-4

Chair: Dana Zoellner(B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany)

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

[SY-F4] Showdown! Pitting computer simulations against time-resolved experimental measurements of grain growth in 3D

Mingyan Wang[1], Nan Wang[2], Jules Dake[1], Søren Schmidt[3], ○Carl Krill[1] （1.Institute of Micro and Nanomaterials, Ulm University, Germany, 2.Dept. of Physics, McGill University, Canada, 3.Dept. of Physics, Technical University of Denmark, Denmark）

[SY-F4] Coarsening and grain-growth in an SOFC-anode under surface and grain boundary self-diffusion: A Multiphase-field approach

○Paul Hoffrogge[1], Daniel Schneider[1,2], Britta Nestler[1,2], Patricia Haremski[2,3], Matthias Wieler[3], Piero Lupetin[3] （1.Karlsruhe University of Applied Sciences, Germany, 2.Karlsruhe Institute of Technology, Germany, 3.Robert Bosch GmbH, Germany）

[SY-F4] Solidification Simulation in Additive Manufacturing Process of Ti-Alloy by ICME approach

○Yusuke SHIMONO, Mototeru Oba, Sukeharu Nomoto （Itochu Techno-Solutions Corp., Japan）

[SY-F4] Phase Field Model of Microstructural Evolution in Metal Alloy for Designing Mechanical Property

Wooju Lee, ○Dongchoul Kim （Dept. of Mechanical Engineering, Sogang Univ., Korea）

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

[SY-F4] Showdown! Pitting computer simulations against time-resolved experimental measurements of grain growth in 3D

Invited

Mingyan Wang[1], Nan Wang[2], Jules Dake[1], Søren Schmidt[3], ○Carl Krill[1] (1.Institute of Micro and Nanomaterials, Ulm University, Germany, 2.Dept. of Physics, McGill University, Canada, 3.Dept. of Physics, Technical University of Denmark, Denmark)

Thanks to dramatic improvements in computational speed, it is now feasible to simulate the coarsening of 3D polycrystalline microstructures containing tens of thousands of grains. Indeed, such calculations have become so powerful that the simulation cells rival—and, in some cases, exceed—sample volumes that can be probed experimentally! But do the computational algorithms underlying these simulations properly capture the physics of microstructural evolution as it occurs in real materials? We have followed a two-pronged strategy to address this question, using (i) three-dimensional x-ray diffraction (3DXRD) microscopy to map the 3D network of grain boundaries in a polycrystalline specimen over the course of stepwise isothermal annealing treatments, and (ii) a phase field model to simulate 3D grain growth starting from the same initial configuration as in experiment. A grain-by-grain showdown between tactic (i) and tactic (ii) offers fresh insights into the phenomenon of grain growth—gleaned not only from discrepancies between measured and simulated size trajectories and grain shapes, but also from instances of agreement.

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

[SY-F4] Coarsening and grain-growth in an SOFC-anode under surface and grain boundary self-diffusion: A Multiphase-field approach

○Paul Hoffrogge[1], Daniel Schneider[1,2], Britta Nestler[1,2], Patricia Haremski[2,3], Matthias Wieler[3], Piero Lupetin[3] (1.Karlsruhe University of Applied Sciences, Germany, 2.Karlsruhe Institute of Technology, Germany, 3.Robert Bosch GmbH, Germany)

Solide oxide fuel cells (SOFCs) convert chemical energy stored in form of a gaseous fuel into electrical energy. Due to the typically high energy-conversion efficiencies achieved, SOFCs are a very promising technology to reduce carbon emission. One of the critical parameters to be economically competitive is the lifetime of an SOFC device. In order to improve the SOFCs long-term performance it is essential to obtain a better understanding of the underlying physical processes leading to a decrease in SOFC performance during operation.
The present study focuses on the evolution of a polycrystalline and porous 3D microstructure of an Ni-YSZ (yttria-stabilized zirconia) SOFC-anode during isothermal coarsening. We employ a multiphase-field model which incorporates self-diffusion of nickel by a grand-chemical formulation to simulate grain-boundary and surface diffusion coupled with simultaneous growth of the inherent Ni-grains. We validate the model by 2D thermal-grooving simulations under surface-diffusion and by a quantitative comparison with analytical results. A comprehensive study of several input parameters such as grain-size on the coarsening behavior of the SOFC-anode is performed. The detailed investigation includes an analysis of the microstructure as a function of particle size, tortuosity and triple-phase boundary length.

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

[SY-F4] Solidification Simulation in Additive Manufacturing Process of Ti-Alloy by ICME approach

○Yusuke SHIMONO, Mototeru Oba, Sukeharu Nomoto （Itochu Techno-Solutions Corp., Japan）

Multi-phase field method (MPFM) coupled with thermodynamics database of calculation of phase diagrams (CALPHAD) is a powerful tool for simulating solidification microstructure evolutions in engineering casting processes. As MPFM is based on local (quasi-)equilibrium assumption in solidification theory, applying MPFM to solidification of additive manufacturing (AM) processes is considered to be difficult because of extremely large cooling rate and temperature gradient.
On the other hand, some researchers have recently reported experimental observations of the columnar-to-equiaxed transition in the solidification of the AM processes. These observations suggested that the local (quasi-)equilibrium assumption can be applied to the solidification of the AM processes.
In this study, AM processes of Ti-alloys are simulated. By using temperature distributions obtained by thermal analyses in finite element method simulations, solidification microstructures are calculated by MPFM. It is confirmed that the microstructures have the columnar-to-equiaxed transitions. The results are summarized in a solidification map for the AM process conditions.

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

[SY-F4] Phase Field Model of Microstructural Evolution in Metal Alloy for Designing Mechanical Property

Wooju Lee, ○Dongchoul Kim （Dept. of Mechanical Engineering, Sogang Univ., Korea）

Precipitation hardening has been widely employed to improve the mechanical properties of metal alloys. During the precipitation hardening, the supersaturated alloying elements in a solid solution phase form secondary precipitate particles. To design the mechanical properties of metal alloy, the relationship between precipitation conditions and morphology of microstructure of secondary phase should be fully understood. The morphology of microstructure in metal alloy is determined by the composition of the alloy and their intermetallic compounds. Here, we investigate the the morphological evolution of microstructures in metal alloy during precipitation. To simulate the temporal evolution of microstructures, a phase field model is employed. By simulations, the effects of anisotropic interfacial energy and lattice mismatch on the morphology of the microstructure are investigated.

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

[SY-M3] Symposium M-3

Chair: Thomas Franosch(University of Innsbruck, Austria)

Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room4

[SY-M3] Heterogeneous thermal properties in a glass from molecular dynamics calculations

○Jean-Louis BARRAT （Univ. Grenoble Alpes, France）

[SY-M3] Structural-dynamical phase transition in the phase space of histories of a polydisperse hard sphere liquid

○Matteo Campo[1,2], Thomas Speck[1] （1.Johannes Gutenberg University Mainz, Germany, Germany, 2.Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany, Germany）

[SY-M3] Time- and History-dependent Structure and Morphology of van-der-Waals Liquids forming Physical Gels and Porous Glasses

○Magdaleno Medina-Noyola, Leticia Lopez-Flores, Jose Manuel Olais-Govea, Benigno Zepeda-Lopez （Instituto de Fisica (Laboratorio Nacional de Ingenieria de la Materia Fuera de Equilibrio), Universidad Autonoma de San Luis Potosi, Mexico）

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room4)

[SY-M3] Heterogeneous thermal properties in a glass from molecular dynamics calculations

Invited

○Jean-Louis BARRAT （Univ. Grenoble Alpes, France）

It is well known that elastic properties of amorphous systems are heterogeneous, leading to peculiarities in vibrational spectra and thermal properties. In this work, we investigate the heterogeneity in thermoelastic properties, and more precisely in the thermal expansion coefficient, in a model metallic glass. We find heterogeneities that are similar - in terms of length scales - to those in elastic constants. It has been suggested that such heterogeneities could be the reason for "cryogenic rejuvenation" processes observed under thermal cycling in several experiments. We investigate this hypothesis by comparing the values of the local yield stresses with the stresses generated by heterogeneities in thermal dilation.

This work was performed in collaboration with Dr Baoshuang Zhang (University Grenoble Alpes and Beijing Computational Science Research Center).

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room4)

[SY-M3] Structural-dynamical phase transition in the phase space of histories of a polydisperse hard sphere liquid

○Matteo Campo[1,2], Thomas Speck[1] （1.Johannes Gutenberg University Mainz, Germany, Germany, 2.Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany, Germany）

The glass transition is a longstanding problem in condensed matter physics. One of the main points of discussion is whether it is possible to characterize the glass transition using structural arguments, together with dynamical ones. In fact, it is known that supercooled liquids do not show major changes in their global (two-point) structure upon cooling while displaying a dramatic change in their dynamical properties. Recent insights have brought attention to the local structure instead. For a wide range of model glassformers, it is possible to identify certain geometric motifs that minimize the local free energy. These motifs are referred to as Locally Favourite Structures (LFS) and are found to be growing in correlation with the slowing-down of the dynamics. Using tools from large deviation theory and statistical mechanics of histories, it was recently possible to identify for some model glassformers a structural-dynamical transition between the supercooled liquid state and a state composed of trajectories rich in LFS with very slow dynamics. We present here a study of this transition for a fundamental atomistic model glassformer, the polydisperse hard sphere liquid. We reveal the first-order nature of the transition by employing finite size scaling on the length of the histories of the system, and a phase diagram is constructed as a function of the density versus the local order, and the density versus the degree of mobility of the system.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room4)

[SY-M3] Time- and History-dependent Structure and Morphology of van-der-Waals Liquids forming Physical Gels and Porous Glasses

○Magdaleno Medina-Noyola, Leticia Lopez-Flores, Jose Manuel Olais-Govea, Benigno Zepeda-Lopez
（Instituto de Fisica (Laboratorio Nacional de Ingenieria de la Materia Fuera de Equilibrio), Universidad Autonoma de San Luis Potosi, Mexico）

In spite of its relevance, no universal principle seems to exist that explains how Boltzmann’s postulate $S = k_B \ln W$ operates for non-equilibrium conditions, predicting, for example, the transformation of liquids into non-equilibrium amorphous solids (glasses, gels, etc.) in terms of molecular interactions. Here, however, we present evidences that the missing fundamental principle to understand non-equilibrium states of matter is provided by Onsager’s description of irreversible processes and thermal fluctuations, adequately combined with Boltzmann’s postulate and extended to genuine non-equilibrium conditions [J. Phys.: Cond. Matter 21: 504103 (2009)]. Formatted as the non-equilibrium self-consistent generalized Langevin equation (NE-SCGLE) theory of irreversible processes in liquids [Phys. Rev. E 82, 061503 (2010)], this approach has been shown to provide a fundamental tool for the understanding of the most essential fingerprints of the transformation of liquids into amorphous solids, such as their aging kinetics or their dependence on the protocol of fabrication [J. Chem Phys. 143, 174505 (2015); Phys. Rev. E 96, 022608 (2017)]. In this work we focus on the NE-SCGLE-predicted scenario of the structural and morphological transformation of van-der-Waals (or "Lennard-Jones--like") simple fluids into hard-sphere glasses at hight densities and temperatures, into physica gels at intermediate densities and low temperatures, into porous glasses at intermediate densities and even lower teperatures, and into cluster-cluster aggregates al very low densities and temperatures. As an illustration, we present the visualization of the non-equilibrium development and arrest of sponge-like structures by arrested spinodal decomposition. The comparison of the theoretical predictions (based on a simple specific model system), with simulation and experimental data measured on similar but more complex materials, suggests the universality of the predicted scenari.

