

Sunday, October 5th

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Registration

Conference reception

Monday, October 6th

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| 07:00 | Breakfast <i>Location: Tent</i> | | | | | |
| 07:15 | | | | | | |
| 07:30 | | | | | | |
| | Chair: Anter Anter El-Azab | | | | | |
| 08:00 | Plenary 1: Dislocation patterns Dr Ladislav Kubin (ONERA, France) <i>Location: Ballroom</i> | | | | | |
| 08:15 | | | | | | |
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| 08:45 | Plenary 2: Rethinking the Meaning of Defect Structure Professor David Srolovitz (University of Pennsylvania) <i>Location: Ballroom</i> | | | | | |
| 09:00 | | | | | | |
| 09:15 | | | | | | |
| 09:30 | Refreshment break <i>Location: Tent</i> | | | | | |
| 09:45 | | | | | | |
| | Ballroom 1 | Ballroom 2 | Ballroom 3 | Ballroom 4 | California | Mariposa |
| | J: Ab initio calculations and microscopic modeling | E: Three dimensional materials science | Joint G/H: Thermally and mechanically activated processes | | D: Modeling of ferritic systems and steels for nuclear applications | C: Electro-chemomechanics in catalysis |
| | Chair: Yang Xiang | Chairs: Javier Segurado and Guillaume Puel | Chairs: Sidney Yip and Javier Llorca | | Chairs: Anna Serra and Pareige Philippe | Chairs: Dane Morgan and Bilge Yildiz |
| 10:00 | (I) Getting Real! Thermodynamics and Statistical Mechanics from First Principles for Materials Science and Engineering Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft | (I) Modeling of a Ni-based superalloy: from micro-pillar compression tests to polycrystalline models Javier Segurado, Polytechnic University of Madrid | (I) Materials Aging at Mesoscale: Activated kinetics and Self-Organized Criticality Sidney Yip, MIT | (I) Long term solute evolution in RPV steels: experimental and modeling convergence? Pareige Philippe, Normandie Université | (I) Mechanics Controls Catalysis (Sometimes) William A Curtin, École Polytechnique Fédérale de Lausanne | |
| 10:15 | | | | | | |
| 10:30 | Two-scale analysis of composite plates with in-plane periodic microstructures Kenjiro Terada, Tohoku University | Simulating the brittle-ductile transition using discrete dislocation plasticity Edmund Tarleton, Oxford University | Low cycle fatigue modeling of dislocation patterning in FCC metals in single and multiple slip by crystal plasticity finite element method Nicolò Grilli, Paul Scherrer Institut | Self-interstitial clusters with C15 Laves phase structure in bcc iron Francois Willaime, CEA, DEN, Service de Recherches de Metallurgie Physique | (I) Strain Effects on Defects and Diffusion in Perovskites Dane Morgan, University of Wisconsin | |

Monday, October 6th

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| 10:45 | <p>SIESTA-PEXSI: Massively parallel method for efficient and accurate ab initio materials simulation Lin Lin, Lawrence Berkeley National Laboratory</p> | <p>Mesoscale modeling of dislocation mechanisms and the effect of nano-sized carbide morphology on the strengthening of advanced lightweight high-Mn steels Seyed Masood Hafez Haghighat, Max-Planck Institute for Iron Research</p> | <p>Modeling dislocation climb at the atomic scale in MgSiO₃ perovskite in the conditions of Earth's lower mantle Pierre Hirel, UMET</p> | <p>The thermal stability and structure of neutron irradiation induced vacancy-solute clusters in iron alloys Monica Chiapetto, SCK-CEN</p> | |
| 11:00 | <p>A coarse grained Gaussian electronic structure model for molecular dynamics studies of materials Glenn Martyna, IBM TJ Watson Research Center</p> | <p>A massively parallel level-set approach for the modelling of 3D anisotropic grain growth in polycrystalline materials Christian Mießen, Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University</p> | <p>Free energy of dislocations: Collective equilibrium behavior and driving forces for dynamics Marleen Kooiman, Eindhoven University of Technology</p> | <p>Flux coupling between vacancies and interstitial solutes (C, N and O) in α-Fe solid solution Thomas Schuler, CEA</p> | <p>An ab initio investigation of the stability of ZnO in an electrochemical environment Mira Todorova, Max-Planck-Institut fuer Eisenforschung</p> |
| 11:15 | <p>A Bayesian Framework for Calibration and Validation of Coarse-Grained Atomistic Models Eric Wright, University of Texas at Austin</p> | <p>Investigations of the effect of grain boundaries shape modeling in three-dimensional actual polycrystalline aggregates Félix Latourte, EDF R&D</p> | <p>Thermally-activated dislocation glide from the atomic scale Laurent Proville, CEA</p> | <p>Atomic Scale Strengthening Mechanisms due to Hard Obstacles in Fe Yury Osetskiy, Oak Ridge National Laboratory</p> | <p>A Multi-Scale Study of the Chemo-Mechanical Behavior of Battery Materials Feifei Fan, Georgia Institute of Technology</p> |
| 11:30 | <p>Assessment of Phase Field Crystal Concepts using Long-Time Molecular Dynamics Kristopher Baker, École Polytechnique Fédérale de Lausanne (EPFL)</p> | <p>Microstructure-sensitive modeling of void nucleation in single-phase polycrystalline materials Evan Lieberman, Carnegie Mellon University</p> | <p>Phase-field model for dislocation climb Alphonse Finel, LEM, Onera/CNRS</p> | <p>Effect of impurities on the mobility of self-interstitial clusters in α-Fe Anna Serra, Universitat Politècnica de Catalunya</p> | <p>Effect of Dislocations on the oxygen ion conductivity in reduced and doped Ceria Lixin Sun, Massachusetts Institute of Technology</p> |

Monday, October 6th

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| 11:45 | <p>Modeling the pressure vessel steel microstructure evolution under neutron irradiation using AKMC in Fe multi component alloys - optimization towards long irradi</p> <p>Christophe Domain, EDF, R&D</p> | <p>(I) Synergies between experiments and simulations: mapping and modelling of LiFePO4 electrodes</p> <p>Katsuyo Thornton, University of Michigan</p> | <p>Atomistic study of dislocation mobility and obstacle hardening in bcc-Fe: versatility of embedded atom method potentials</p> <p>Seyed Masood Hafez Haghighat, Max-Planck Institute for Iron Research</p> | <p>Combined Molecular Dynamics and Object Kinetic Monte Carlo simulations of ion implantation in Fe thin films</p> <p>María José Aliaga Gosálvez, Universidad de Alicante</p> | <p>First-Principles Study of Oxygen Reduction Reaction on Bulk Metallic Glasses</p> <p>Zhengzheng Chen, California State University, Northridge</p> | |
| 12:00 | <p>Kinetics and micromechanics associated with crack growth in brittle materials</p> <p>Mohamed Chabaat, Civil Engg. Faculty, U.S.T.H.B.</p> | | <p>A 3D dislocation dynamics analysis of the development of size effects at high temperature during micropillar compression of LiF [111] single crystals</p> <p>Javier Llorca, Polytechnic University of Madrid & IMDEA Materials Institute</p> | <p>Development of object kinetic Monte Carlo models for nanostructural evolution under irradiation in iron alloys</p> <p>Monica Chiapetto, SCK: CEN</p> | <p>Role of solvation dynamics in influencing nanoscale corrosion and passive oxide breakdown</p> <p>Subramanian Sankaranarayanan, Argonne National Lab</p> | |
| 12:15 | <p>Quantum-Atomic-Continuum-Coupled Model for the Thermo-mechanical Behavior in Micro-nano Simulation</p> <p>Tiansi Han, LSEC, ICMSEC, Academy of Mathematics and Systems Science, Chinese Academy of Sciences</p> | | <p>Dislocation Interactions in a Continuum Dislocation Dynamics Formulation</p> <p>Katrin Schulz, Karlsruhe Institute of Technology</p> | <p>Prediction of the Effects of Radiation For Reactor pressure vessel and in-vessel Materials using multi-scale modelling - 60 years foreseen plant lifetime</p> <p>Christophe Domain, EDF R&D</p> | <p>Diagnosis of the Mechanism of Anodic Oxide Film Growth on Platinum in H₂SO₄</p> <p>Feixiong Mao, Northeastern University Shenyang</p> | |
| 12:30 | <p>Lunch</p> <p><i>Location: Tent</i></p> | | | | | |
| 13:00 | | | | | | |
| 13:30 | | | | | | |
| | Ballroom 1 | Ballroom 2 | Ballroom 3 | Ballroom 4 | California | Mariposa |
| | J: Rare events and multiscale modelling | B: Multiscale mechanics of polymers, soft and biological materials (microscale; molecular) | G: Atomic scale and defect processes | H: Hydrogen embrittlement and fatigue | D: Modeling of mechanical properties and plasticity in nuclear and functional materials | C: Electrochemomechanics in corrosion processes |
| | Chair: Yang Xiang | Chairs: Markus Hütter and Lambért C A van Breemen | Chairs: Peter Gumbsch and M. Carmen Miguel | Chair: Anthony Rollett | Chairs: Jaime Marian and Pritam Chakraborty | Chairs: Gary Was and Rouzbeh Shahsevari |

Monday, October 6th

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| 14:00 | (I) Extending accelerated molecular dynamics methods to larger and more complex systems Arthur Voter, Los Alamos National Laboratory | (I) Molecular Description of Mechanical Behavior for a Semicrystalline Polymer Gregory Rutledge, MIT | Atomistically informed discrete dislocation dynamics simulations and the origin of anomalous slip in tungsten Peter Gumbsch - Fraunhofer IWM | (I) Protocols for designing H resistant alloys through multiscale modelling: The HeMS Project Pedro E J Rivera, University of Cambridge | (I) Stress and irradiation effects on solute diffusion to dislocations Dallas Trinkle, Univ. Illinois, Urbana-Champaign | (I) Nano-Mechanics of Pit Initiation on Metals and Alloys Digby Macdonald, University of California at Berkeley |
| 14:15 | | | Screw Dislocation Cross-Slip at Cross-Slip Plane Jogs and Screw Dipole Annihilation in FCC Cu,Ni Investigated via Atomistic Simulations Satish Rao, UES Inc. | | | |
| 14:30 | (I) Bifurcation diagram and thermally assisted magnetization reversals in spin-torque driven nanomagnets Eric vanden-eijnden, Courant Institute, NYU | Tracking a glassy polymer on its energy landscape in the course of small time-dependent deformations. Maxime Delhorme, Eindhoven University of Technology | From atomic to mesoscale diffusion equations for alloys Maylise Nastar, CEA | Hydrogen Effects on Dislocation Dynamics and Metal Plasticity Ryan Sills, Stanford University | Inverse Relation between Strain Rate and Yield Strength of Dislocation-Obstacle Interaction in bcc Fe Yue Fan, MIT | Emergent Piezoelectricity in Mono- and Bilayers of Inorganic Two-Dimensional Crystals Karel-Alexander Duerloo, Stanford University |
| 14:45 | | Multiscale modelling of unfolded proteins Patrick Onck, University of Groningen | Thermal properties of point defects and their clusters in bcc Fe Matthias Posselt, 1Helmholtz-Zentrum Dresden-Rossendorf | Effect of microstructure on hydrogen trapping in bcc Fe-Ti-C steel - A quantitative parameter study Peter Lang, University of Cambridge | Interactions between mobile dislocations and radiation induced loops: a multiscale approach Laurent Dupuy, CEA Saclay | (I) Chemistry in the double layer: Implications for developing better microkinetic models in electrochemistry, corrosion research and alloy design Santanu Chaudhuri, University of Illinois at Urbana-Champaign |