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

[SY-M4] Symposium M-4

Chair: Leticia Lopez Flores(University of San Luis Potosi, Mexiko)

Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room4

[SY-M4] Mechanical behavior and emerging morphologies in active matter

○Ignacio Pagonabarraga （CECAM, EPFL, Switzerland）

[SY-M4] Time dependent interaction between intruders in granular media

○Hisao Hayakawa [1], Takahiro Tanabe[2] （1.Yukawa Institute for Theoretical Physics, Kyoto Univeristy, Japan, 2.Graduate School of Advanced Mathematical Sciences, Meiji University, Japan）

[SY-M4] Hystory-dependent shear jamming of granular materials under oscillatory shear

○Michio Otsuki[1], Hisao Hayakawa[2] （1.Graduate School of Engineering Science, Osaka Univ., Japan, 2.Yukawa Institute for Theoretical Physics, Kyoto Univ., Japan）

[SY-M4] Structural predictor for nonlinear sheared dynamics in simple glass-forming liquids

○Trond S. Ingebrigtsen, Hajime Tanaka （University of Tokyo, Japan）

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room4)

[SY-M4] Mechanical behavior and emerging morphologies in active matter

Invited

○Ignacio Pagonabarraga （CECAM, EPFL, Switzerland）

Flocks of birds, schools of fishes, or bacterial colonies constitute examples of living systems that coordinate their motion. In all these systems their constituent elements generate motion due to energy consumption and can exchange information or react sensitively to chemical cues in order to move together or to react collectively to external signals. Artificial systems, such as nanorobots, exploit the heterogeneous compositions of their surface to displace as a result of the heterogeneous chemical processes that take place in the presence of appropriate chemical substances.

All these systems are intrinsically out of equilibrium in the absence of any external driving. Their collective properties result as a balance between their direct interactions and the indirect coupling to the medium in which they displace, and a self-consistent dynamical approach is required to analyze their evolution. The mechanical balance that determines the states they develop spontaneously make these systems very versatile and have a natural tendency to for large scale aggregates.

I will consider simple statistical models to address fundamental questions associated to these systems and will analyze the implications the generic self-propulsion has in the emergence of structures in suspensions of model self-propelled particles. I will discuss the potential of schematic models to address fundamental questions, such as the connection of the effective phase diagram and pressure with effective equilibrium concepts. I will analyze the collective behavior of these emerging morphologues and their response to external forcings, as well as how we can understand the resistance to deformation in this type of systems.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room4)

[SY-M4] Time dependent interaction between intruders in granular media

○Hisao Hayakawa [1], Takahiro Tanabe[2] （1.Yukawa Institute for Theoretical Physics, Kyoto Univeristy, Japan, 2.Graduate School of Advanced Mathematical Sciences, Meiji University, Japan）

In this presentation, we will discuss the interactions between two intruders in two dimensional granular environment from DEM (discrete element method) simulation and phenomenological theory. Through the DEM simulation, we found that the interaction is repulsive if there exists a steady flow or the amplitude of an external oscillation is small enough, but the interaction becomes attractive if the amplitude of the oscillation is large. Such an attractive interaction is known as depletion effect or Casimir effect nearly equilibrium environments, but it is interesting that both attractive and repulsive interactions can be observed in out-of-equilibrium systems such as granular media. We also develop a phenomenology based on an analogous equation to Boltzmann-Enskog equation. The phenomelogy can explain the drag force acting on one intruder in granular environment and the repulsive interaction between two intruders under a steady flow, but is still far away to describe the attractive interaction between two intruders in highly oscillated situations.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room4)

[SY-M4] Hystory-dependent shear jamming of granular materials under oscillatory shear

○Michio Otsuki[1], Hisao Hayakawa[2] (1.Graduate School of Engineering Science, Osaka Univ., Japan, 2.Yukawa Institute for Theoretical Physics, Kyoto Univ., Japan)

Granular materials have rigidity above a critical density [1]. Such rigidity transition, known as the jamming transition, has attracted much attention among researchers in these days. It is well-known that frictionless grains under small strain exhibit a continuous transition of the shear modulus G, while recent studies have revealed that G of frictional grains with harmonic repulsive interaction discontinuously emerges at the critical density [2].
In this talk, we present our recent numerical results on the shear modulus of frictional grains under oscillatory shear. It is confirmed that the shear modulus depends on the amplitude of the initial oscillatory shear before the mesurament. Even at densities below the transition point, where isotropic jamming occurs without shear, the initial oscillatory shear can induce the finite shear modulus. This behavior is consistent with a transition known as shear jamming [3]. We also discuss the evolution of the force chain network under the initial oscillatory shear and the conection with the discontinuous shear thickenning.

[1] M. van Hecke, J. Phys.: Condens. Matter 22, 033101 (2009).
[2] M. Otsuki and H. Hayakawa, Phys. Rev. E 95, 062902 (2017).
[3] D. Bi, J. Zhang, B. Chakraborty, and R. Behringer, Nature (London)
480, 355 (2011).

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room4)

[SY-M4] Structural predictor for nonlinear sheared dynamics in simple glass-forming liquids

○Trond S. Ingebrigtsen, Hajime Tanaka (University of Tokyo, Japan)

Glass-forming liquids subjected to sufficiently strong shear universally exhibit striking nonlinear behavior; for example, a power-law decrease of the viscosity with increasing shear rate. This phenomenon has attracted considerable attention over the years from both fundamental and applicational viewpoints [1, 2, 3, 4]. However,
the out-of-equilibrium and nonlinear nature of sheared fluids have made theoretical understanding of this phenomenon very challenging and thus slower to progress. We find here [5] that the structural relaxation time as a function of the two-body excess entropy, calculated for the extensional axis of the shear flow, collapses onto
the corresponding equilibrium curve for a wide range of pair potentials ranging from harsh repulsive to soft and finite. This two-body excess entropy collapse provides a powerful approach to predicting the dynamics of nonequilibrium liquids from their equilibrium counterparts. Furthermore, the two-body excess entropy scaling suggests that sheared dynamics is controlled purely by the liquid structure captured in the form of the two-body excess entropy along the extensional direction, shedding light on the perplexing mechanism behind shear thinning.

References

[1] D. J. Evans, H. J. M. Hanley, and S. Hess. Phys Today 37, 26 (1984).
[2] R. Yamamoto, and A. Onuki. Phys. Rev. E 58, 3515 (1998).
[3] V. Lubchenko. Proc. Natl. Acad. Sci. U.S.A. 106, 11506 (2009).
[4] X. Cheng, J. H. McCoy, J. N. Israelachvili, and I. Cohen. Science 333, 1276 (2011).
[5] T. S. Ingebrigtsen, and H. Tanaka. Proc. Natl. Acad. Sci. U.S.A. 115, 87 (2018).

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

[SY-O3] Symposium O-3

Chairs: Momoji Kubo(Tohoku University, Japan), Michael Moseler(Fraunhofer Institute for Mechanics of Materials IWM, Germany)

Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room5

[SY-O3] Scale Dependence of Friction: How Elasticity Destroys Superlubricity

Joseph Monti[1], Lars Pastewka[2], ○Mark Owen Robbins[1] （1.Dept. of Physics and Astronomy, Johns Hopkins University, United States of America, 2.University of Freiburg, Germany）

[SY-O3] Coarse-Grain Simulations of Polymer Solutions with Hydrodynamics and Long-range Interactions

○Hitoshi Washizu[1,2], Hiroaki Yoshida[3], Soma Usui[1], Taiki Kawate[1] （1.Univ. Hyogo, Japan, 2.Kyoto Univ., Japan, 3.Toyota Central R&D Labs., Inc., Japan）

[SY-O3] A Multi-Scale Approach for the Design of Novel Lubricants

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

[SY-O3] Impact of ionic liquid ordering on their triborheological properties

○Konstantinos Gkagkas[1], Andras Vernes[2,3] （1.Advanced Material Research Division, Toyota Motor Europe NV/SA, Belgium, 2.AC2T research GmbH, Austria, 3.Institute of Applied Physics, TU Wien, Austria）

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room5)

[SY-O3] Scale Dependence of Friction: How Elasticity Destroys Superlubricity

Invited

Joseph Monti[1], Lars Pastewka[2], ○Mark Owen Robbins[1] (1.Dept. of Physics and Astronomy, Johns Hopkins University, United States of America, 2.University of Freiburg, Germany)

Friction in single-asperity contacts is studied as a function of contact radius *a*, substrate stiffness *G*, atomic structure, adhesive strength and adsorbed layers. Friction between bare, rigid surfaces can be obtained by a simple sum over atomic forces. When surfaces are aligned and have the same periodicity, the forces add in phase and the friction force *F* rises linearly with area *A*. When the two surfaces are misaligned or disordered, so that there is no common periodicity, forces add out of phase and $F \sim A^x$ with *x* less than or equal to *1/2*. This is known as structural superubricity and implies that friction vanishes in the limit of large contact sizes. Most surfaces do not share a common period but friction is almost always observed at macroscopic scales. We use an efficient Greens function technique to study contacts with dimensions of micrometers while resolving atomistic interactions at the surface. A new formulation that includes dynamic effects explicitly will be described. For small tips and high loads the contact area follows predictions for contact of rigid surfaces, *x=1* for identical aligned surfaces, *x=1/2* for random surfaces and *x=1/4* for incommensurate crystals. Elasticity becomes important when *a* exceeds the core width b_{core} of interfacial dislocations. For $a>b_{core}$ parts of the contact can advance independently. The friction for identical aligned surfaces drops as a power law and then saturates at the Peierls stress for edge dislocations. The friction on incommensurate and disordered surfaces saturates at nearly the same value. Thus for all geometries *x=1* in large contacts. While this means that elasticity destroys superlubricity, the friction between bare surfaces drops exponentially with the ratio of substrate stiffness to local interfacial shear stress. In contrast, when adsorbed layers are included between surfaces, all geometries have *x=1* with a large prefactor.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room5)

[SY-O3] Coarse-Grain Simulations of Polymer Solutions with Hydrodynamics and Long-range Interactions

○Hitoshi Washizu[1,2], Hiroaki Yoshida[3], Soma Usui[1], Taiki Kawate[1] (1.Univ. Hyogo, Japan, 2.Kyoto Univ., Japan, 3.Toyota Central R&D Labs., Inc., Japan)

Polymer solution is used as lubricant in Tribological purpose. Viscosity index improver is used to normalize temperature dependence of viscosity of the lubrication oil. Here we show our numerical simulation approach to investigate the dynamics of polymer solution. The numerical scheme is for simulating the dynamics of suspensions of Brownian particles, coupling molecular motion treated by Langevin equation and hydro-dynamics treated by lattice Boltzmann method.

In order to simulate bulk properties of polymers under shear, we apply periodic external field so that to make shear field. The external force is applied to the fluid dynamics part. Polymer is dragged to the region where the shear force is strongest, and changes its shape. The structure change is described by the radius of gyration which decreases with time.

In order to describe confined system, non-slip boundary is adopted in bottom line and moving wall is set in top line. During the simulation, the polymer are pull to upper layer where the shear field is large. To show the orientation of the molecule, order parameter is calculated. Due to the effect of external field, the orientation

of the polymers changed to the direction of the shear force.
In above simulation, the chemical properties of the polymers are not discussed. We simulate the equilibrium structure of polymer using point dipole interactions. We use Monte Carlo Brownian Dynamics method for time integration.The radius of gyration of non-polar polymers are same as analytical theory. The structure of the polymers with functional groups is calculated. The interaction between functional groups make tight structure in low temperature and show high viscosity index than non-polar polymers. The polar polymer shows strong initial distribution dependence.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room5)

[SY-O3] A Multi-Scale Approach for the Design of Novel Lubricants

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

Friction accounts for ~15% of fuel energy losses in conventional vehicles. A deeper understanding of lubrication mechanisms in engineering systems and how to accurately model them is therefore necessary. Atomistic simulations can provide fundamental insights in the fluid behaviour under extreme contact conditions, at a high computational cost. On the other hand, continuum methods, while capable of efficiently solving macroscopic problems, cannot resolve features and flow patterns at the nanometer scale, due to the breakdown of the continuum assumption [1]. In this work, we employ a multi-scale approach that combines continuum and particle-based descriptions for simulating hydrodynamic lubrication systems, while seeking ideal designs of virtual lubricants that maximise load carrying capacity and minimize friction.

Inspired by computational [2] and experimental [3] studies of ionic liquids as lubricants, we emulate their layering behaviour and near-wall solidification [2] on the continuum domain by introducing an inhomogeneous viscosity field in the Navier-Stokes equations. Using an Evolutionary Algorithm, optimal viscosity profiles leading to the minimisation of specific friction are identified. By doing so, a potential improvement in friction performance up to 65% was found for a converging hydrodynamic slider.

The study is then extended to nano-hydrodynamic lubrication using Coarse Grain Molecular Dynamics simulations, which can help in selecting specific molecule typologies featuring the aforementioned viscosity variations - and thus the potential for significant friction reduction - under severely loaded contact conditions.

1. I. Cosden and J. Lukes, Comput. Phys. Commun. 184 (8) (2013)

2. K. Gkagkas, V. Ponnuchamy, M. Dašić, and I. Stanković, Tribol. Int. 113 (2016)

3. J. Qu, D. Bansal, B. Yu, J. Howe, H. Luo, S. Dai, H. Li, P.J. Blau, B. Bunting, G. Mordukhovich and D. Smolenski, ACS Appl. Mater. Interfaces 4 (2) (2012)

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room5)

[SY-O3] Impact of ionic liquid ordering on their triborheological properties

○Konstantinos Gkagkas[1], Andras Vernes[2,3] （1.Advanced Material Research Division, Toyota Motor Europe NV/SA, Belgium, 2.AC2T research GmbH, Austria, 3.Institute of Applied Physics, TU Wien, Austria）

The development of novel lubrication concepts is a multi-scale challenge that requires the correlation of nano- and meso-scale features, such as molecule structure and their ordering, with macro-scale properties such as observed friction. Ionic Liquids (ILs) are interesting lubricants that are shown to have a positive impact on friction reduction. A feature that plays an important role in their behaviour is the Coulombic interaction between ions leading to layering in the transverse direction to the sliding and to a near-wall solidification, as seen both experimentally [1] and numerically [2]. At the same time, in-plane crystalline structures are also formed [3, 4, 5].

In this contribution, we quantify the impact of the internal structure on the triborheological properties of ILs. More precisely, both structure factors and bond-orientational order parameters will be calculated on coarse grain MD models of ILs in order to describe the ion ordering and formation of crystalline structures under bulk and confined conditions. Then an attempt will be made to correlate the detected ordering with internal (ion shapes and sizes), external (wall structure, pressure and shearing velocity) and constitutive (e.g., coefficient of friction) system parameters. Through such quantification, we expect an improved understanding of the underlying physico-chemical mechanisms, guiding us towards the design of optimised tribological systems.

1. A. M. Smith, K. R. J. Lovelock, N. N. Gosvami, P. Licence, A. Dolan, T. Welton, and S. Perkin, J. Phys. Chem. Lett. 4, 378 (2013).
2. K. Gkagkas, and V. Ponnuchamy, Model. Simul. Mater. Sci. Eng. 25 (6), 064004 (2017).
3. K. Gkagkas, V. Ponnuchamy, M. Dašić, and I. Stanković, Tribol. Int. 113, 83 (2016).
4. R. Capozza, A. Vanossi, A. Benassi and E. Tosatti, J. Chem. Phys. 142, 064707 (2015).
5. O. Fajardo, F. Bresme, A. Kornyshev, and M. Urbakh, Sci. Reports 5, 7689 (2015).

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

[SY-O4] Symposium O-4

Chairs: Aiichiro Nakano(Univ. of Southern California, United States of America), Shandan Bai(KYOCERA Corp., Japan)

Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room5

[SY-O4] Molecular simulation to better understand soot-detergent interactions in engine oils

○Sophie LOEHLE[1], Elias Gebremedhn[2], Michael Mazarin[1], Stephan Steinman[2], Carine Michel[2] （1.Total M&S, France, 2.ENS Lyon, France）

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

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

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

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

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

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

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room5)

[SY-O4] Molecular simulation to better understand soot-detergent interactions in engine oils

Invited

○Sophie LOEHLE[1], Elias Gebremedhn[2], Michael Mazarin[1], Stephan Steinman[2], Carine Michel[2] (1.Total M&S, France, 2.ENS Lyon, France)

In the engine, soot is formed as a result of incomplete combustion. Some of the formed soot is absorbed into the lubricating oil film present until a certain level is reached in which it precipitates. This lead not only to the increase of the lubricant's viscosity but also it adsorbs on the metallic surface, thus increasing engine wear. Most automotive enhancement additives contain, among other additives, detergents which help control the agglomeration and deposition of soot particles and other corrosive contaminants. A typical detergent molecule features a head part with constituting polar functional groups and a long hydrocarbon tail group [1]. The common perception is that the detergents do the job as dispersants and/or through formation of protective coating on steel surfaces. However, little is known about the complex physicochemical and structural details of the soot-detergent interfaces, and it seems that such details are too difficult to capture using conventional experimental techniques alone. In this respect, molecular modeling can fill the gap by providing atomistic level understandings on soot-detergent interactions and interfacial structural features.Finding an atomistic representation of the soot is the crucial step in modeling soot-detergent interactions. First, we show how we developed reliable soot model using experimental data [2-4], we employed a deterministic structural elucidation method to automatically generate representative soot structures. Following, we show how we assessed physisorption energies between the soot models and some polar detergent-head groups using the latest semi-empirical PM7 method, and how the result can be used to complement experimental screening techniques.

References:

1- J.D. Burrington, J. K. Pudelski, J. P. Roski, Chapter 18: Challenges in detergents and dispersants - *Practical Advances in Petroleum Processing* **2007**
2- Christine Esangbedo, Andre L. Boehman, Joseph M. Perez, *Tribology International* **2012**, 47, 194
3- A. La Rocca, F. Bonatesta, M. W. Fay, F. Campanella, *Tribology International* 86 (**2015**) 77-84
4- I. Z. Jenei et al., *Nanotechnology* n°8, Vol 29 (**2018**)

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room5)

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

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

Diamond-like carbon (DLC) is a promising solid lubricant and widely used as a lubricant coating in various industrial applications such as engine, hard-disk, and space instruments. Hydrogenated DLC coatings show the much better low-friction properties and lubricity than the non-hydrogenated DLC coatings. However, wear of the hydrogenated DLC coatings causes the reduction of the durability of DLC coatings and limits their utilization. For the further improvement of the hydrogenated DLC coatings, the deep and

comprehensive understandings of the wear mechanisms of the hydrogenated DLC are very essential; nevertheless, these understandings are still lacking because the experiments are difficult to observe the complicated atomic-scale friction processes and tribochemical reactions at the interface. To handle these difficulties, we employ a molecular dynamics method to investigate the wear mechanisms of the hydrogenated DLC. We perform friction simulations in the vacuum by using the DLC models with a hydrogen concentration of 0%, 20%, 30%, 40%, and 50%. From the simulation results, we observe two wear mechanisms of DLC: 1) chemical wear as the generation of hydrocarbons desorbing from DLC surface and 2) mechanical wear as the transfer of carbon atoms to the counter substrates. The chemical and mechanical wear co-decide the wear behaviors of DLC. Furthermore, with increasing the hydrogen concentration in DLC, chemical wear increases and mechanical wear decreases, causing a parabolic-like hydrogen dependence of the total wear with a minimum value at the hydrogen concentration of 30%. Our simulations successfully give fundamental understandings about the wear mechanisms of the hydrogenated DLC and provide the theoretical instructions to improve the anti-wear properties of DLC coatings.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room5)

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

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

Diamond-like carbon (DLC) coatings possess excellent frictional properties. However, the wear of DLC coatings is still a problem. To improve the properties of DLC, clarification of the wear mechanisms is required. It is reported that the wear of DLC under the water lubrication is lower than that in the air. To expound the wear mechanisms, clarification of this phenomenon is strongly demanded. However, the detailed mechanism is still unclear due to the complicated tribochemical reactions. Therefore, we studied the wear mechanisms of DLC under both vacuum and water environment by using the molecular dynamics method. The DLC model is made of two hemispherical substrates, to simulate real rough surfaces. The friction simulations were carried out by sliding two substrates. During the friction, under both environments the transfer of carbon atoms to their counter substrates was observed, indicating the adhesive wear of DLC. The number of transferred carbon atoms under vacuum condition was much larger than that under water lubrication, suggesting that the water environment suppresses the wear of DLC. Considering that interfacial C-C bonds which connect two DLC substrates promotes the transfer of carbon atoms, we investigated the number of interfacial C-C bonds. The number of interfacial C-C bonds under water lubrication was less than that in vacuum, indicating that the formation of the interfacial C-C bonds was suppressed by the water. To understand the cause of the suppression effect of water on the interfacial C-C bonds formation, we investigated the chemical reactions during friction process. With friction time going, the increase in the C-H and C-O bonds and the decrease in water molecules were observed, indicating the reaction between water molecules and carbon atoms. We suggest that these chemical reactions increase H and OH terminations on the DLC substrates and suppress the formation of the interfacial C-C bonds, and therefore the adhesive wear is inhibited.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room5)

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

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

Water lubrication has the characteristic of low environmental burden. It is known that silicon carbide (SiC) shows quite low friction coefficient by the formation of a tribofilm on the surface of SiC during water lubrication. Understanding of its mechanism is essential to improve friction characteristic for practical use and application. However, it is difficult to observe directly such a complicated phenomenon including friction and chemical reaction by experiments. Therefore, in this study, molecular dynamics method which can simulate chemical reaction was conducted to analyze the structure and formation mechanism of tribofilm in the friction process of amorphous SiC under water environment.