Monday, October 6th

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| 15:00 | Sampling saddle points on the free energy surface Amit Samanta, Lawrence Livermore National Lab | Prediction and Validation of Viscoelastic Properties of Polyurea with Systematically Coarse-Grained Molecular Dynamics Jay Oswald, Arizona State University | Theory of solid solution strengthening in High Entropy Alloys Celine Varvenne, LAMMM, Swiss Institute of Technology Lausanne (EPFL) | Cyclic and High-Strain Rate Plasticity in Penta-Twinned Silver Nanowires – Atomistic Experiments and Modeling Horacio Espinosa, Northwestern University | Modeling of Tensile Deformation in Irradiated RPV steel Pritam Chakraborty, Idaho National Laboratory | |
| 15:15 | Enhanced sampling of rare events in molecular dynamics simulations by nonlinear manifold learning Behrooz Hashemian, UPC-BarcelonaTech | Mechanical Properties of Biological Nanotubes with Multiscale Coarse-grained Models Roderick Melnik, M2NeT Lab, Wilfrid Laurier University, Waterloo | Presentation withdrawn | 3D mesoscopic simulation of fatigue-crack shielding and blunting in FCC metals Laurent Korzeczek, Onera | Multiscale simulations of strengthening induced by small dislocation loops Ghiath Monnet, EDF-R&D | Ionic motion during field-assisted oxidation of aluminium studied by molecular dynamics simulations Barend Thijssse - Delft University of Technology |
| 15:30 | Refreshment break <i>Location: Tent</i> | | | | | |
| 15:45 | | | | | | |
| 16:00 | Numerical methods for high-dimensional problems in computational materials science Johannes Bulin, Fraunhofer Institute for Algorithms and Scientific Computing SCAI | Molecular Dynamics study on moisture-dependent properties of amorphous cellulose extended to poromechanical model Karol Kulasinski, ETH Zurich | Creep modeling in Olivine by 2.5D dislocation dynamics simulations Francesca Buioli, UMET, University of Lille1 | Role of plasticity-induced crack closure in fatigue crack growth in metals Jesus Toribio, University of Salamanca | Simulation for dislocation core structure of solute atom clusters using generalized stacking fault energy Toshiharu Ohnuma, Central Research Institute of Electric Power Industry | The Volcano of Hydrogen Pickup in Zirconium Alloys Explained by p-type Doping of the Passive Oxide Layer Mostafa Youssef, MIT |
| 16:15 | A Path Factorization Approach to Multiscale Stochastic Simulations Manuel Athènes, CEA | Synchronized molecular dynamics via macroscopic heat and momentum transfer for non-isothermal polymeric flows Shugo Yasuda, University of Hyogo | Deformation and failure of curved nanocrystalline shells M. Carmen Miguel, University of Barcelona | Theoretical study of hydrogen interacting with TiC nanoparticles in iron. Christian Elsässer, Fraunhofer IWM | Defect-induced plasticity in CuNb nanocomposites Enrique Martinez Saez, LANL | Multiscale Corrosion Modeling and Computational Design of Aerospace Coatings Systems Erik Sapper, The Boeing Company |

Monday, October 6th

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| 16:30 | (I) Overcoming Temporal and Spatial Multiscale Challenges in Materials Modeling and Computing Mitchell Luskin, University of Minnesota | Mechanical and Thermal Properties of Cross-Linked Phenolic Resins: Towards a Multiscale Approach for Thermal Protection Materials for Space Vehicles Joshua Monk, NASA Ames | (I) The many contributions of Ladislav Kubin to dislocation theory and plasticity B. Devincre, A. El Azab and friends. | Ab initio modeling of secondary slip in zirconium Nermine Chaari, SRMP, CEA Saclay | Multiscale cleavage fracture initiation model accounting for material microstructure and effects of irradiation Anssi Laukkanen, VTT | Prediction of Crack Growth Rate in Type 304 Stainless Steel Using Artificial Neural Networks and the Coupled Environment Fracture Model Jiangbo Shi, Tianjin University |
| 16:45 | | Linking Composition and Topology to Mechanical Properties of Biopolymer Networks Erik Van der Giessen, Zernike Institute for Advanced Materials | | Presentation withdrawn | | Growth and breakdown of iron sulfide passivating corrosion films: Towards a mechanistic, multiscale model Aravind Krishnamoorthy, Massachusetts Institute of Technology |
| 17:00 | Poster Intros: B, C & D Chair: Andrew Minor | | | Poster Intros: G & H Chair: Vasily Bulatov | | |
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| 20:30 | Poster session 1 and beer reception | | | | | |
| 21:00 | <i>Location: Tent</i> | | | | | |
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October, Tuesday 7th

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| 07:00 | Breakfast <i>Location: Tent</i> | | | | | |
| 07:15 | | | | | | |
| 07:30 | | | | | | |
| | Chair: Jaime Marian | | | | | |
| 08:00 | Plenary 3: Modeling of neutron irradiation embrittlement of reactor pressure vessel steels Dr Naoki Soneda (Central Research Institute of Electric Power Industry, Japan) <i>Location: Ballroom</i> | | | | | |
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| 08:45 | Plenary 4: Over a Decade of Folding@home: how citizen science has lead to key new advances in biophysics and fighting disease Professor Vijay Pande (Stanford University) <i>Location: Ballroom</i> | | | | | |
| 09:00 | | | | | | |
| 09:15 | | | | | | |
| 09:30 | Refreshment break <i>Location: Tent</i> | | | | | |
| 09:45 | | | | | | |
| | Ballroom 1 | Ballroom 2 | Ballroom 3 | Ballroom 4 | California | Mariposa |
| | J: Mechanics of materials II | B: Multiscale mechanics of polymers, soft and biological matter (mesoscale; soft matter/polymer physics) | | H: Dislocation energetics: glide and interactions | F: Friction, Lubrication and Wear across the Scales I | C: Electro-chemomechanics in cracking |
| | Chair: Christian Linder | Chairs: Gregory C Rutledge and Patrick R Onck | | Chair: Chris Weinberger | Chair: Lars Pastweka | Chairs: Erik Sapper and Mostafa Youssef |
| 10:00 | (I) Phase transformations in solids driven by mechano-chemically non-convex free energies Krishna Garikipati, University of Michigan | (I) Almost Ab Initio Nonlinear Rheology of Entangled Polymers Jay Schieber, IIT | | (I) Physical modeling on size-dependent yield strength with dislocation pile-up and surface effects in finite single-crystal samples Bo Pan, Osaka University | (I) Nanoscale superlubricity, peeling and fracture at carbon and silicon interfaces Naruo Sasaki, Department of Engineering Science, University of Electro-Communications | (I) Multiscale Nature of Stress Corrosion Cracking Gary Was, University of Michigan |
| 10:15 | | | | | | |
| 10:30 | (I) Combined Atomistic/Continuum Modeling of Strain Localization in Metallic Glass Michael Falk, Johns Hopkins University | (I) Large scale Brownian dynamics simulations of complex viscoelastic Soft Matter Wim Briels, Twente University | | Modeling thermal activation of dislocation glide in cementite at low temperature Nils Garvik, UMET | Atomistic modeling friction on graphene: effects of hydrogenation, substrate roughness and electron-phonon coupling Yalin Dong, University of Akron | (I) Multiscale simulation of stress corrosion effects and surface response to charging Peter Gumbsch, Karlsruhe Institute of Technology KIT |

October, Tuesday 7th

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| 10:45 | | | | M111 dislocation of high Peierls stress in BCC Ta Keonwook Kang, Yonsei University | Presentaion withdrawn | |
| 11:00 | Strain Functionals for Characterizing Atomistic and Other Geometries Edward Kober, Los Alamos National Laboratory | Dynamic Phase diagram of soft colloids Sudipta Gupta, JCNS-SNS-Oak Ridge National Laboratory | | Studying the Effect of Stress Relaxation and Creep on Lattice Strain Evolution of Magnesium Alloy AZ31 under Tension and Compression Huamiao Wang, LANL | Simulation of a Dental Tribological System at a Microscopic Scale Christian Nutto, Fraunhofer IWM | Multiscale modelling of materials chemomechanics: from catastrophic brittle fracture to stress corrosion cracking James Kermode, King's College London |
| 11:15 | In-situ Neutron Measurement and Modeling of Martensitic Phase Transformation Carlos Tome, LANL | Thermodynamics of reductions in multiscale modeling Miroslav Grmela, Ecole Polytechnique de Montreal | | Ab initio investigation of the Peierls potential of screw dislocations in bcc iron and its consequences on the dislocation-carbon interaction David Rodney, University of Lyon | Nano scale contribution to features occurring at the macro scale in lubricated contacts Philippe Vergne, LaMCoS CNRS INSA Lyon | (I) Self-healing materials and damage from shock induced nanobubble collapse: reactive molecular dynamics simulations Priya Vashishta, University of Southern California |
| 11:30 | Smart use of Density Functional Theory calculations to drive Newtonian dynamics Reese Jones, Sandia National Laboratory | A materials genome approach to engineering functional suprabiomolecular nanotubes Luis Ruiz, Northwestern University | | Predicting the Rate of Dislocation Cross Slip in FCC Metals William Kuykendall, Stanford University | Molecular dynamics study of automotive lubricants: linking molecular structure and friction Michael Doig, University of Edinburgh | |
| 11:45 | Structural phase transformations in solids - Atomistic insight on mechanisms and interface properties Jutta Rogal, ICAMS, Ruhr-Universität Bochum | Self-regulation in structure formation Peter Roozmond, Eindhoven University of Technology | | Molecular dynamics simulation of dislocation motion in high-entropy alloys Shaoqing Wang, Institute of Metal Research, CAS | Shear-induced amorphization of silicon crystals Gianpietro Moras, Fraunhofer Institute for Mechanics of Materials IWM | Mapping Strain Rate Dependence of Dislocation-Defect Interactions in Zirconium Bilge Yildiz, MIT |

October, Tuesday 7th

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| 12:00 | <p>Three-dimensional iso-geometric solutions to Toupin's gradient elasticity theory at finite strains and its application to study of dislocation cores and defects Shiva Rudraraju, University of Michigan</p> | <p>Local stress calculations in biomembranes: importance of force decomposition Alejandro Torres-Sánchez, LaCàN, UPC-BarcelonaTech</p> | | <p>Grain Scale Models of Plasticity in BCC iron: Describing the Role of Temperature, Strain Rate and States of Stress on Yield Christopher Weinberger, Drexel University</p> | <p>Friction Process of Silicon Carbide under Water Lubrication: Quantum Chemical Molecular Dynamics Approach Yoshihiko Kobayashi, Tohoku University</p> | <p>(I) Decoding the chemomechanics of friction and scratch in complex granular hydrated oxides Rouzbeh Shahsavari, Rice University</p> |
| 12:15 | <p>A concurrent atomistic-continuum study of sequential slip-transfer reactions for dislocation pile-ups at grain boundaries David McDowell, Georgia Tech</p> | <p>Rheology and shear-induced diffusion in dense suspensions of red blood cells Fathollah Varnik, Ruhr-University Bochum</p> | | <p>Probing Micro-Mechanics of Flow in Metals through Crackling Noise and Mean Field Theory Xiaoyue Ni, California Institute of Technology</p> | <p>Atomistic Control of Chemical Reaction Dynamics during Chemical Mechanical Polishing of Gallium Nitride: Quantum Chemical Molecular Dynamics Simulations Kentaro Kawaguchi, Fracture and Reliability Research Institute, Tohoku University</p> | |
| 12:30 | <p>Lunch</p> | | | | | |
| 13:00 | <p><i>Location: Tent</i></p> | | | | | |
| 13:30 | <p><i>Location: Tent</i></p> | | | | | |
| | Ballroom 1 | Ballroom 2 | Ballroom 3 | Ballroom 4 | California | Mariposa |
| | <p>B: Multiscale mechanics of polymers, soft and biological materials (macroscale; solids composites)</p> | <p>E: Synergies at the atomistic scale</p> | <p>G: Surface and interfacial phenomena</p> | | <p>D. Simulations of microstructural evolution and texture under irradiation (in honor of Prof CH Woo)</p> | <p>A: Multiscale modeling of material microstructure</p> |
| | <p>Chairs: Jay D Schieber and Erik van der Giessen</p> | <p>Chairs: Katsuyo Thornton and Guillaume Puel</p> | <p>Chairs: Nasr M Ghoniem and Scott Norris</p> | | <p>Chairs: Sergei Dudarev and Yuri Osetsky</p> | <p>Chair: R Krishna</p> |
| 14:00 | <p>(I) Meso-scale Dynamic of Polymeric Glasses: Constitutive Models that Acknowledge Dynamic Heterogeneity J M Caruthers, Purdue University</p> | <p>Defect Character at Grain Boundary Facet Junctions: A Combined HRSTEM and Atomistic Modeling Study of a $\Sigma=5$ Grain Boundary in Fe Douglas Medlin, Sandia National Laboratories</p> | <p>(I) Theory, Modeling and Experiments of Nano-structured Surfaces by Plasma Ions Nasr M Ghoniem, University of California</p> | | <p>(I) White-noise quantum heat bath for MD and SLD simulations in magnetic materials Chung H. Woo, City University of Hong Kong</p> | <p>(I) Toward mastery of microstructural degrees of freedom in engineering design Dennis Dimiduk, Air Force Research Laboratory</p> |

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| 14:15 | | <p>Using Atomistic Reconstructions of 3D Atom Probe Tomography Data to Study the Interactions of Dislocations with γ'-Precipitates in a Ni-base Superalloy Erik Bitzek, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)</p> | | | | |
| 14:30 | <p>Predicting segmental relaxation in quiescent and deformed polymer glasses Anton Smessaert, University of British Columbia</p> | <p>Measuring and Modeling Strain Fields in High Angle Graphene Grain Boundaries Colin Ophus, Lawrence Berkeley National Laboratory</p> | <p>Predicting interface dislocation structure and energy using anisotropic elasticity theory Niaz Abdolrahim, Massachusetts Institute of Technology</p> | | <p>Effects of magnetism and strain relaxation on the phase stability of multi-component alloys Jan Wrobel, CCFE</p> | <p>(I) Image Based Crystal Plasticity FE Models for Predicting Fatigue in Polycrystalline Metals and Alloys: Addressing the ICMSE Initiative Somnath Ghosh, Johns Hopkins University</p> |
| 14:45 | <p>Filled polymer glasses; the sum of its parts? Sam Krop, Eindhoven University of Technology</p> | <p>Atomistic Determination of Grain Boundary Mobility in Fe-He Alloys Aulia Tegar Wicaksono, The University of British Columbia</p> | <p>Thin film buckling on substrate: effect of pressure and plasticity Antoine Ruffini, ONERA</p> | | <p>Effect of point defect sinks on irradiation-induced compositional patterning Pascal Bellon, University of Illinois at Urbana-Champaign</p> | |
| 15:00 | <p>Hierarchical composites reinforced with microscopic fibers and nanotubes: the modelling challenge. Valentin Romanov, KU Leuven - Materials Engineering</p> | <p>Ultrafast melting of laser-excited gold nanofilms: Combining experiment and atomistic modelling Alexander Shluger, University College London (UCL)</p> | <p>A microstructural phase field approach to shock-induced martensitic transitions in iron Aurélien Vattré, CEA, DAM, DIF</p> | | <p>Radiation induced grain boundary flow - Effects of grain boundary segregation Yinon Ashkenazy, Racah Institute of Physics, The Hebrew University of Jerusalem</p> | <p>Impact of Spatially Non-Random Solutes on the Strength of Aluminum Alloys Alban de Vaucorbeil, University of British Columbia</p> |

October, Tuesday 7th

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| 15:15 | Concurrent two-scale model for the elasto-viscoplastic behavior of silica-filled rubber Markus Hütter, Eindhoven University of Technology | Modeling of nanocalorimetry experiments in self-amorphized ion implanted silicon Manuel Ruiz, University of Valladolid | Phase Field Modeling of Widmanstatten structures Benoit Appolaire, LEM - ONERA/CNRS | | Ion-Irradiation Induced Vacancy and Interstitials Clusters in Fe Investigated by X-Ray Diffuse Scattering and by Continuum and Molecular Dynamics Simulations Ben Larson, Oak Ridge National Laboratory | Hierarchical crystal plasticity Fe model for nickel-based superalloys: sub-grain microstructures to polycrystalline aggregates Shahriyar Keshavarz, Civil Department of Johns Hopkins University |
| 15:30 | Refreshment break | | | | | |
| 15:45 | <i>Location: Tent</i> | | | | | |
| 16:00 | Micromechanics modeling of the linear viscoelasticity of nano-reinforced polymers with an interphase Julie Diani, CNRS UMR 8006 | Molecular-dynamics simulations and experimental investigation of the migration of tilt and mixed grain boundaries in pure Aluminum Luis Barrales-Mora, IMM | Presentation withdrawn | | Modeling of swelling under electron, ion, and neutron irradiation Stanislav Golubov, ORNL | Vi(CA)2T – Virtual Cement & Concrete Aging Analysis Toolbox Nhu Cuong Tran, EDF / R&D (Research and Development) |
| 16:15 | Coupled Digital Image Correlation and Fracture Mechanics analysis for the identification of cohesive models in polymers at the micron scale Rafael Estevez, University Grenoble / SIMAP | Modeling and experimental characterization of {311} defects in silicon Luis Alberto Marqués, University of Valladolid | A Phase-field model for Displacive Phase Transformations in Elastically Anisotropic and Inhomogeneous Polycrystals Tae Wook Heo, Lawrence Livermore National Laboratory | | Ductility and work hardening in nano-sized and irradiated metallic glasses David Chen, California Institute of Technology | Decoding Cement Hydrate: Hierarchical Modeling from Electrons to Microstructures Rouzbeh Shahsavari, Rice University |
| 16:30 | A Thermodynamically Consistent Finite Deformation Enhanced Strain Formulation for the Coupled Diffusion in Gels Christian Linder, Stanford University | Molecular dynamics modelling of mechanically loaded interfaces of single-walled carbon nanotubes and palladium Steffen Hartmann, TU Chemnitz | (I) Multi-scale Modeling of Irradiation-Induced Morphology Evolution Scott Norris, Southern Methodist University | | Modelling self trapping and trap mutation in tungsten using DFT and Molecular Dynamics with an empirical potential based on DFT Julien Boisse, Université de Lorraine | FTMP-based Continuum Description of 4D Discrete Dislocation Systems Tadashi Hasebe, Kobe University |