In the simulation, we prepared the model consisting of two amorphous SiC substrates sandwiching water molecules. The substrates have rough surfaces and the two of substrate surfaces can be in contact during the friction. The substrates were given a constant pressure (3 GPa) and slid for 1000 ps at 100 m/s.

We performed the sliding simulation of SiC under water lubrication. In the initial structure, the surface of the substrates was corrugated. However, the rough surface of the substrates was smoothed while Si atoms from the a-SiC substrate reacted with water molecules and formed bonds with O atoms of H_2O during friction. Firstly, we investigated the change in number of water molecules and Si-O-Si bonds during friction. It was found that the number of water molecules decreased constantly while the number of Si-O-Si bonds increase correspondingly. This result shows that Si reacts with H_2O to form a SiO_2 layer. Next, we investigated the change in the distribution ratio of C and Si before and after friction. The ratio of C was increased around the substrate surfaces and that of Si was increased on the substrates indicating that the bilayer tribofilm of the SiO_2 and C rich SiC was generated on the substrate by the tribo-chemical reaction.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A3] Symposium A-3

Chair: Katsuyo Thornton(University of Michigan, Ann Arbor, United States of America)

Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room6

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

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

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

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

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

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

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

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

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room6)

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

Invited

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

We consider multiple crystalline plasticity model constructs that address evolution of dislocation structures over a broad range of length and time scales, from atomistic modeling and coarse-graining strategies through discrete dislocation theory to reduced order generalized and local continuum models. The predictive character of each construct is considered, along with the notion of uncertainty of modeling phenomena at various scales and for two-scale transitions, either concurrent or hierarchical in nature. In each case, we list the set of phenomena that each model construct addresses. Challenges to modeling the evolution of the dislocation network are discussed, including the important role of the entropic barrier to collective dislocation bypass of obstacles. Gaps and future challenges are summarized.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room6)

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

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

Continuum dislocation dynamics models, which are proposed to conquer the restrictions of high computational cost that discrete dislocation dynamics models generally experience, have made great progress in the past decades. However, it is inevitable that certain dislocation microstructure information is ‘lost’ during the averaging/coarse graining process ('upscaling'), for example, dislocation short range interactions. This information, however, is crucial for a correct prediction of the structure-property relation in continuum simulations. We will show a new type of multiscale analysis which is based on the energy density of 2D systems, where we identify the ‘missing’ information during coarse graining for arbitrary averaging resolution. This methodology can be directly generalized to 3D systems of curved dislocations. Furthermore, based on our database, we will be able to benchmark a number of existing 2D continuum formulations for dislocation interaction. Last but not least, we will show that our data base also will be a useful starting point for recovering statistical information of (ensembles of) discrete dislocations from continuum field data during 'downscaling'.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room6)

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

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

Discrete Dislocation Dynamics (DD) is a well-established simulation technique aimed at reproducing the collective behavior of dislocations at the mesoscale. Despite the considerable progresses made in last decades, DD simulations are still unable to precisely reproduce the microstructure of large poly-crystals and, especially, of irradiated polycrystalline materials. An important step in the development of predictive simulations of this class of materials is the improvement of the numerical capabilities of DD codes to model dislocation properties in large volumes representative of the materials microstructures.
Here we propose a promising strategy based on the coupling between two advanced simulation tools. First, the Discrete-Continuous Model (DCM) is employed [O. Jamond et al., Int. J. Plast. 80,19(2016)]. This numerical model based on the Eigenstrain theory, couples an extensive DD simulation code (microMegas), to an elastic solver dedicated to boundary value problems resolution. The DCM allows for the rigorous solution of dislocation-surface and -interfaces interactions and has been proven to efficiently model plasticity in nano- and micro-objects. Nevertheless, its application has been limited to samples of few mm in size. Second, to overcome this difficulty, we employ a solver based on Fast Fourier Transform (FFT) calculation [Bertin et al. Modelling Simul. Mater. Sci. Eng. 23,065009 (2015)]. In particular, we employ AMITEX_FFTP, a new distributed parallel elastic solver based on FFT calculation. Using this approach, the stress state definition in the simulated volumes can be increased from a 64x64x64 grid to a 1024x1024x1024 one, hence allowing the simulation of realistic dislocation density in a multi-grains periodic volume over significant plastic strains (5-10%). In summary, we aim at improving mechanical properties predictions by taking into account both the complexity of multi-crystalline materials microstructure and the local properties of dislocations.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room6)

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

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

A Fast Fourier Transform (FFT) based hybrid discrete dislocation dynamics
(DDD) and cluster dynamics (CD) tool is introduced to study plasticity and microstructure evolution in polycrystalline media. The overall intent of the work is to introduce a unified modeling platform applicable at the tens of micron scale that allows for the validation and calibration of constitutive models and rate theory models used at higher length scales. In addition, the proposed framework aims at leveraging novel/advanced characterization methods. As such the model will be able to be directly compared against in-situ characterization methods (TEM, X-Ray diffraction). With regards to the modeling framework, in addition to its common treatment of plasticity, DDD in combination with FFT methods allows for the description of dislocations both as discrete and as continuous objects, thereby providing an ideal linkage with higher order constitutive modeling, which will be demonstrated by taking the example of grain boundary/dislocation interactions and in bicrystals and polycrystals. Further, an application of this framework to the case of twin propagation in hcp metals will be shown. Finally, the coupling between DDD and CD provides for a treatment of the role of dislocation microstructures on the evolution of radiation-induced damage as well as for the quantification of plasticity induced by irradiation. This will be illustrated in the case of pure body centered cubic Iron in which a mapping of the dominant deformation processes as a function of temperature, stress and irradiation condition will be presented.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A4] Symposium A-4

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

Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room6

[SY-A4] Effective Transport Properties of Polycrystalline Materials

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

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

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

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

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

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

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

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room6)

[SY-A4] Effective Transport Properties of Polycrystalline Materials

Invited

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

Most solid materials have surfaces, interfaces, and grain boundaries that enhance or hinder transport; as a result, the properties of polycrystalline solids can be vastly different from their intrinsic properties, especially in nanocrystalline materials. Diffusion in polycrystalline materials plays an important role in a wide range of material systems, including those found in batteries and solid oxide fuel cells. Due to the computational expense in explicitly considering the grain boundary network, establishing rational design rules for nanocrystalline materials with desired transport properties remains a challenge. We apply the Smoothed Boundary Method to evaluate the effective diffusivity of polycrystalline materials with a range of grain morphologies. We find that the anisotropy of grain morphologies plays a critical role in the overall transport behavior, which cannot be quantified using the classical mean field theories. The results are used to obtain an expression for mixed-pathway transport that is capable of universally predicting the effective diffusivity in complex polycrystalline solids without the use of computationally intensive simulations. Such an approach enables efficient simulation of transport in larger-scale systems while accurately capturing the effects of grain morphologies.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room6)

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

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

Effective medium polycrystal models provide a computationally efficient tool for simulations of elastic and visco-plastic deformation of aggregates. In particular, visco-plastic self-consistent (VPSC) schemes have been widely and successfully applied to predictions of texture, stress-strain, and dislocation density evolution during large strain deformation. In addition, VPSC schemes have been implemented in finite element codes as material subroutines to simulate various metal forming operations. However, a limitation of VPSC models is that they only address deviatoric stress and strain and neglect elastic contributions. As a consequence, they cannot be used to predict internal Cauchy stress evolution (as measured with neutron or X-ray diffraction), or to study constitutive behavior during complex loading scenarios (such as Bauschinger or spring-back) where the contribution of elasticity needs to be accounted for.

Several formulations have been proposed in the last 20 years that empirically combine visco-plastic and elastic regimes to formulate elasto-visco-plastic (E-VPSC) effective medium models. A disadvantage of these formulations is that they increase considerably the computation time, which makes them unwieldy for using in forming simulations.

Here we present a new approximate E-VPSC formulation that, by treating elasticity as a perturbation to the VPSC scheme of Lebensohn and Tomé [1], seems to capture the best of both worlds: efficient numerical processing while providing access to the evolution of Cauchy stress in the grains.

In this presentation we describe such E-VPSC formulation, compare it to previous ones, and provide a simple application - based on Voce hardening - to predictions of stress strain and internal stress evolution in steel subjected to tension-compression reversal tests. In a companion paper [2] we present several applications of this new E-VPSC formulation.

[1] R.A. Lebensohn, C.N. Tomé, “A self-consistent anisotropic approach for the simulation of plastic deformation and texture development of polycrystals: application to zirconium alloys”, Acta Metallurgica et Materialia 41(9) (1993) 2611-2624

[2] Y. Jeong, C.N. Tomé, “A new E-VPSC formulation: applications”, this conference

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(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room6)

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

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

In this presentation we implement an elasto-visco-plastic (E-VPSC) polycrystal formulation described in a companion paper [1]. In this formulation the contribution of elasticity is introduced as an eigen strain rate into the visco-plastic regime of each grain. The VPSC model of Lebensohn and Tomé [2] provides the implementation platform for the new E-VPSC formulation. The new model is validated by conducting several applications as follows:
Simple uniaxial tension test to validate the model and to demonstrate the numerical performance in comparison with the VPSC model [2], a separate E-VPSC model [3], and a rate insensitive EPSC model [4].
Large strain cyclic shear of low-carbon steel using Voce hardening law to demonstrate the Bauschinger effect. The results are compared with the VPSC-RGVB model [5], where the back-stress is linked to evolution of dislocation structures. Relaxation of internal stress in steel subjected to strain holds during tensile testing.