October, Tuesday 7th

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| 16:45 | <p>Micromechanical modeling of elastoplastic damage behavior of the human femur under compression loading Hakim Naceur, LAMIH, Université de valenciennes</p> | <p>Investigating the limits of discrete dislocation descriptions of inclined twin boundaries in the presence of hydrogen Christopher O'Brien, Sandia National Laboratories</p> | | | <p>Inert-gas defects and trapping of helium in bcc transition metals: Ab initio predictions and thermal desorption spectroscopy validation Duc Nguyen-Manh, Culham Centre for Fusion Energy</p> | <p>Hot-working Multiscale Simulations Using Multi-phase-field Finite Element Dynamic Recrystallization Model Tomohiro Takaki, Kyoto Institute of Technology</p> |
| 17:00 | | | | | | |
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| 19:00 | <p>Conference Banquet at the UC Berkeley Faculty Club. Coaches to depart from outside the hotel at 19:00</p> | | | | | |
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| 07:00 | Breakfast <i>Location: Tent</i> | | | | | |
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| | Chair: Peter Gumbsch | | | | | |
| 08:00 | Plenary 5: Comparisons of 3D Experiments and Simulations on Plastic Deformation of Metals Anthony D Rollett (Carnegie Mellon University) <i>Location: Ballroom</i> | | | | | |
| 08:15 | | | | | | |
| 08:30 | | | | | | |
| 08:45 | Plenary 6: Role of Multiscale Materials Modeling in Integrated Computational Materials Engineering Professor Mark Asta (University of California, Berkeley) <i>Location: Ballroom</i> | | | | | |
| 09:00 | | | | | | |
| 09:15 | | | | | | |
| 09:30 | Refreshment break <i>Location: Tent</i> | | | | | |
| 09:45 | | | | | | |
| | Ballroom 1 | Ballroom 2 | Ballroom 3 | Ballroom 4 | California | Mariposa |
| | J: Mathematical modeling and analysis | E: Synergies at the grain scale | G: Experiments and models for mesoscale plasticity | H: High temperature and strain rate deformation | D: Method development to bridge the time and space scale gap in irradiation damage simulations | A: Integrated methods for materials design and optimization |
| | Chair: Jianfeng Lu | Chairs: Franz Roters and Jean-Hubert Schmitt | Chairs: Richard LeSar and Istvan Groma | Chair: Tony Paxton | Chairs: Guido Roma and Haixuan Xu | Chair: D McDowell |
| 10:00 | (I) A theory and challenges for coarsening in microstructure David Kinderlehrer, Carnegie Mellon University | (I) Simulation analysis of stress and strain partitioning in dual phase steel based on real microstructures Franz Roters, MPI für Eisenforschung | Probing Deformation on the Mesoscale Using Submicron-Resolution 3D X-Ray Microscopy and Dislocation Dynamics Simulations Ben Larson, Oak Ridge National Laboratory | (I) Lattice dynamics and solid-state plasticity experiments at high pressures and strain rates Bruce Remington, LLNL | (I) Multiscale Modeling of Defect Cluster Evolution in Irradiated Structural Materials Brian Wirth, University of Tennessee | (I) Search for substitutes of critical materials with targeted properties by scale-bridging and high-throughput modelling and simulation Christian Elsaesser, Fraunhofer IWM |
| 10:15 | | | | | | |
| 10:30 | Interfaces in Discrete Environments Nung Kwan Yip, Purdue University | Resolving the evolution of pore structures in 304-L laser welds James Foulk III, Sandia National Laboratories | Multiplication mechanisms and topology changes of interacting dislocation densities investigated by Discrete Dislocation Dynamics Markus Stricker, KIT-IAM Karlsruhe Institute of Technology - Institute for Applied Materials | Grain boundary dynamics from atomistic simulations Christian Brandl, Karlsruhe Institute of Technology | Prediction of material behavior after irradiation for reactor pressure vessel steels and reactor internals : modeling aspects and implementation in the PERFORM Félix Latourte, EDF R&D | Modeling the Behavior of Cellular Silicone Pads in the Structure-Continuum Transition Chris Hammetter, Sandia National Laboratories |

Wednesday, October 8th

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| 10:45 | <p>A degenerate Ising model for atomistic simulation of crystal-melt interfaces Tim Schulze, University of Tennessee</p> | <p>Understanding how oxidized grain boundaries fail: A combined experimental and crystal plasticity finite element approach Judith Dohr, University of Oxford</p> | <p>The Discrete-Continuum Model: An important breakthrough to simulate the mechanical properties of dislocated crystals with complex boundary conditions Riccardo Gatti, LEM, UMR 104 CNRS-ONERA</p> | <p>Experimental investigation of metals at high strain rates Jonathan Crowhurst, Lawrence Livermore National Laboratory</p> | <p>The necessary initial conditions for simulation of damage cascades under neutron irradiation Mark Gilbert, CCFE</p> | <p>Analysis of electronic subgap states in amorphous semiconductor oxides on the example of Zn-Sn-O systems Christian Elsaesser, Fraunhofer IWM</p> |
| 11:00 | <p>Continuum framework for dislocation structure, energy and dynamics of dislocation arrays and low angle grain boundaries Yang Xiang, Hong Kong University of Science and Technology</p> | <p>Cyclic deformation experiments and plasticity modeling of three Ti microstructures Benjamin Smith, Boeing</p> | <p>Numerical Simulation of Glide Dislocations in Persistent Slip Band Miroslav Kolář, FJFI CVUT v Praze</p> | <p>Temperature and high strain rate dependence of tensile deformation behavior in single crystal iron from dislocation dynamics simulations Jaime Marian, Lawrence Livermore National Laboratory</p> | <p>Elastic trapping of dislocation loops in ion-irradiated tungsten foils Daniel Mason, CCFE</p> | <p>Materials Design and Discovery: Role of Atomic-Scale Modeling Susan Sinnott, University of Florida</p> |
| 11:15 | <p>Analysis of force-based multiscale method Jianfeng Lu, Duke University</p> | <p>The Deformation Induced Martensitic Transformation of Metastable Austenite Chad Sinclair, The University of British Columbia</p> | <p>Dislocation-Dynamics based constitutive equations for crystalline plasticity of BCC metals at low temperature Ghiath Monnet, EDF-R&D</p> | <p>Multiscale modeling of high-rate plastic deformation of polycrystalline bcc metals Robert Rudd, Lawrence Livermore National Lab</p> | <p>(I) Defect Interaction and Evolution in Iron and Its-based Alloys Haixuan Xu, University of Tennessee</p> | <p>Thermodynamics of α-Fe solid solution: interplay between vacancies and interstitial solutes (C, N and O) Thomas Schuler, CEA</p> |
| 11:30 | <p>Multiscale analysis of non-linear dislocation models Tom Swinburne, Imperial College</p> | <p>Microstructure based continuum modeling of highly anisotropic metals Rodney McCabe, Los Alamos National Laboratory</p> | <p>Discrete dislocation analysis of dislocation interactions with voids and precipitates Lynn Munday, Army Research Lab</p> | <p>High-Temperature Discrete Dislocation Plasticity Amine Benzerga, Texas A&M University</p> | | <p>OpenKIM.org: Ensuring reliability, reproducibility and transferability in multiscale and atomistic simulations Ellad Tadmor, University of Minnesota</p> |

Wednesday, October 8th

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| 11:45 | A parameter identification problem for random heterogeneous materials Frederic Legoll, Ecole des Ponts | Strain Gradient Crystal Plasticity Modelling – An Efficient Approach to Capture Experimental and Discrete Dislocation Dynamics Observations? Eric Bayerschen, Karlsruhe Institute of Technology | Anisotropic elasticity in dislocation dynamics Sylvie Aubry, LLNL | Tuning Ideal Tensile Strengths and Intrinsic Ductility of BCC Refractory Alloys Liang Qi, Department of Materials Science and Engineering, University of California, Berkeley | Diffuse interface modeling of void growth in irradiated materials. Mathematical, thermodynamic and atomistic perspectives Anter El-Azab, Purdue University | Grain boundary segregation as a route to stabilize nanocrystalline alloys: A phase field study Fadi Abdeljawad, Sandia National Laboratories |
| 12:00 | Homogenization of heat diffusion in a cracked medium Peigney Benjamin-Edouard, CEA | Intermittent and heterogeneous plasticity in hcp alloys: correlations between experimental results and multiscale models Jean-Loup Strudel, Mines-ParisTech | Discrete dislocation dynamics with anisotropic elasticity Richard LeSar, Iowa State University | DD Simulations of Temperature Effects on Tungsten Micro-pillar Compression with a Semi-phenomenological Dislocation Mobility Formulation David Rivera, UCLA | Constrained ab initio method for non-collinear magnetic excitations Pui Wai Ma, Culham Centre for Fusion Energy | Scale bridging modelling of hydride formation Robert Spatschek, Max-Planck Institute for Iron Research |
| 12:15 | Multiscale modeling of spin transfer torques in ferromagnetic multilayers Jingrun Chen, UCSB | Grain-scale Experimental Validation of Crystal Plasticity Finite Element Simulations of Tantalum Oligocrystals Hojun Lim, Sandia National Laboratories | Statistical properties of the velocity of dislocations Istvan Groma, Eotvos University Budapest | The subsonic / transonic transition of rectilinear edge dislocations: predictions from a field-based equation of motion Yves-Patrick Pellegrini, Commissariat à l'Énergie Atomique | Ab initio study of threshold displacement energies in tungsten Pär Olsson, KTH Royal Institute of Technology | Material and microstructure based design of anisotropic linear elastic properties of cubic crystal aggregates using zeroth-, first- and second-order bounds Mauricio Lobos, Karlsruhe Institute of Technology (KIT) |
| 12:30 | Excursions | | | | | |
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Thursday, October 9th

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| 07:00 | Breakfast <i>Location: Tent</i> | | | | | |
| 07:15 | | | | | | |
| 07:30 | | | | | | |
| | Chair: Ju Li | | | | | |
| 08:00 | Plenary 7: Contact and Friction of Rough Adhesive Surfaces Professor Mark Robbins (Johns Hopkins University) <i>Location: Ballroom</i> | | | | | |
| 08:15 | | | | | | |
| 08:30 | | | | | | |
| 08:45 | Plenary 8: Multiscale Modeling in Mesoscale Materials Dr George W Crabtree (Argonne National Laboratory) <i>Location: Ballroom</i> | | | | | |
| 09:00 | | | | | | |
| 09:15 | | | | | | |
| 09:30 | Refreshment break <i>Location: Tent</i> | | | | | |
| 09:45 | | | | | | |
| | Ballroom 1 | Ballroom 2 | Ballroom 3 | Ballroom 4 | California | Mariposa |
| | | A/E: Integration of computations with experiment | | H: Microstructure and plasticity | D: Modeling oxides, fuels, and cladding materials | K: Simulation Methodology and Defect Properties |
| | | Chairs: Cem Tasan, Claudio Zambaldi and P Gumbsh | | Chair: Pedro Rivera | Chairs: Michael Tonks and Blas Uberuaga | Chair: Ju Li |
| 10:00 | | (I) Integrated experimental-numerical methodology to map microstructural strain and stress evolution in bulk nanostructured alloys Cem Tasan, Max-Planck Institute for Iron Research | | (I) Multiscale Modeling of Forming and Fracture - Industry Perspective Raj Misra, GM RandD Center | (I) Role of Microstructure on Fuel Performance: Macroscale Insights from Atomic-resolution Simon Phillpot, University of Florida | (I) A Multiscale Atomistic Method for Defects in Ionic Materials Kaushik Dayal, Carnegie Mellon |
| 10:15 | | | | | | |
| 10:30 | | Microstructure-sensitive modeling of the mechanical behavior of polycrystalline materials with direct input from emerging 3-D characterization methods Ricardo Lebensohn, Los Alamos National Laboratory | | Quantitative study of the role of twin-parent and twin-twin interactions on the mechanical response of hexagonal materials Pierre-Alexandre Juan, Georgia Institute of Technology | Interatomic potentials accuracy: how do they bridge the scales? U-Mo fuel case Vladimir Stegaylov, JIHT RAS | Presentation withdrawn |
| 10:45 | | Computational Process-Structure-Properties Modeling of Thermal Sprayed Coatings Tatu Pinomaa, VTT Technical Research Centre of Finland | | Presentation withdrawn | Atomistically-informed cluster dynamics modeling of void and loop nucleation in irradiated UO2 Sarah Khalil, UW-Madison | |

Thursday, October 9th

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| 11:00 | | <p>An inverse optimization strategy to determine single crystal mechanical behavior from polycrystal tests: application to Mg alloys Javier Llorca, Polytechnic University of Madrid & IMDEA Materials Institute</p> | <p>A multi-scale model for transformation induced plasticity and the numerical calibration of its material parameters Thomas Antretter, Montanuniversitaet Leoben</p> | <p>Radiation growth in Zr under Frenkel-pair produced irradiation Alexander Barashev, UT</p> | <p>First-principles molecular dynamics transport in Li3InBr6: Tools for High-Throughput Screening Nicole Adelstein, Lawrence Livermore National Lab</p> |
| 11:15 | | <p>Identification of constitutive parameters by inverse simulation of indentation in single crystals and close to grain boundaries Franz Roters, MPI für Eisenforschung</p> | <p>A Mechanistic Study of Intergranular Cracking in Stainless Steels Esteban Busso, ONERA</p> | <p>Presentation withdrawn</p> | <p>Conductivity of doped ceria from non-equilibrium molecular dynamics Johan O Nilsson, Royal Institute of Technology (KTH)</p> |
| 11:30 | | <p>Building realistic atomic models of kerogen using Hybrid Reverse Monte Carlo simulations Colin Bousige, Massachusetts Institute of Technology</p> | <p>Linking Computational Stacking Fault Energies with Plasticity Mechanisms in High Temperature Carbide Ceramics Gregory Thompson, University of Alabama</p> | | <p>First-principles and molecular dynamics simulation for diffusion problem of YSZ and Ni/YSZ in solid oxide fuel cells Yoshitaka Umeno, The University of Tokyo</p> |
| 11:45 | | <p>Integrated Computational and Experimental Structure Determination for Nanoparticles Min Yu, University of Wisconsin-Madison</p> | <p>A Multi-Scale Framework to Simulate Dynamic Recrystallization in Magnesium Alloys Kaan Inal, University of Waterloo</p> | <p>First principles study of anisotropy of point defect diffusion barriers in HCP Zr German Samolyuk, Oak Ridge National Laboratory</p> | <p>Atomistic simulations of thermal transport in nanostructured semiconductors Yuping He, University of California, Davis</p> |
| 12:00 | | <p>Towards efficient fatigue simulation and parameter identification using models with multiple time scales Guillaume Puel, Ecole Centrale Paris / CNRS UMR8579</p> | <p>Hierarchical multi-scale model: from texture and substructure to evolution of plastic anisotropy and complex hardening Jerzy Gawad, KU Leuven - Dept. Computer Science</p> | <p>Radiation damage evolution in nanostructure materials Blas Uberuaga, Los Alamos National Laboratory</p> | <p>Stability and kinetics of Se overlayers on Mo(110) and the role of Na impurities: from ab initio data to thermodynamics and kinetics Guido Roma, CEA-Saclay and Uni-Mainz</p> |

Thursday, October 9th

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| 12:15 | | A coupling method for stochastic polycrystalline models at different scales Regis Cottureau, Laboratoire MSSMat, Ecole Centrale Paris, CNRS | | Molecular Statics and Molecular Dynamics Simulations of Dislocation Behavior in a Model FCC Multicomponent Concentrated Solid Solution Alloy Satish Rao, UES Inc. | Ab initio prediction of point defect properties in materials for energy production Fabien Bruneval, CEA | A self-consistent first-principles approach model carrier mobility in organic materials Wolfgang Wenzel, Karlsruhe Institute of Technology |
| 12:30 | Lunch | | | | | |
| 13:00 | <i>Location: Tent</i> | | | | | |
| 13:30 | | | | | | |
| | Ballroom 1 | Ballroom 2 | Ballroom 3 | Ballroom 4 | California | Mariposa |
| | J: Mechanics of materials I | E: Microstructure evolution and phase transformation | G: Continuum theory of defects in deformation | A: Components and tools for integrated computational materials | F: Friction, Lubrication and Wear across the Scales II | K: Energy harvesting |
| | Chair: Christian Linder | Chairs: Vesselin Yamakov and Remi Dingreville | Chairs: Laurent Capolungo and Stefan Sandfeld | Chair: J Neugebauer | Chairs: Ashlie Martini and Momoji Kubo | Chair: Ju Li |
| 14:00 | (I) Comparison of 3D phase field and Peierls-Nabarro modeling of dislocation dissociation, glide and twinning in fcc systems Bob Svendsen, RWTH Aachen | Dislocation-induced elastic distortion fields in deformed FCC crystals: Discrete dislocation dynamics simulations and experimental measurements Anter El-Azab, Purdue University | (I) Grain boundary modeling using an elasto-plastic theory of dislocation and disclination fields Claude Fressengeas, LEM3 CNRS | Banding, grain fragmentation and texture formation in f.c.c. polycrystals: 'stack of domains' model Arul Kumar Mariyappan, Los Alamos National Laboratory | (I) On the importance of timescales in the atomistic modelling of friction Danny Perez, Los Alamos National Laboratory | (I) Thermal Transport Modeling on Low-Dimensional Semiconducting Nanostructures Yong-Wei Zhang, Institute of High Performance Computing |
| 14:15 | | Metal-rich Ceramic Phase Stability and Microstructures in Group IV and V Carbides and Nitrides Xiaoxiang Yu, The University of Alabama | | Multiscale simulations and modeling for integrated materials engineering Gerard Paul Leyson, Max-Planck-Institut für Eisenforschung | | |

Thursday, October 9th

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| 14:30 | Defect Nucleation in Crystals Terry Delph, Lehigh University | (I) Computational Multiscale Modeling and Experimental Characterization of Martensitic Transformations in CoNiAl Alloys Vesselin Yamakov, National Institute of Aerospace | Numerical Method and Applications for Generalized Disclination Theory Chiqun Zhang, Carnegie Mellon University | Multiscale modeling of a multi-component system: towards the understanding of Oxide Dispersion Strengthened steels Caroline Barouh, DEN/DMN/SRMP, CEA Saclay | Atomic scale modelling of third body formation and wear in hard carbon materials Michael Moseler, Fraunhofer Institute for Mechanics of Materials IWM | Understanding fracture in Si anodes: Experiments and Simulations Katerina Aifantis, University of Arizona |
| 14:45 | Atomistic Modeling at Experimental Strain Rates: Plasticity in Amorphous Solids Harold Park, Boston University | | A Fast Fourier Transform Based Elasto-Viscoplastic Model for Polycrystalline Plasticity using Field Dislocation and Disclination Mechanics Laurent Capolungo, Georgia Institute of Technology | The use of discrete harmonics in direct multi-scale embedding of polycrystal plasticity Nathan Barton, Lawrence Livermore National Laboratory | Tight-Binding Quantum Chemical Molecular Dynamics Study on Tribo-Chemical Reaction of Diamond-Like Carbon under Water Lubrication Shandan Bai, Tohoku University | Exotic phase group IV nanoparticles and Si-ZnS nanocomposites: new paradigms to improve the efficiency of MEG solar cells Gergely Zimanyi, University of California Davis |
| 15:00 | Spectral finite-element based methodology for large scale electronic-structure calculations using density functional theory Jonathan Lind, Lawrence Phani Motamarri, University of Michigan | Stagnation of microstructure features in simulated grain growth Jonathan Lind, Lawrence Livermore National Laboratory | Computational modelling of dislocation patterns and strain hardening in deformed metals Shengxu Xia, Purdue University | Dislocation dynamics simulations of HCP beryllium single crystals at high strain rates Moono Rhee, Lawrence Livermore National Lab. | Tribochemical interactions between DLC coatings and hydrocarbon gases Julien Fontaine, Ecole Centrale de Lyon | PEC H2 production: is it PV + electrolysis or not? Tadashi Ogitsu, LLNL |
| 15:15 | Enabling strain hardening modeling via efficient time-integrators in dislocation dynamics simulations Amin Aghaei, Stanford University | Massively Parallel Cellular Automata Algorithms for the Simulation of Primary Recrystallization Markus Kühbach, Institute for Physical Metallurgy and Metal Physics | Pair correlations and self-correlations in systems of curved dislocations Thomas Hochrainer, Universität Bremen | Impact of magneto-vibrational couplings on the thermodynamic properties of iron: A hierarchical ab initio approach Fritz Körmann, Max-Planck-Institut GmbH Düsseldorf | Smoothed Particle Hydrodynamics Simulations of Abrasive Flow Machining Claas Bierwisch, Fraunhofer IWM | Efficiency assessment of novel materials based flexible thermoelectric devices Malika Bella, STMicroelectronics |
| 15:30 | Refreshment break | | | | | |
| 15:45 | <i>Location: Tent</i> | | | | | |
| 16:00 | A numerical and computational framework for hierarchical multi-scale simulations on large scale computers Jaroslav Knap, Army Research Laboratory | Validating Phase Field Models using Microstructural Experimental Data Michael Tonks, Idaho National Laboratory | FTMP-based Flow-Evolutionary Hypothesis and Its Application to Self-evolving Dislocation Substructures Tadashi Hasebe, Kobe University | Uncertainty Analysis of Materials Phase Diagrams Kristin Lennox, Lawrence Livermore National Laboratory | Multiscale-Multiphysics Approach to Polyelectrolyte Brush Friction Hitoshi Washizu, Toyota Central R&D Labs., Inc. | Better photovoltaic performance through randomised nanowires Thomas Edwards, Imperial College London |

Thursday, October 9th

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| 16:15 | Acceleration of microscale polycrystal plasticity models using GPUs Andrew Richards, Los Alamos National Laboratory | Understanding deformation mechanisms of a dense hydrous magnesium silicate (Phase A) Karine Gouriet, Unité Matériaux et Transformations, CNRS UMR 8207 | A Continuum Approach Towards Formation of Persistent Slip Bands During Cyclic Deformation Stefan Sandfeld, University of Erlangen-Nürnberg, Institute of Materials Simulation (WW8) | First principles thermodynamics of magnetically disordered materials: defect formation in iron and steel Vsevolod Razumovskiy, Materials Center Leoben Forschung G.m.b.H. | Instabilities at Frictional Interfaces: Creep Patches, Nucleation and Rupture Fronts Yohai Bar Sinai, Weizmann Institute of Science | Synergistic Behavior of Tubes, Junctions and Sheets Imparts Mechano- and Thermo-Mutable Functionality in 3D Porous Multifunctional Boron Nitride Nanostructures Rouzbeh Shahsavari, Rice University |
| 16:30 | 3D phase field modeling for nanowire growth by vapor-liquid-solid mechanism Yanming Wang, Stanford University | Recent progresses on the characterization of crystal plasticity behavior of nuclear structural materials Félix Latourte, EDF R&D | (I) Continuum theory of dislocations : coarse-graining and correlations Alphonse Finel, LEM (ONERA/CNRS) | Multi-scale Modeling of Heat Transport in Glasay and Amorphous Materials Mohammad Javad Abdolhosseini Qomi, MIT | Effects of atomic-scale geometry on rough contact Tristan Sharp, Johns Hopkins University | Ab initio lattice thermal conductivity in pure and doped half-Heusler thermoelectric materials. Luc Andrea, ONERA - The French Aerospace Lab |
| 16:45 | | | | Modeling Multiple-site Brittle Fracture in Tungsten During Thermo-mechanical Transients with Discrete Volterra Dislocation Arrays Andrew Sheng, University of California, Los Angeles | Rate-dependent contact mechanics of polymer composites Lambert van Breemen, Eindhoven University of Technology | |
| 17:00 | Poster Intros: F, J & K | | | Poster Intros: A & E | | |
| 17:30 | Chair: Martin Dienwiebel | | | Chair: Tom Arsenlis | | |
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| 20:30 | Poster session 2 and beer reception | | | | | |
| 21:00 | <i>Location: Tent</i> | | | | | |
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Friday, October 10th