[1] C.N. Tomé, Y. Jeong, “A new E-VPSC formulation: fundamentals”, this conference

[2] R.A. Lebensohn, C.N. Tomé, “A self-consistent anisotropic approach for the simulation of plastic deformation and texture development of polycrystals: application to zirconium alloys”, Acta Metallurgica et Materialia 41 (1993) 2611-2624

[3] H. Wang, P.D. Wu, C.N. Tomé, Y. Huang, “A finite strain elastic-viscoplastic self-consistent model for polycrystalline materials”, Journal of the Mechanics and Physics of Solids 58 (2010) 594-612

[4] P.A. Turner, C.N. Tomé, "A study of residual stresses in Zircaloy-2 with rod texture", Acta metall mater 42 (1994) 4143-53

[5] W. Wen, M. Borodachenkova, C.N. Tomé, G. Vincze, E.F. Rauch, F. Barlat, J.J. Gracio, “Mechanical behavior of low carbon steel subjected to strain path changes: experiments and modeling”, Acta Materialia 111 (2016) 305-314

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room6)

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

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

Material variability from heterogeneous microstructure, such as grain and pore morphologies, can have significant effects on component behavior and creates uncertainty around performance. Current engineering material models typically do not incorporate microstructural variability explicitly, rather functional forms are chosen based on intuition and parameters are selected to reflect mean behavior. Conversely, mesoscale models that capture the microstructural physics, and inherent variability, are impractical to utilize at the engineering scale. An enhanced design methodology must be developed for materials with significant variability, such as current additively manufactured (AM) metals, to predict the ensemble response.

To address these challenges we have developed a method based on the Embedded Uncertainty formulation, Sargsyan, Najm, Ghanem (2015) to calibrate distributions of material parameters from high-throughput experimental data. With this method, material variability is directly associated with commonly-used material parameters using a chosen nominal model. One of the benefits of this approach is that expert knowledge can be extended to interpret the effect of (hidden) microstructure on variable mechanical response. In a complementary effort, we are developing machine learning techniques to handle the large volume of data from high-throughput methods. The focus of this aspect is on adapting common machine learning models, such as neural networks, to obey the same exact properties and symmetries as traditional constitutive models while representing features in the data in a flexible, bias-less manner, Tensor Basis Neural Network in Ling, Jones, Templeton (2016). Classical constitutive modeling provides guidance in selecting appropriate microstructural descriptors as inputs and functional frameworks for outputs. Examples of application of these techniques to polycrystalline, porous metals, motivated by current AM materials, will be given.

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

[SY-I3] Symposium I-3

Chair: Peter Voorhees(Northwestern University, United States of America)

Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room7

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

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

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

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

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

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

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room7)

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

Invited

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

Solutes can strongly interact with grain boundaries (GBs) and impact their thermodynamic and kinetic properties. Some of the most interesting effects of solute segregation include the segregation-induced GB phase transformations and the solute drag/pinning effect. An even more interesting is the effect of GB motion on GB phase transformations. Studying these effects by molecular dynamics is highly problematic due to the limited time scale of the method. The talk will present two alternative methods for studying phase transformations in moving GBs. One method is based on a semi-analytical discrete GB model in a binary solid solution. The regular solution model predicts first-order phase transformations in GBs, which can be shown by a GB phase coexistence line and GB spinodals of the bulk phase diagram. The model overcomes the time-scale limitation and treats both GB thermodynamics and GB dynamics within a unified framework. It gives direct access to the solute drag force and the GB free energy, which are difficult to compute by atomistic simulations. GB migration can be modeled on different timescales and over a wide range of velocities in both the transient and steady-state regimes. The simulations reveal interesting effects, such as kinetic stabilization of metastable or even unstable GB phases, dynamic GB phase transformations, and the dynamic GB hysteresis. Other interesting effects include the break-way events in which the GB leaves the segregation atmosphere behind and forms a new segregation. This new segregation atmosphere can represent the same of a different GB phase. It is shown how the discrete model reduces to phase-field model in the limit of wide segregation region. The phase-field simulations within this model yield similar results as the discrete model but have certain computational advantages. The results of this study can be broadly interpreted in terms of extremum principles of non-equilibrium thermodynamics, which predict dynamic stabilization of thermodynamically unstable but kinetically favored phases. Extension of the models to 2D and 3D systems and more accurate thermodynamic treatments will be discussed.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room7)

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

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

Grain boundary segregation is a phenomenon studied both experimentally and theoretically for decades. The interest in this phenomenon is evoked not only by its close relationship to temper embrittlement but also by its ability to stabilize nanocrystalline structures by solute segregation in the concept of Grain Boundary Engineering.

A full description of the exact temperature and solute concentration dependence of grain boundary segregation requires reliable values of segregation enthalpy and entropy as well as solute interaction coefficients. However, experimental studies of all these values are rather limited, and theoretical studies are usually restricted to segregation energy at zero Kelvin. It is obvious that such a database does not allow a full description of the grain boundary segregation in most systems of interest.

In this contribution we present a semi-empiric method enabling prediction of all required thermodynamic parameters - ideal enthalpy, ideal entropy and real binary interaction (Fowler) coefficient - which, in combination, describe fully the segregation of any segregant at any temperature and at individual grain boundaries. This method is based on the relationship between the segregation enthalpy and the solid solubility limit, and on the enthalpy-entropy compensation effect. The data for numerous solutes in alpha iron are predicted and they are compared to available data in the literature.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room7)

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

Invited

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

Segregation of solute atoms to grain boundaries is a well-known phenomenon which can modify grain boundary structure, energy and mobility among other properties. In this talk, we present computations of the segregation of Au at grain boundaries in Pt and corresponding experimental validation. The existence of a grain boundary phase transformation between high- and low-segregation states will be demonstrated. The impact of this segregation on the mechanical response of both individual grain boundaries and grain boundary networks will be examined. This work shows that for nanocrystalline samples, the stability of the grain structure against thermal or deformation induced grain growth is enhanced, but that ductility is reduced.

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

[SY-I4] Symposium I-4

Chairs: Shen J Dillon(University of Illinois, USA), Daniel Pino Munoz(Mines ParisTech / PSL Research University, France)

Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room7

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

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

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

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

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

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

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

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

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room7)

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

Invited

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

Due to their low sputtering yield, low intrinsic tritium retention, high melting point, and high thermal conductivity, W and W alloys are promising candidates for the divertor region in a magnetic fusion device. Transmutation reactions under neutron irradiation lead to the formation of He and H particles that potentially degrade material performance and might lead to failure. High He fluxes ultimately lead to the formation and bursting of bubbles that induce swelling, a strong decrease in toughness, and a nanoscale microstructure that potentially degrades the plasma. Understanding the behavior of He in polycrystalline W is thus of significant importance as one avenue for controlling the material properties under operating conditions. In this work we study the interaction of both substitutional and interstitial He atoms with various grain boundaries in pure W and the effect of the He presence on the system response to external loading. We observe that He segregates to all the interfaces tested and decreases the cohesion of the system at the grain boundary. Upon tension normal to the interface, the presence of He significantly decreases the yield stress, which depends considerably on the bubble pressure. Increasing pressure reduces cohesion, as expected. More complex stress states result in more convoluted behavior, with He hindering grain boundary sliding upon simple shear.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room7)

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

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

Grain boundaries (GBs) are one of the key factors to manipulate the material properties. The solute segregation and solute drag effects are remarkable for the thermodynamic properties of GBs, where the microscopic atomic and electronic structures affect the macroscopic behaviors of GB evolution. We have developed the local analysis method to get the local-energy and local-stress of each atom [1], which is of assistance to unveil the microscopic mechanism. In the present study, we firstly focused on the Σ11(332) and Σ3(111) <110> symmetrical tilt GBs in bcc Fe with 3d-transition-metal (TM) solutes. We performed ab-initio calculations together with the local analysis, and observed that the segregation behaviors of 3d-TM solutes can be classified into early TMs (Sc, Ti and V), middle TMs (Cr and Mn), and late TMs (Co, Ni and Cu). The early and late TMs prefer to segregate at the looser and tighter sites of GBs, respectively. The local-energy decomposition indicates that the segregation of early TMs is dominated by the stabilization of surrounding Fe atoms at a GB, while that of late TMs is dominated by the repulsion from the bulk as well as the stabilization of a TM-atom itself. Furthermore, corresponding to the segregation energy of each 3d-TM segregated to the looser or tighter site of GBs, by the multiscale modeling, we estimated the solute drag effects on the mobility and interface energy of GBs, and the grain growth rate. Finally, we discuss the cases of

general GBs, and compare the results with experiment.

[1] Y. Shiihara et al., Phys. Rev. B 81, 075441 (2010). S. Bhattacharya et al., J. Mater. Sci. 49, 3980 (2014).

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room7)

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

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

Predictions of the ferrite to austenite or austenite to ferrite transformation kinetics during heating and/or cooling of ternary Fe-C-X alloys is challenging because diffusion coefficients of interstitial and substitutional elements are very different in both phases. The model described in this paper, is based on the prediction of (i) concentration profiles for all elements and (ii) interface velocity, that corresponds to the minimization of the Gibbs energy (*i.e.* phase field approach). The total energy of the system is given *via* a dynamic coupling with Thermocalc database.

The ferrite/austenite interface is assumed to have a finite width. This allows to deal with a unique diffusion profile for all species. Element fluxes are derived from their chemical potential gradient. Another advantage of such an approach is the possibility of introducing a potential depth within the interface, leading to solute atoms segregation, that is believed to control transformation kinetics in ternary systems.

During the transformation, it is observed that the model automatically switches between different equilibrium conditions (from out-of-equilibrium transformation to para-equilibrium, local equilibrium with and without partitioning until ortho-equilibrium). To our knowledge, it constitutes a real improvement in phase transformation modeling. This model has been calibrated on decarburization experimental kinetics reported in the literature in various Fe-C-X systems. This model shows an interface motion slowing down with the addition of a potential depth at the interface in agreement with experimental observations. By extension, the model has been used on isothermal and non-isothermal heating for complex Dual Phase steels and compared with experiments.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room7)

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

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

Powder metallurgy is a processing technology that uses metal powder compacts to produce near net shape parts through sintering and is suitable for mass production. Quantitative prediction of microstructure evolution and sintering kinetics during powder sintering is of great significance for understanding the sintering mechanism and optimizing the sintering process.