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| 07:00 | Breakfast <i>Location: Tent</i> | | | | | |
| 07:15 | | | | | | |
| 07:30 | | | | | | |
| | Chair: Pedro Rivera-Diaz-Del-Castillo | | | | | |
| 08:00 | Plenary 9: Transformation induced inhomogeneity and its effects on creep, fatigue and deformation of titanium alloys | | | | | |
| 08:15 | Dr Rui Yang (Institute of Metals Research, China) | | | | | |
| 08:30 | <i>Location: Ballroom</i> | | | | | |
| 08:45 | Plenary 10: The Materials Genome: Overview, Success Stories and Outlook | | | | | |
| 09:00 | Dr Kristin Persson (Lawrence Berkeley National Laboratory) | | | | | |
| 09:15 | <i>Location: Ballroom</i> | | | | | |
| 09:30 | Refreshment break | | | | | |
| 09:45 | <i>Location: Tent</i> | | | | | |
| | Ballroom 1 | Ballroom 2 | Ballroom 3 | Ballroom 4 | California | Mariposa |
| | J: Numerical methods | E: Microstructure characterization and reconstruction | G: Spatio-temporal instabilities and patterning in plasticity | H: Size effects and methods | F: Friction, Lubrication and Wear Across the Scales III | K: Energy Storage |
| | Chair: Jianguf Lu | Chairs: Joel Bernier and Richard Karnesky | Chairs: Michael Zaiser and Jaafar El-Awady | Chair: Pedro Rivera | Chair: Martin Dienwiebel | Chair: Jiangyu Li |
| 10:00 | (I) Generalized Irving-Kirkwood formula for the calculation of continuum quantities in molecular dynamics models Zhijian Yang, Wuhan University | (I) Capturing the Response of Polycrystalline Materials at the Mesoscale: Measurements, Modeling and Data Mining Joel Bernier, Lawrence Livermore National Laboratory | (I) Power laws distributions as a signature of complexity: models from materials science Garani Ananthakrishna, Materials Research Centre, Indian Institute of Science | (I) Accelerated Multiscale Simulations of Incipient Plasticity using Hyper-QC Ellad Tadmor, University of Minnesota | (I) Coupled Experiments and Simulations of Atomic Stick-Slip Friction: Effects of Sample Dimensionality and Sliding Speed Robert Carpick, University of Pennsylvania | (I) Large-Scale First-Principles Molecular Dynamics Simulations of Materials for Energy Conversion Francois Gygi, University of California |
| 10:15 | | | | | | |
| 10:30 | A concurrent parallel multiscale algorithm for large 3d continuum/atomic simulations at finite temperature using lammps Fabio Pavia, EPFL | Interaction between toughness anisotropy and loading conditions of a drawn wire Jean-Hubert Schmitt, Ecole Centrale Paris | Portevin - LeChatelier like phenomena in confined compression of snow Michael Zaiser, FAU Erlangen-Nuremberg | Molecular Dynamics Simulation Study of the Effect of Temperature and Grain Size on the Deformation Behavior of Poly-crystalline Cementite Seunghwa Ryu, KAIST | (I) Shear-induced Effects in Boundary Film Formation on Copper Wilfred Tysoe, UW-Milwaukee | in situ Nanomechanics of Electrode Failure in Lithium-Ion Batteries Ting Zhu, Georgia Institute of Technology |

Friday, October 10th

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| 10:45 | <p>Analysis of an energy localization method used in kinetic Monte Carlo simulations of heteroepitaxial growth Kyle Golenbiewski, University of Tennessee</p> | <p>Virtual X-Ray and Electron Diffraction Characterization of Surfaces and Interfaces in Alumina Douglas Spearot, University of Arkansas</p> | <p>Dislocation Pattern Evolution and Strain Hardening in FCC Metals through Discrete Dislocation Dynamics Simulations Jaafar El-Awady, Johns Hopkins University</p> | <p>Fast Fourier Transform based Multi-scale Probabilistic Model of Twinning in HCP Materials Arul Kumar Mariyappan, Los Alamos National Laboratory</p> | | <p>A Multiscale Analysis of Ion Conductivity in Non-Equilibrium Environment Christian Neuen, Fraunhofer SCAI</p> |
| 11:00 | <p>Frozen Gaussian approximation for wave propagation in periodic media Xu Yang, UC Santa Barbara</p> | <p>Theoretical and experimental X-ray spectroscopy of graphene-based supercapacitor electrodes under realistic operating conditions Brandon Wood, Lawrence Livermore National Laboratory</p> | <p>Quantification and Comparison of Random Structures Jeremy Mason, Bogazici University</p> | <p>Mechanical properties of nanopillars containing a single homo- or heterogeneous interface Zachary Aitken, California Institute of Technology</p> | <p>Friction and wear of nanocrystalline copper Ao Li, University of Wisconsin Madison</p> | <p>Composition and catalytic activity of Au/Cu electrocatalytic nanoalloys in solution: A combination of DFT and accurate neural network potentials Nongnuch Artrith, Massachusetts Institute of Technology</p> |
| 11:15 | <p>Semiclassical Models for Quantum Systems and Band Crossings Lihui Chai, UCSB</p> | <p>A hierarchical study of grain boundary energy distribution using high-energy x-ray diffraction microscopy Shiu Fai Li, LLNL</p> | <p>Spatiotemporal correlations between plastic events in the shear flow of amorphous solids: from molecular dynamics to mesoscopic models Joerg Rottler, University of British Columbia</p> | <p>Scaling laws in the ductile fracture of metals Michael Baskes, Mississippi State University</p> | <p>Tribological behaviors of C18 fatty acids blended in PAO 4: coupling experimental and computational studies Sophie Loehlé, TOTAL</p> | <p>A Multiscale Design Strategy for Advance Polymer Dielectrics Ghanshyam Pilonia, Los Alamos National Laboratory</p> |
| 11:30 | <p>An efficient rescaling algorithm for simulating the evolution of precipitates in an elastic media Shuwang Li, Illinois Institute of Technology</p> | <p>3D Digital Reconstruction and Numerical Modeling of Microstructurally Small Fatigue Cracks in an Aluminum Alloy from Synchrotron-Based Measurements Ashley Spear, University of Utah</p> | <p>Spatial structure and time evolution of breaking bursts in a fiber bundle model of disordered materials Ferenc Kun, University of Debrecen, Department of Theoretical Physics</p> | <p>Increasing grain boundary cohesion to improve ductility of bcc transition metals Lorenz Romaner, Materials Center Leoben GmbH</p> | <p>Shear accommodating third body layers between metallic nano-asperity contacts Pedro Antonio Romero, Fraunhofer IWM</p> | <p>Unveiling role of salt in Li-ion transfer through boundary between SEI and liquid electrolyte in Li-ion battery: a multi-thousand-atom DFT study Shuji Ogata, Nagoya Institute of Technology</p> |

Friday, October 10th

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| 11:45 | Scalable parallel kinetic Monte-Carlo without approximation Tomas Ooppelstrup, Lawrence Livermore National Lab | Three-dimensional imaging and numerical reconstruction of graphite/epoxy composite microstructure based on ultra-high resolution X-ray computed tomography Michael Czabaj, University of Utah | Field Dislocation Mechanics in the tectonic and sub-inter-supersonic regimes Xiaohan Zhang, CMU | Size Dependent Strength of Nanoparticles – A Combined Experimental/Computational Study Dan Mordehai, Technion | Atomistic Modeling and Simulation of Mechanical and Sliding Properties of Cu-S and Cu-Fe-S Crystal Systems Ken-ichi Saitoh, Kansai University | Unlocking the potential of cation-disordered oxides for lithium batteries Alexander Urban, Massachusetts Institute of Technology |
| 12:00 | OptiDis: a MPI/OpenMP Dislocation Dynamics Code for Large Scale Simulations Arnaud Etcheverry, INRIA | Identification of a crystalline constitutive law using multimodal full-field measurements in grain scale Wang Chow, Ecole Centrale Paris | (I) Instabilities & Patterning in Plasticity: Review and Perspectives Elias Aifantis, Aristotle University of Thessaloniki | Linking Atomistic, kinetic Monte Carlo and Crystal Plasticity simulations of single-crystal Tungsten strength David Cereceda Senas Lawrence Livermore National Laboratory | Multi-physical contact between elastic and elasto-plastic solids with fractal surfaces Vladislav Yastrebov, Centre des Matériaux, MINES ParisTech, CNRS UMR 7633 | Ab-initio-based Cluster Expansion Study of the Phase Transformation and Voltage Fade of the Layered Li_xMnO₃ Eunseok Lee, University of Alabama in Huntsville |
| 12:15 | Fast Multipole Method with Application in Dislocation Dynamics Chao Chen, Stanford University | | | Modelling Mechanical Behaviour of Quantum Solids using Path-integral Monte Carlo Simulations Maurice de Koning, Universidade Estadual de Campinas | Multiscale Modeling of Surface Texture Effect on Hybrid Bearing Shiyuan Pei, Xi'an Jiaotong University | |
| 12:30 | Depart | | | | | |
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| 15:00 | | | | | | |