In this paper, the packing structure model of nano copper particles was established using the discrete

element method as a powder compact. The solid phase sintering of the powder compact was studied by molecular dynamics simulation using embedded atom method. The sintering mechanism and densification kinetics of the nano powders were analyzed and compared with the experimental results. The effects of diffusion mechanism and grain growth on the sintering densification process are discussed in detail.

Keywords: powder sintering, diffusion, grain growth, discrete element, molecular dynamics

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

[SY-L3] Symposium L-3

Chairs: Peter M Derlet(Paul Scherrer Institut, Switzerland), Cynthia Reichhardt(Los Alamos National Laboratory, United States of America)

Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room8

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

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

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

○Lasse Laurson （Aalto University, Finland）

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

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

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room8)

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

Invited

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

The relationship between dislocation network stucture and plasticity is studied via a linear stability analysis of the evolving dislocation configuration. This is done for a simplified one dimensional model of interacting dislocation pile-ups, which exhibits a mean-field depinning transition at yield, and for a two dimensional dislocation dynamics model always in a state of criticality that is well described by a jamming transition. We find that the obtained eigen-modes prior to a plastic event play an important role in characterizing the discrete micro-plastic regime of simulation, reflecting the degree of criticality the system is in, the nature of how a plastic event occurs and its eventual evolution into an avalanche.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room8)

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

Invited

○Lasse Laurson (Aalto University, Finland)

First, I will present an overview of our recent studies focusing on the statistical properties of strain avalanches in crystal plasticity as observed in discrete dislocation dynamics (DDD) simulations. These encompass various scenarios, including two and three dimensional DDD models, and considering systems with and without an additional quenched pinning field (due to, e.g., precipitates) interacting with the dislocations. I discuss the results from the perspective of two main mechanisms affecting the nature of dislocation dynamics and hence the deformation process: dislocation (de)pinning and dislocation (un)jamming.

Second, I will briefly present our very recent efforts to apply machine learning to predict the properties of the stress-strain curves of individual microscale samples using features of the initial, pre-exisiting dislocation network as input. The resulting predictability of the deformation process is found to evolve with strain in a non-monotonic fashion, something we attribute to the stochastic nature of the deformation avalanches.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room8)

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

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

Due to the difficulties of tensile/compressive tests at small length scales, nanoindentation is widely used towards unveiling crystalline mechanical properties. However, crystal plasticity limits the understanding of

nanoindentation results at depths below 500nm: the Indentation Size Effect (ISE) in these scales leads to very noisy and unclear data, with the measured hardness/stiffness being difficult to ‘translate’ into features of the material microstructure. In this work, we demonstrate two statistical approaches to investigate the ultra-nano regime of FCC metals towards unveiling crystalline properties: First, we notice that indentation together with in-plane tension consist of a phase diagram of the sample elasto-plastic property. The elastic-plastic transition during indentation is naturally continuous for large dislocation densities. In the large dislocation density regime, through the development of scaling functions for an appropriately defined plasticity order parameter, we connect statistically the bulk crystal plasticity transition with nanoindentation. Second, for low dislocation densities, we utilize the noise of the load-depth nanoindentation curves and the post-indent nanoindentation images to statistically connect experiments with 3D discrete dislocation dynamics simulations. We develop a machine-learning approach that can be used for nanoindentation and predict experimentally relevant pre-existing dislocation densities in single crystalline FCC grains.

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

[SY-L4] Symposium L-4

Chair: Lasse Laurson(Aalto University, Finland)

Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room8

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

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

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

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

[SY-L4] Temporal and spatial plastic instability of micrometer-scaled materials

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

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room8)

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

Invited

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

We examine driven dislocation assemblies and show that they can exhibit a set of dynamical phases remarkably similar to those of driven systems with quenched disorder such as vortices in superconductors, magnetic domain walls, and charge density wave materials. These phases include pinned-jammed, fluctuating, and dynamically ordered states, and each produces distinct dislocation patterns as well as specific features in the noise fluctuations and transport properties. Our work suggests that many of the results established for systems with quenched disorder undergoing plastic depinning transitions can be applied to dislocation systems, providing a new approach for understanding pattern formation and dynamics in these systems.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room8)

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

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

It is well-known from micropillar and acoustic emission experiments that plastic strain accumulates in sudden avalanche-like events. Based on the statistical analysis of these bursts it is now apparent that plastic deformation can be described as a critical phenomenon. A lot of subsequent attention has been paid to understand the fundamental nature of this criticality: whereas the analysis of experiments suggests that scale-free behavior is characteristic only to the onset of yield, discrete dislocation dynamic (DDD) simulations hint at a more involved picture. Namely, the dynamics of the system is of glassy nature, where power-law distributions arise irrespective of the distance to the yielding threshold. These DDD simulations represent pure systems where neither Peierls stress nor any kind of impurities impede dislocation motion. In the talk we will discuss how addition of these realistic ingredients affect the critical behavior in terms of relaxation properties, avalanche statistics, dynamic correlations and system size dependence.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room8)

[SY-L4] Temporal and spatial plastic instability of micrometer-scaled materials

Invited

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

Suppressing plastic instability is a critical goal to improve deformability and ductility in a wide variety of engineering applications. At temporal scale, plastic instability is manifested as intermittent burst and dislocation avalanches, leading to uncontrollable deformation. At spatial scale, plastic instability is manifested as the onset of flow localization, leading to sudden failure. While insight in the physical origin of plastic instability accumulates, the need for a quantitative description of temporal and spatial plastic instability remains challenged due to the lack of clear quantitative relation correlating deformation behavior with microstructural features. Here, we will discuss the quantitative description method of temporal and spatial plastic instability, and present a very simple model to predict them based on the idea of stochastic activation of dislocations sources. Combined with systematic discrete dislocation dynamics simulations, we will present that even though power law scaling is widely used to describe the statistical distribution of strain burst magnitude, power law scaling does not tell the whole story at temporal scale. At spatial scale, highly-irradiated materials will be taken as an example. We will unravel the mystery of how and why irradiation-induced defects enhance or inhibit plastic instability, and how and why dislocation channels arise, and what governs their width.

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

[SY-H1] Symposium H-1

Chair: Turab Lookman(Los Alamos National Laboratory, United States of America)

Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room9

[SY-H1] **Multiscale modeling of electro-responsive gels**

○Masao Doi （Beihang University, China）

[SY-H1] Non-monotonic particle size effect on the glass transition in polymer-particle blends and its application to shape memory polymers

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

[SY-H1] **Thermomechanical behavior of shape-memory polyurethane copolymer : A coarse-grained molecular dynamics simulation**

○SUNGWOO PARK, JUNGHWAN MOON, BYUNGJO KIM, MAENGHYO CHO （Seoul National University, South Korea, Korea）

[SY-H1] **Investigation of photo-mechanical behavior of azobenzene-based polymer: A coarse-grained molecular dynamics study**

○Junghwan Moon[1], Byungjo Kim[1], Joonmyung Choi[2], Maenghyo Cho[1,3] （1.Divison of Multiscale Mechanical Design, School of Mechanical and Aerospace Engineering, Seoul National University, Korea, 2.Mechatronics R&D center, SAMSUNG ELECTRONICS CO., LTD, Korea, 3.Institute of Advanced Machines and Design, Seoul National University, Korea）

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room9)

[SY-H1] Multiscale modeling of electro-responsive gels

Invited

○Masao Doi （Beihang University, China）

Certain kind of ionic gels show electro-mechanical coupling: the gel deforms when electric field is applied, and, conversely, electric field is created when the gel is deformed. Such phenomena may be used for actuators and sensors. In this talk, I will discuss the physical modeling of the electro-mechanical coupling in ionic gels.

[References] Masao Doi, Fluid transport in gels, Oxford Handbook of Soft Condensed Matter, Oxford

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room9)

[SY-H1] Non-monotonic particle size effect on the glass transition in polymer-particle blends and its application to shape memory polymers

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

Both via experiments and molecular dynamics simulations, it is shown that adding small molecules enhances the dynamics of structural relaxation in polymer melts and glasses [1]. While this effect is a monotonic function of concentration [1], it is found to be a non-monotonic function of particle size [2]. A detailed survey of non-Gaussian parameter for small molecules and polymer beads reveals a separation of time scales for cooperative motion between the above two species. This is indicative of a decoupling of the fast dynamics of small molecules from the chains’ relaxation dynamics and a resulting weak effect. The dynamics of large particles, on the other hand, is strongly coupled to that of polymer. However, since large particles are only slightly more mobile than the polymer beads, their enhancing effect is also relatively weak. For intermediate particle sizes, the particles are sufficiently fast and the coupling to polymer strong enough to induce a large enhancement of the chains' relaxation kinetics. This non-monotonic effect occurs both for entangled and non-entangled polymers, hinting towards local packing effects as the main origin of the phenomenon [1]. It is shown that the effect can be explored in shape memory polymers to tune the triggering temperature of the shape recovery process in a non-monotonic manner.

[1] Elias M. Zirdehi, Axel Marquardt, Gunther Eggeler and Fathollah Varnik, Molecular dynamics simulations of entangled polymers: The effect of small molecules on the glass transition temperature, Procedia Computer Science 198C, 265 (2017).

[2] Elias M. Zirdehi and Fathollah Varnik, Non-monotonic particle size effect on the glass transition in polymer-particle blends (submitted).

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room9)

[SY-H1] Thermomechanical behavior of shape-memory polyurethane copolymer : A coarse-grained molecular dynamics simulation

○SUNGWOO PARK, JUNGHWAN MOON, BYUNGJO KIM, MAENGHYO CHO （Seoul National University, South Korea, Korea）

Shape-memory polymers (SMPs) are smart materials that react to external stimuli to restore their original shape. The stimuli can be various things such as light, heat, humidity, and so on. Segmented polyurethane copolymer is a representative thermo-responsive SMP which are synthesized with a polyol and an isocyanate. The hard-segment which is clustered together helps to memorize the original shape by stabilizing the network, and the soft-segment which can achieve polymer crystallization acts as a switching-segment which fixes the temporary shape and induces the shape-memory effect. This dual-segment system is a necessary condition for shape-memory behavior of polyurethane. Full-atom molecular dynamics (MD) simulation can cover the atomistic structures and shape-memory properties, but it has limitations on observing mesoscale phenomena such as polymer crystallization, and micro-phase separation. To overcome this issue, we have developed a coarse-grained (CG) MD model with reduced degrees of freedom by treating multiple atoms as a single bead. Full-atom MD simulation was performed to obtain intra- and inter-bead potential of the CG model via iterative Boltzmann inversion (IBI) method. As a result, we could observe the crystallinity and shape-memory properties of SMPU models with different hard-segment contents. Then, the effect of microstructure on the mechanical deformation and shape memory behavior were investigated. We expect this study provides an insight to design the segmented polyurethane copolymer with enhanced shape recovery performance.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room9)

[SY-H1] Investigation of photo-mechanical behavior of azobenzene-based polymer: A coarse-grained molecular dynamics study

○Junghwan Moon[1], Byungjo Kim[1], Joonmyung Choi[2], Maenghyo Cho[1,3] （1.Divison of Multiscale Mechanical Design, School of Mechanical and Aerospace Engineering, Seoul National University, Korea, 2.Mechatronics R&D center, SAMSUNG ELECTRONICS CO., LTD, Korea, 3.Institute of Advanced Machines and Design, Seoul National University, Korea）

Photo-active deformable structures have drawn great attention because they can exhibit complex 3D deformations without any electronic circuit. Among the photo-responsive polymers (PRPs), liquid crystalline polymers (LCPs) doped with photochromic azobenzene molecules have diverse applications for soft micro-mechanical actuators because of a reversible photo-isomerization under ultraviolet (UV)/visible light illumination. The micro-scale photo-mechanical behavior of the polymer network can be greatly represented using conventional molecular dynamics (MD) simulations. However, MD simulation cannot be applied to examine the meso-scale phenomena occurred in the photo-deformable structure because too much degrees of freedom (DOFs) are required for full-atomistic description. To overcome this limitation, we propose a multi-scale/multi-physics computational framework based on a coarse-grained (CG) molecular dynamics simulation, which combines molecular switching induced by the photo-isomerization, and overall shape change of the polymer network. The structure-based iterative Boltzmann inversion (IBI) method was utilized to systematically represent the photo-chemical reaction-induced change of the polymeric structure, and effectively expand time- and length-scales of the atomistic simulations. As a result, we could observe the transition between three different liquid crystalline phases (smectic A - nematic - isotropic) under light irradiation, which cannot be reproduced using the all-atom MD simulations. Also, we investigated a unique photo-deformation of the smectic LCP network and its effect on the mechanical properties. We expect the proposed multiscale modeling and simulations to be a guideline for mechanically designing the photo-

responsive smart materials.

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

[SY-H2] Symposium H-2

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

Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room9

[SY-H2] **Hydrogels with Dynamic Sacrificial Bonds - From Toughness to Adhesion to Composites -**

○Jian Ping Gong[1,2] （1.Faculty of Advanced Life Science, Hokkaido University, Japan, 2.Soft Matter GI-CoRE, Hokkaido University, Japan）

[SY-H2] Elastic properties and effective interactions of *in silico* realistic microgels

○Lorenzo Rovigatti[1,2], Nicoletta Gnan[1,2], Emanuela Zaccarelli[1,2] （1.Institute for Complex Systems, Uos Sapienza - CNR, Italy, 2.Dipartimento di Fisica, Sapienza Università di Roma, Italy）

[SY-H2] Controlling the mechanics of a synthetic hydrogel with motor-like internal contractility

Marcos Fernandez-Castano Romera[1], Rint P Sijbesma[1],
○Cornelis Storm[1] （1.Theory of Polymers and Soft Matter, Technische Universiteit Eindhoven, The Netherlands）

[SY-H2] **Study on viscoelastic behavior of natural rubber with multiscale approach**

○Byungjo Kim, Junghwan Moon, Maenghyo Cho （Seoul National University, Korea）

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room9)

[SY-H2] Hydrogels with Dynamic Sacrificial Bonds - From Toughness to Adhesion to Composites -

Invited

○Jian Ping Gong[1,2] (1.Faculty of Advanced Life Science, Hokkaido University, Japan, 2.Soft Matter GI-CoRE, Hokkaido University, Japan)

Invention of the tough double network hydrogels (DN gels), consisting of interpenetrated rigid/brittle network and soft/stretchable network, shows that the effective energy dissipation by the breaking of the covalent bond of the brittle network prevents catastrophic crack propagation upon deformation, and thus, gives the extraordinarily high toughness of the material. Such sacrificial bond effect has been successfully applied to develop tough double network hydrogels of diverse chemistry and also to double and triple network elastomer materials. Thus, sacrificial bond concept is proved to be a general approach for developing tough soft materials. As the internal rupture of DN gels is due to the irreversible breaking of the covalent bonds of the brittle network, the conventional DN gels deteriorate gradually after repeated deformation. To address this problem, many recent works have replaced the covalent bonds with non-covalent bonds to allow the sacrificial bonds to be reformed. In this talk, novel hydrogels with reversible sacrificial bonds developed in author's group are reviewed and their excellent mechanical behaviors such as high toughness, self-healing, adhesion to biological tissues, and fast underwater adhesion are demonstrated. Furthermore, this principle is extended to develop tough composites using tough hydrogels as energy dissipative soft matrix.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room9)

[SY-H2] Elastic properties and effective interactions of *in silico* realistic microgels

○Lorenzo Rovigatti[1,2], Nicoletta Gnan[1,2], Emanuela Zaccarelli[1,2] (1.Institute for Complex Systems, Uos Sapienza - CNR, Italy, 2.Dipartimento di Fisica, Sapienza Università di Roma, Italy)

The bulk behaviour of colloidal suspensions depends crucially on the microscopic details of the particle-particle interaction[1]. For polymer-based building blocks, the interactions depend on a large number of parameters such as the particle microstructure, its composition and related physico-chemical properties (solvophobicity, charge density, *etc.*). Among the huge variety of available systems, stimuli-responsive microparticles built out of polymer networks, so-called microgels, have emerged as one of the most interesting class of soft particles, for both a theoretical and applicative standpoint[2].
Here we build upon a recently-developed method[3] to generate and simulate realistic *in silico* microgels. We first look at the single-particle mechanics by calculating the elastic moduli in the small-deformations regime. We then use Umbrella Sampling and a generalised Widom insertion method to accurately estimate the two-body effective interaction.
We show for the first time that the Hertzian theory works well for large separations, and that in this regime the single-particle elastic moduli can predict the amplitude of *V(r)* for a wide range of network topologies. However, for smaller separations the two microgels start to strongly interact and change their shape and *V(r)* deviates from the predicted Hertzian behaviour.
This work establishes a clear link between the microscopic network properties and the resulting microgel-microgel interactions, paving the way for a deeper understanding of the bulk behaviour of microgel

suspensions.

[1] C. N. Likos, Phys. Rep., **348**, 267 (2001)
[2] A. Fernandez-Nieves, H. Wyss, J. Mattsson, D. A. Weitz, *Microgel Suspensions: Fundamentals and Applications*; John Wiley &Sons (2011)
[3] N. Gnan, L. Rovigatti, M. Bergman, E. Zaccarelli, Macromolecules, **50**, 8777 (2017)

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room9)

[SY-H2] Controlling the mechanics of a synthetic hydrogel with motor-like internal contractility

Marcos Fernandez-Castano Romera[1], Rint P Sijbesma[1],
○Cornelis Storm[1] （1.Theory of Polymers and Soft Matter, Technische Universiteit Eindhoven, The Netherlands）

Stiffening due to internal stress generation is common in living materials and regulates many biomechanical processes. For example, cells stiffen their surrounding matrix by pulling on collagen and fibrin fibers. At the subcellular level, molecular motors prompt fluidisation and stiffening of the cytoskeleton by sliding polar actin filaments in opposite directions. I will present results showing that synthetic materials, likewise, are able to change their stiffness in response to internally generated and externally applied forces. Theoretical and experimental results are presented for a system where chemical crosslinking of thermoresponsive poly(N-isopropylacrylamide) (PNIPAM) into a fibrous matrix of synthetic semi-flexible polymers allows for internal stress generation upon induction of coil-to-globule transition, resulting in a macroscopic stiffening response spanning up to three orders of magnitude. Strikingly, the forces generated by PNIPAM collapse are sufficient to drive a fluid material into a stiff gel within a few minutes. Rigidified networks dramatically stiffen in response to applied stress featuring power law rheology with exponents that match those of reconstituted actomyosin networks pre-stressed by molecular motors. This concept holds potential for the rational design of responsive synthetic materials that are fluid at room temperature and rapidly rigidify at body temperature to form hydrogels mechanically compatible to cells or tissues.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room9)

[SY-H2] Study on viscoelastic behavior of natural rubber with multiscale approach

○Byungjo Kim, Junghwan Moon, Maenghyo Cho （Seoul National University, Korea）

In this study, the viscoelastic behavior of natural rubber is investigated with the aid of a coarse-grained (CG) molecular dynamics (MD) simulation. It is challenging to understand the long-term nature of polymeric materials using a conventional MD simulation due to the inherent limitation in the time and length scale. To overcome the drawback in terms of scalability in time and length, the CG model can offer a way to assess the long-term physical behavior by substantially reducing a degree of freedoms with the implementation of bead particles which are equivalent to the specific group of atoms. To describe the inter- and intra-interactions between the beads consisting of the system, the iterative Boltzmann inversion (IBI) method is employed. As an important viscoelastic behavior of elastomer, the time-dependent shear relaxation modulus is calculated

using the stress autocorrelation function. The dynamic modulus in a frequency domain is further studied with using the Fourier transformation. The influence of vulcanization and chain length of natural rubber is taken into account. Plus, the spherical shape of SiO_2 nanoparticles are considered as filler materials, and the behavior of filler-rubber is also studied for varying filler loading conditions. With the present work, the viscoelastic nature of rubber is understood by employing CG MD simulations which can enhance the scale of computation in terms of length and time. Further, this work can be extended to examine more complex polymeric system regarding the long-term physical nature or thermodynamic property.