Poster session 1

Monday, October 6th

Symposium B

- P1 **Multiscale modeling and simulation of the mechanical behavior of hierarchical bovine enamel**
Swantje Bargmann, Hamburg University of Technology
- P2 **Correlating the Free-Volume Evolution to Plastic Deformation of Highly Cross-Linked Polymers from Large Scale Coarse-Grained MD Simulations**
Amin Aramoon, Johns Hopkins University
- P3 **Universal Structure-Material-Property Map for Natural and Biomimetic Platelet-Matrix Composites and Stacked Heterostructures**
Rouzbeh Shahsavari, Rice University
- P4 **Scaled dynamics of nanoparticles in semi-dilute polymer solution**
Sudipta Gupta, JCMS-SNS-Oak Ridge National Laboratory
- P5 **Welding and healing of polymer interfaces: Connecting structure, dynamics and strength**
Mark Robbins, Johns Hopkins University
- P6 **Multiscale Analysis of Multilayer Composite Pipes**
Dinh Chi Pham, Institute of High Performance Computing, A*STAR
- P7 **Nucleation barrier to registration of lipid bilayer domains**
John Williamson, Georgetown University
- P8 **Molecular Mechanism of viscoelasticity in aligned polyethylene**
Ali Hammad, Imperial College London
- P9 **Mesoscale Modeling of the Interfacial Mechanics of Nanocellulose with Glassy Transparent Polymers**
Luis Ruiz, Northwestern University
- P10 **The Microscopic Effect of Filler on Rubber Reinforcement : A Coarse-Grained Molecular Dynamics Study II**
Kentaro Nagaya, Toyota Technical Development Corporation
- P11 **Multiscale strain field measurement in fibrous membrane of connective tissue with photobleaching**
Michel Coret, GEM/Ecole Centrale de Nantes
- P12 **The Mechanism Underpinning Biological Ferroelectricity**
Matthew Zelisko, University of Houston

Symposium C

- P13 **Hybrid quantum-classical simulation of the reaction of breaking bond by water molecules in silica glass**
Takahisa Kouno, Nagoya Institute of Technology
- P14 **Simulation of impurity atom segregation formation kinetic in the vicinity of dislocations and crack tips**
Andrei Nazarov, National research nuclear university (MEPhI)
- P15 **Understating pitting in the passive layer of carbon steel starting from first principles study of its point defects**
Mostafa Youssef, MIT

Poster session 1

Monday, October 6th

Symposium D

- P16 **Void Dynamics in Phase Field Modeling**
San-Qiang Shi, Department of Mechanical Engineering, The Hong Kong Polytechnic University
- P17 **Vacancy assisted diffusion and clustering of interstitial solutes in α -Fe from first principles**
Caroline Barouh, DEN/DMN/SRMP, CEA Saclay
- P18 **Poster withdrawn**
- P19 **Molecular dynamics study on interaction between an edge dislocation and a Frank loop in Fe-10%Ni-20%Cr alloy**
Akiyoshi Nomoto, Central Research Institute of Electric Power Industry
- P20 **Stability of SIA clusters in Fe: the role of substitutional atoms – ab initio study**
Christophe Domain, EDF R&D
- P21 **Nucleation of point defect clusters in displacement cascades near edge and screw dislocations in fcc metals subjected to fast particle irradiation**
Alexander Volkov, Russian Research Centre 'Kurchatov Institute'
- P22 **Mesoscale simulation of phonon mediated thermal transport in UO₂: Perturbation theory based Monte Carlo solution of Boltzmann Transport Equation**
Ahmed Hamed, Purdue University
- P23 **Examination of multiscale concept for swelling description of metals and alloys**
Alexey Yanilkin, All-Russia Research Institute of Automatics
- P24 **Assessment of the influence of elastic anisotropies on dislocation loops sink strength: a phase-field approach**
Rouchette Hadrien, Unité Matériaux et Transformation
- P25 **Towards a quantitative modeling of radiation induced segregation in alloys**
Maylise Nastar, CEA
- P26 **Point defect modeling in materials : coupling ab initio and elasticity approaches**
Celine Varvenne, LAMMM, Swiss Institute of Technology Lausanne (EPFL)
- P27 **Multiscale modeling of dislocation-precipitate interactions: implementing precipitate pinning in Discrete Dislocation Dynamics**
Arttu Lehtinen, Aalto University
- P28 **Multiscale modeling of helium-induced nano-fuzz formation on tungsten surfaces**
Barend Thijssse, TU Delft
- P29 **Molecular dynamical investigation of the interaction of edge dislocations with carbides in BCC Fe; Parametrization for DDD-simulations**
Fredric Granberg, Department of Physics
- P30 **Mesosopic Investigation of Homogeneous to Heterogeneous Deformation Transitions in Irradiated BCC Crystals**
Tom Arsenlis, Lawrence Livermore National University

Poster session 1

Monday, October 6th

Symposium G

- P31 **A continuum theory for defect dynamics in metallic glasses**
Amit Acharya, Carnegie Mellon University
- P32 **Continuum Dislocation Dynamics simulation of dislocation structure evolution in torsion of micro-pillars**
Alireza Ebrahimi, BIME - Bremer Institut für Strukturmechanik und Produktionsanlagen, Universität Bremen
- P33 **Free energy of steps on the surface of faceted solids**
Rodrigo Moura Freitas, UC Berkeley
- P34 **Anisotropic geometrical damage for dynamic processes**
Ioan Ionescu, University Paris 13, LSPM
- P35 **Poster withdrawn**
- P36 **Scale-free dynamics in dislocation systems**
Péter Dusán Ispánovity, Department of Materials Physics, Eötvös University
- P37 **Atomistic Modeling on Elastic Heterogeneities Evolution and Elementary Activations in Metallic Glass**
Yue Fan, ORNL
- P38 **Dislocation Pattern Evolution and Strain Hardening in FCC Metals through Discrete Dislocation Dynamics Simulations**
Ahmed Hussein, Johns Hopkins University
- P39 **Poster withdrawn**
- P40 **The evolution of plastic flow localization from the micro- to macroscale level**
Lev Zuev, Institute of Strength Physics and Materials Science
- P41 **Numerical Simulation of Dislocation Annihilation by Cross-Slip**
Michal Benes, Czech Technical University in Prague
- P42 **A numerical spectral approach for solving elasto-static field dislocation and g-disclination mechanics**
Stephane Berbenni, CNRS, LEM3 UMR 7239
- P43 **A Multiscale Study of Solidification: Interfacial atomistic properties and their consequences at the mesoscale microstructures**
Tomorr Haxhimali, Lawrence Livermore National Laboratory
- P44 **Modeling of dislocation mechanisms and the influence of the γ/γ' lattice misfit on the dislocation assisted creep of high temperature Ni-base superalloys**
Seyed Masood Hafez Haghighat, Max-Planck Institute for Iron Research
- P45 **Microstructural characterization and petro-physics from natural heterogeneous rocks and the upscaling of properties**
Jie Liu, University of Western Australia

Poster session 1

Monday, October 6th

- P46 **A mesoscopic stochastic model for micron-scale plasticity**
Dániel Tüzes, ELTE Department of Materials Physics
- P47 **Vacancy-solute clusters and cavities evolution in α -Fe solid solutions**
Thomas Schuler, CEA
- P48 **A continuum model for dislocation dynamics in three dimensions**
Yichao Zhu, The Hong Kong University of Science and Technology
- P49 **Modeling polycrystal plasticity using field disclination and dislocation mechanics**
Vincent Taupin, LEM3
- P50 **A phase field model coupling cracks and dislocations at finite strain**
Antoine Ruffini, ONERA
- P51 **Reaction pathway analysis for the partial dislocation mobility in 3C-SiC**
Jing Yang, University of Tokyo
- P52 **Solid phase recrystallization of Si and Ge nanowires**
Matthias Posselt, Helmholtz-Zentrum Dresden-Rossendorf
- P53 **Large-scale molecular dynamics simulation of microstructure formation during plasma spray process**
Tao Wang, ICAMS, Ruhr-Universität Bochum

Symposium H

- P54 **Unexpected material response in nanoimprinting simulations**
Yunhe Zhang, Delft University of Technology
- P55 **Fatigue hot spot simulation of a Ti Widmanstätten microstructure**
Benjamin Smith, Boeing
- P56 **Screw Dislocations in Layered, Complex Hydrated Oxides**
Rouzbeh Shahsavari, Rice University
- P57 **Phase Field Crystal Simulation of Strain Effects on Dislocation Movement of Premelting Grain Boundaries at High Temperature**
Gao Yingjun, Guangxi University
- P58 **Comparative study of the size of the plastic zone produced by nanoindentation**
Yu Gao, University Kaiserslautern
- P59 **A phase field model coupling cracks and dislocations at finite strain**
Antoine Ruffini, ONERA
- P60 **Revisiting continuum modelling of hydrogen diffusion and trapping in metals for the purposes of hydrogen assisted fracture analysis**
Jesus Toribio, University of Salamanca

Poster session 1

Monday, October 6th

- P61 **Dislocation mobility laws with several character angles in FCC Aluminum**
Jaehyun Cho, École polytechnique fédérale de Lausanne EPFL / ENAC-IIC, STI-IMX, Computational Solid Mechanics Laboratory
- P62 **A Unified Framework for Localization and Fracture in Extreme Environments**
Elias Aifantis, Aristotle University of Thessaloniki
- P63 **Screw dislocation core structure as a function of lattice expansion and contraction in bcc transition metals**
Lucile Dezerald, CEA
- P64 **Peierls Potential for $1/2\langle 110 \rangle\{110\}$ in MgO: unusual effect of high pressure**
Philippe Carrez, University of Lille 1
- P65 **Computational Investigations into the Hardness of Metal Carbides**
Xiaoxiang Yu, The University of Alabama
- P66 **Dislocation diffusion of hydrogen in fcc metal: A molecular dynamics study**
Kenji Nishimura, AIST
- P67 **First-principles prediction of ductility in rhenium-based alloys from elastic constants, twin boundary energies and surface energies**
Mark Asta, UC Berkeley
- P68 **Surface Roughness Evolution under Thermo-mechanical Cycling Loads in FCC Metals - Discrete Dislocation Dynamics Simulations**
Ahmed Hussein, Johns Hopkins University
- P69 **Peierls stress, Pile-ups and Inertia effects in Field Dislocation Mechanics**
Xiaohan Zhang, CMU
- P70 **Increasing Elongation by Secondary Twinning in Magnesium Nanowires**
Chang Ni, Shanghai Jiao Tong University
- P71 **On the effect of dislocation emission on intergranular fracture in Ni**
Guoqiang Xu, MIT
- P72 **Dislocation-obstacle interactions and effects on glide from atomistic simulations**
Roberto Gomes de Aguiar Veiga, University of São Paulo
- P73 **Atomistic Modeling of Dislocation Slip in Alpha-Iron towards the Development of a Multi-Scale Model of Dislocation Plasticity**
Jonathan Zimmerman, Sandia National Laboratories
- P74 **Ab initio prediction of screw dislocation motion in bcc transition metals: kink-pair formation enthalpies and Schmid law deviation**
François Willaime, CEA