Symposium | J. Multiscale Modeling of Heterogeneous Layered Media

[SY-J3] Symposium J-3

Chairs: Ramesh Talreja(Texas A&M University, United States of America), Tong-Earn Tay(National University of Singapore, Singapore)

Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room10

[SY-J3] Fundamentals of Generalized Particle (GP) Multiscale Methods with Applications to Analyses of Alternatively-Arranged Soft and Hard Layers

○Jinghong Fan （Kazuo Inamori School of Engineering, Alfred University, United States of America）

[SY-J3] The effect of layer thickness ratio on the plastic deformation mechanisms of nonoindented Ti/TiN nanolayered composite: A molecular dynamics study

○Georges Y Ayoub[1], Wei yang[2], Iman Salehinia[3], Bilal Mansoor[2], Hussein Zbib[4] （1.Dept. of Industrial and manufacturing system Engineering, Univ. of Michigan, United States of America, 2.Dept. of Mechanical Engineering, Texas A&M Univ., United States of America, 3.Dept. of Mechanical Engineering, Northern Illinois Univ., United States of America, 4.School of Mechanical and Materials Engineering, Washington State Univ., United States of America）

[SY-J3] The attenuation of stress wave propagation in multilayer structure

○Fengyuan Yang, Zhanli Liu （Tsinghua University, China）

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

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

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room10)

[SY-J3] Fundamentals of Generalized Particle (GP) Multiscale Methods with Applications to Analyses of Alternatively-Arranged Soft and Hard Layers

Invited

○Jinghong Fan （Kazuo Inamori School of Engineering, Alfred University, United States of America）

Alternatively-placed soft and hard layers are investigated using multiscale generalized particle methods, namely the GP and/or XGP methods (Fan 2009, Xu, Fan et al. 2016, Fan et al. 2017). In the methods, material models are divided as several domains with generalized particle of different scales. The distinguished characteristics of the GP methods are that each higher scale particle is formed by lumping the lower scale particle or atoms but their structures are all the same as the atomistic one, such as BCC, FCC and HCP. The fundamentals of this type of multiscale analysis are based on the local bottom-up multiscale analysis. Specifically, the position, mass and physical property of the upper-level particle is determined by all lower-level particles (e.g. atoms) within the individual particle’s neighbor link cell (NCL), thus the material behavior naturally follows the displacement and motion of these atoms consisted of the material and the numerical algorithm follows the typical molecular dynamics.
Extrinsic and intrinsic size effects has been successfully investigated to confirm the accuracy and efficiency of the proposed multiscale methods. Among several interesting observations of the atomistic/multiscale simulations, results show that defects in the soft, hard layers and their interface due to loading and manufacturing determine, to a large extent, their deformation and failure behavior. It has been found that some observations are different from previous predictions in the literature for a long period. For instance, simulations show that Langford’s famous prediction (1977) of dislocations appearance in cementite layer is not fully accurate. In addition, a direct check of the dislocation pile-up theory proposed by Eshelby, Frank and Nabarro (1951) indicate that the simulation-determined interface stress is much lower than their theory-predicted one.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room10)

[SY-J3] The effect of layer thickness ratio on the plastic deformation mechanisms of nonoindented Ti/TiN nanolayered composite: A molecular dynamics study

○Georges Y Ayoub[1], Wei yang[2], Iman Salehinia[3], Bilal Mansoor[2], Hussein Zbib[4] （1.Dept. of Industrial and manufacturing system Engineering, Univ. of Michigan, United States of America, 2.Dept. of Mechanical Engineering, Texas A&M Univ., United States of America, 3.Dept. of Mechanical Engineering, Northern Illinois Univ., United States of America, 4.School of Mechanical and Materials Engineering, Washington State Univ., United States of America）

Molecular dynamics simulations were performed to identify the underlying deformation mechanisms controlling the plastic behavior of nanoindented nanoscale multilayered Ti/TiN. MD simulations were conducted on pure Ti and pure TiN as well as on four different layer-thickness ratios of Ti/TiN multilayers, Ti:TiN=1, 2.5, 4, and 7.5. The Ti layer thickness varied from 2nm to 15nm. The plastic deformation of nanoindented pure Ti was dominated by the formation of dislocation loops resulting from basal partial dislocations, while very few perfect dislocations that tie dislocation loops together were observed. The plastic

deformation of nanoindented pure TiN was controlled by the activation of perfect dislocation propagation along the *111* plane that dissociates into two partials. Depending on the thickness ratio, either dislocation pile-up or single dislocation crossing through the interface was the controlling plastic deformation mechanism of nanoindented Ti/TiN multilayers. For metal layer thicknesses above 5nm, significant dislocation pile-ups were observed at the interface of the quad-layered samples. The Ti/TiN multilayer with a thickness ratio of 1:1 with individual layer thickness of 2nm exhibited the highest strain-hardening rate. At this length scale, the activation of dislocation sources requires very high stresses, and the single dislocation crossing process is the most dominant deformation mechanism. The initiation of plasticity in the TiN layer occurs at a high level of stress since there is no dislocation pile-up at the interface.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room10)

[SY-J3] The attenuation of stress wave propagation in multilayer structure

○Fengyuan Yang, Zhanli Liu （Tsinghua University, China）

In recent years, many biological structures with excellent impact resistance have been studied, such as the stomatopod dactyl club, fish scales, etc. These biological structures have a multi-layered structure and each layer structure has different material properties. These specific bio-layered structures not only have higher hardness and modulus, but also have higher dissipative stress wave performance. In this paper, the influence of the material properties and the arrangement order of the multilayer structure on the propagation of stress waves is studied, in order to obtain a multilayer structure with higher attenuation stress wave energy. The propagation of stress wave in the material of viscoelastic layer changes with the frequency of stress wave. The transmission coefficient of the stress wave in the multilayer structure has frequency effect and size effect.

(Tue. Oct 30, 2018 9:45 AM - 11:00 AM Room10)

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

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

Using multiscale modelling approach we performed molecular-dynamics simulations of both coarse-grained and detailed atomistic (polyimide R-BAPB) amorphous polymer melts consisting of non-entangled, non-crosslinked polymer chains. The inorganic filler surfaces were mimicked either by solid walls, or by explicit insertion of the filler particles. The rise in the glass-transition temperature with increase of the filler fraction was accompanied by a monotonic slowing-down of the relaxation of the incoherent scattering function on all simulated length scales. The filler surface roughness could also lead to slower segmental relaxation. Higher dynamic fragility was observed for smaller film thicknesses.
The cyclic shear deformation is performed to characterize macroscopic properties of the systems before and after filler insertion. The reported coarse-grained simulations show a strong decrease of the nanocomposites storage modulus with increasing strain amplitude, which is accompanied by a maximum in the loss modulus (the so-called Payne effect); the onset of the softening is observed in the linear regime of deformation at

strain amplitude of about 0.01. Moreover, the dependence of the storage modulus on the instantaneous strain exhibits both softening and hardening regimes, in agreement with Large Amplitude Oscillatory Shear (LAOS) experiments. The observed hardening is caused by the shear-induced decrease of the non-affine diffusion of the polymer segments due to filler particles acting as effective crosslinks between polymeric chains and, hence, hindering diffusion. Moreover, the formation of glassy immobile layers at the nanoparticle interface strongly increases the storage modulus at low strain amplitudes. The strain softening with increasing strain amplitude is connected to the mobilization of these glassy layers and an ***increase in the dynamic heterogeneity*** of the polymer matrix.

Symposium | J. Multiscale Modeling of Heterogeneous Layered Media

[SY-J4] Symposium J-4

Chairs: Brian Cox(Arachne Consulting Inc., United States of America), Tomonaga Okabe(Tohoku University, Japan)

Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room10

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

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

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

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

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

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

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room10)

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

Invited

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

Validation of analytical models for ply cracking of general symmetric composite laminates

Polymer matrix composites (PMCs) that have high specific strength and specific rigidity have been used in aerospace fields. Laminates made by stacking unidirectional fiber-reinforced lamina, which have predefined mechanical properties, are commonly used. Fiber-reinforced laminates have a specific fracture mode such as transverse cracking, delamination, and breakage of the fiber. Of these fracture modes, transverse cracking occurs in the earliest stage. In laminates with plies in different fiber orientations, transverse cracks can form from defect in a given ply, and grow traversing the thickness of the ply and running parallel to the fibers in that ply. The most direct effect of transverse cracking is reduction of the thermomechanical properties of the laminate, including changes in the effective values of Young's moduli, Poisson's ratios, and thermal expansion coefficients. Substantial transverse cracking may give rise to more deleterious forms of damage, or provide pathways for the entry of moisture and corrosive liquids. Thus, although this damage mode is not critical from a final fracture point of view, it can result in significant degradation in the properties of laminates. Therefore, it is necessary to understand the mechanical behavior of laminate including transverse cracks. The continuum damage mechanics (CDM) is considered to be a valid approach to this issue. This approach utilizes the internal state variable and damage variable to consider the effect of transverse cracks on the reduction of stiffness.

In this study, the three-dimensional local stress field (3-D LSF) model was formulated at first. Secondly, a Tohoku continuum damage mechanics (TCDM) model, which is an energy-based model of ply cracking of general composite laminates, was presented using the 3-D LSF model and the CDM approach. Especially, the damage variable d_2 in the direction normal to the fiber was derived for the ply including transverse cracking as a function of transverse crack density using the 3-D LSF model. Finally, the validity of the TCDM model was estimated by comparing the NPL model and the experiment results.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room10)

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

Invited

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

A fully coupling model for diffusion induced finite elastoplastic bending of bilayer electrodes in lithium-ion batteries is proposed. The effect of mechanical stress on lithium diffusion is accounted for by the mechanical part of chemical potential derived from Gibbs free energy along with use of logarithmic stress and strain. Eight dimensionless parameters, which govern the stress-assisted diffusion and the diffusion induced elastoplastic bending, are identified. It is found that the finite plasticity starting from the interface of bilayer

increases the chemical potential gradient and thereby facilitates lithium diffusion. The full plastic flow makes the abnormal lithium concentration distribution possible that the concentration at the lithium inlet is lower than the concentration at the interface (downstream). The increase in thickness of active layer during charging is much larger than the eigen-stretch due to lithiation, and this excess thickening is found to be caused by the lithiation induced plastic yield.

(Tue. Oct 30, 2018 11:15 AM - 12:30 PM Room10)

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

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

In the contribution, we discuss the model of solidification of melt occupying pores of the porous medium with grains intact but participating in the heat transfer. The research motivation is given by development of advanced materials as well as by climate changes. The model is based on coupled heat conduction equation and the phase-field. We present the model and several computational studies.

Solidiffication inside the porous medium is accompanied by complex processes affected by the material composition, micro-scale interfaces between phases within the medium, bulk properties of the presented phases, and ambient physical conditions. Volumetric changes of the liquid presented in pores subjected to phase change conditions is one of crucial phenomena. Due to the generic inhomogeneity of volume occupied by the solidifying porous medium, we focus on treating the phase transition at microscale. We have developed a micro-scale model describing mechanical, thermal, and phase change processes within a small sample of a porous medium. The phase change is described in the Lagrangian framework by means of the energy, Navier, and phase-field equations. A coupling of multi-physics and multiple phases is introduced. The model provides spatio-temporal dependencies of primary variables, the resulting forces exerted on grain surfaces by the change in specific volume due to phase transition, and possibly, the mean values of the key quantities useful for upscaling. The role of the model is demonstrated on several computational studies which follow recently published results [1-2].

[1] Žák A., Beneš M. and Illangasekare T.H. Analysis of Model of Soil Freezing and Thawing, IAENG International Journal of Applied Mathematics, Volume 43, Issue 3, pp. 127--134, September 2013

[2] Žák A., Beneš M., Illangasekare T. H., Trautz A. Mathematical Model of Porous Medium Freezing at Micro-Scale, to appear in Communications in Computational Physics, 2018