Poster session 2

Thursday, October 9th

Symposium A

- P1 **Development of Multi-phase-field Crystal Plasticity Model for Grain Boundary Bulging during Dynamic Recrystallization**
Takato Yamaguchi, Kyoto Institute of Technology
- P2 **Analytical method for estimating the thermal expansion coefficient at high temperature**
So Takamoto, the University of Tokyo
- P3 **Dynamic Recrystallization Modeling by Multi-phase-field Method Considering Misorientation Dependent Interface Properties**
Eisuke Miyoshi, Kyoto Institute of Technology
- P5 **Computational model verification using multiplexed photonic doppler velocimetry for high-velocity projectile impact on steel targets**
Mohamed Trabia, University of Nevada, Las Vegas
- P6 **A multiphase-field model with Onsager reciprocal relations**
Reza Darvishi Kamachali, ICAMS - Ruhr-Uni-Bochum
- P7 **Modelling nonlinear behavior of heterogeneous geomaterials by extended finite-element method**
Naima Belayachi, University of Orleans (PRISME)
- P8 **Crack Propagation Simulations in Polycrystal by Multi-phase-field-crack Model**
Shinya Mori, Kyoto Institute of Technology
- P9 **Impact of extended defects on the mobility of grain boundaries: A molecular dynamics study**
Sherri Hadian, Max-Planck institute
- P10 **On the strength properties of ductile porous solids with a Mohr-Coulomb matrix: theoretical formulation and numerical assessment**
Kokou Anoukou, Institut Jean Le Rond d'Alembert (UPMC)
- P11 **Diffusion of oxygen in TiNiHf high temperature shape memory alloy**
Hak-SungLee, Korea Institute of Materials Science
- P12 **Phase transformations in Fe-C bulk and nanowire systems: molecular dynamics simulation and free-energy calculations**
Emilia Sak-Saracino, University Kaiserslautern
- P13 **Principal component analysis of necking in sintered nanoparticles**
Amlan Dutta, S. N. Bose National Centre for Basic Sciences
- P14 **Reversible multiscale homogenization for obtaining effective strength-elastic properties of composite materials with incomplete set of initial data**
Alexandr P. Sokolov, Bauman Moscow State Technical University
- P15 **Bridging Crack Propagation at Atomistic and Mesoscopic Scale with Hybrid Multiscale Methods**
Jinghong Fan, Alfred University
- P16 **Modeling of buckling under residual stresses by arlequin method and asymptotic numerical method: application to rolling of thin sheet metal**
Kékéli Kpogan, Université de Lorraine

Poster session 2

Thursday, October 9th

Symposium E

- P17 **Crystal plasticity analysis of scale dependent mechanical properties of ferrite/cementite fine lamellar structure in pearlite steel**
Yohei Yasuda, Kitami Institute of Technology
- P18 **Grain Growth in Porous Oxides: Diffuse Interface Modeling and Experiments**
Karim Ahmed, Purdue University
- P19 **Through-process Modeling for Alloy Design and Process Optimization for Cold Spray Processing**
Danielle Belsito, Worcester Polytechnic Institute
- P20 **Experimental Verification of Through-Process Modeling of Cold Spray Al Alloys**
Baillie McNally, Worcester Polytechnic Institute
- P21 **Experimental investigation and modeling of the plastic behavior of halite single crystals at room temperature and 400°C: in-situ approach**
Jean Raphanel, LMS CNRS Ecole polytechnique
- P22 **Solute segregation and dislocation mobility in binary alloys from dynamical variational Gaussian calculations**
Evgeniya Dontsov, Department of Materials Engineering, University of British Columbia
- P23 **Stability of a quadruple node in the interfacial network in 3D**
Vasily Bulatov, Lawrence Livermore National Laboratory
- P24 **Phase transitions in metallic grain boundaries**
Timofey Frolov, University of California, Berkeley
- P25 **Molecular Origins of the Mechanical Behavior of Hybrid Molecular Materials**
Reinhold Dauskardt, Stanford University
- P26 **Influence of Interfaces on the Intrinsic Growth Stresses in Nanoscale Metallic Thin Films**
Gregory Thompson, University of Alabama
- P27 **Microscale plastic strain distribution in slip dominated deformation of Mg alloys**
Chad Sinclair, The University of British Columbia
- P28 **Formation and structure of first water monolayer on TiO₂ rutile surface**
Natalia Skorodumova, The Royal Institute of Technology (KTH)
- P29 **The Origin of Oxygen Strengthening Effect in α -Titanium**
Liang Qi, University of California
- P30 **WC-Co microstructure degradation study in rotary-percussive drilling**
Dmitry Tklich, NTNU
- P31 **Gas Adsorption in Microporous Materials: Ab Initio Based Grand Canonical Monte Carlo Simulations**
Rouzbeh Shahsavari, Rice University
- P32 **Ultrahigh strength of nanotwinned Ag-Cu dilute alloys by atomistic simulations**
Linh Nguyen, Lawrence Livermore National Laboratory

Poster session 2

Thursday, October 9th

- P33 **Comparison of dislocation-based model of recovery and cross-correlation based EBSD measurements in single crystals**
István Groma, Eötvös Loránd University (ELTE)
- P34 **Prediction of Microstructural Evolution during Sintering Process using Meso-scale Simulation and FIB/SEM Tomography**
Shotaro Hara, The University of Tokyo

Symposium F

- P35 **Wear, plasticity, and rehybridization in tetrahedral amorphous carbon**
Matthias Posselt, Helmholtz-Zentrum Dresden-Rossendorf
- P36 **Quantifying touch-feel perception: Tribological Aspects on a new artificial finger design**
Hui Niu, University of Warwick
- P37 **Multiscale estimating technique of rubber friction on surface asperities depending on sliding velocity**
Hiro Tanaka, University of Tokyo
- P38 **Nanoindentation and wear of graphene-covered surfaces**
Andreas Klemenz, Fraunhofer IWM
- P39 **Seamless elastic boundaries for atomistic calculations**
Lars Pastewka, Fraunhofer IWM
- P40 **Improving Estimates of Fretting Wear Rates through Microscale Simulations**
Areg Hayrapetian, Massachusetts Institute of Technology
- P41 **Theoretical modeling and molecular dynamics simulation of atomic scale wear: a combined study**
Yuchong Shao, Johns Hopkins
- P42 **Multiscale Modelling for Atomic Force Microscopy**
Yasuhiro Senda, Yamaguchi University
- P43 **Density Functional Study of Gold-Coated Iron Nanoparticles (Potential for Medical Applications)**
Eyachew Misganewl, Debre Tabor University
- P44 **Computational Chemistry Study on Resin/Metal Interface: Tribochemical Reaction and Its Effect on Friction**
Tasuku Onodera, Hitachi Research Laboratory, Hitachi., Ltd.
- P45 **Piston pin lubrication**
Hannes Allmaier, Virtual Vehicle Research Center
- P46 **Roughness induced hysteretic behavior of adhesive contacts.**
Giuseppina Recchia, Politecnico di Bari
- P47 **Molecular dynamics of study of automotive lubricants: linking molecular structure and friction**
Michael Doig, University of Edinburgh

Poster session 2

Thursday, October 9th

Symposium J

- P48 **Mathematical Model of Anisotropic Surface Diffusion**
Dieu Hung Hoang, Czech Technical University in Prague
- P49 **Insights on micro-mechanisms of damage in a cement-based geomaterial under uniaxial compression from multiscale modelling**
Duc-Phi Do, University Orleans
- P50 **A multiscale approach for 3D mixed mode crack propagation**
Anthony Gravouil, LAMCOS - INSA LYON
- P51 **Matched asymptotics of dislocation pile-ups against an interface in a coated solid**
Roman Voskoboynikov, ANSTO
- P52 **Hybrid continuum-atomistic simulations on the Bloch point dynamics in a single-crystalline ferromagnet**
Christian Andreas, Université de Strasbourg
- P53 **An efficient fast multipole evaluation of the elastic stress field and energy of a dislocation ensemble.**
Pierre Blanchard, Inria Bordeaux - Sud-Ouest
- P54 **Progresses towards coupling MD and FEM for the simulation of MEMS containing nanoelectromechanical components**
Michel Devel, Femto-ST, ENSMM
- P55 **Multi-scale quantum mechanical calculations of solute-grain boundary interaction**
Liam Huber, University of British Columbia
- P56 **Computing traction force of dislocation stress field on free surfaces and grain boundaries in anisotropic crystals**
Bing Liu, Lawrence Livermore National Laboratory
- P57 **Accelerated molecular dynamics simulation of dislocation glide in magnesium**
Peng Yi, Johns Hopkins University
- P58 **A Scale-Bridging Elastoviscoplasticity Proxy Application for Exascale Co-design**
Milo Dorr, Lawrence Livermore National Laboratory
- P59 **Intersecting slip for dislocation dynamics in 2-dimensions**
Wei Cai, Stanford University
- P60 **Polyethylene-based nanocomposites with carbon reinforcements: atomistic and coarse-grained approaches**
Nikita Orekhov, Joint Institute for High Temperatures of Russian Academy of Sciences
- P61 **Identification of dislocations by singular value decomposition of the Nye tensor**
Fuzhi Dai, Tsinghua University
- P62 **First-principles study on the mechanical property of high-entropy alloys by MaxEnt modelling**
Shaoqing Wang, Institute of Metal Research, CAS
- P63 **Numerical Simulation of Three-Dimensional Anisotropic Crystal Growth**
Pavel Strachota, FJFI CVUT v Praze

Poster session 2

Thursday, October 9th

- P64 **Multiscale Dynamic Simulations and Microstructure of Dipole Colloid**
Jianwei Zhang, School of Physics, Tongji University
- P65 **Adaptive Resolution Simulation of an Atomistic Protein in MARTINI Water**
Matej Praprotnik, National Institute of Chemistry
- P66 **Multiscale simulation of atomic structure in the neighborhood of nanovoids**
Andrei Nazarov, National Research Nuclear University (MEPhI)

Symposium K

- P67 **Defect substitution energies in cubic barium titanate**
Juan J. Melendez-Martinez
- P68 **Nanostructuring Bi₂Te₃: influence on the phonon thermal conductivity**
Christian Elsässer, Fraunhofer-IWM
- P69 **A study of iron impurities interacting with grain boundaries in photovoltaic silicon using density functional theory**
Benedikt Ziebarth, Karlsruher Institut für Technologie
- P70 **Passivation of silicon surfaces by aluminum oxide layers: a simulation study**
Christian Elsässer, University of Freiburg and Fraunhofer IWM
- P71 **A hybrid quantum classical simulation on the diffusivity of Li's in the graphite**
Shuji Ogata, Nagoya Institute of Technology