Sunday October 9th, 2016

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16:00	**Registration** *Foyer*
18:00 - 20:00	**Welcome reception** *Grands Echézeaux Hall*

Monday October 10th, 2016

MMM 2016

08:00	**Registration** *Foyer*								
Plenary session 1 *R1 Amphi Romanée Conti* *Chair: François Willaime, CEA, France*									
08:30	**Welcome** François Willaime, CEA, France								
08:40	(plenary) **Model-reduction in multiscale problems for composite and polycrystalline materials** Pierre Suquet, CNRS Marseille, France								
09:30	(plenary) **The effect of dislocation junctions on the work hardening rate of face-centered cubic metals** Wei Cai, Stanford University, USA								
10:20	**Coffee break** *Foyer Bar and Hall D'Accueil*								
10:50	**A1** *R8 Mercurey* *Chair: Jim Belak, Lawrence Livermore National Laboratory, USA*	**C1** *R3 Santenay-Chablis* *Chair: James Kermode, University of Warwick, UK*	**D1** *R4 Musigny + R5 Pommard* *Chair: Joerg Rottler, University of British Columbia, Canada*	**E1** *R2 Morey Saint Denis* *Chair: Byeong-Joo Lee, POSTECH, South Korea*	**F1** *R9 Saint Romain* *Chair: Tony Lelièvre, Ecole des Ponts ParisTech, France*	**G1** *R1 Amphi Romanée Conti* *Chair: Ghiath Monnet, EDF-R&D, France*	**M1** *R7 Givry+Savigny* *Chair: Döme Tanguy, CNRS-Lyon1, France*	**N1** *R6 Volnay* *Chair: Gianpietro Moras, Fraunhofer Institute for Mechanics of Materials IWM, Germany*	
	(invited) **Designing the mechanical response of additively manufactured silicone cellular solids with ordered porous architectures** Todd Weisgraber, Lawrence Livermore National Laboratory, USA	(invited) **Coarse graining interatomic potentials with machine learning** Gabor Csanyi, University of Cambridge, UK	(invited) **Non-equilibrium first order transition marks the mechanical failure of glasses** Peter Schall, University of Amsterdam, Netherlands	(invited) **Multiscale modeling of coherent precipitation in interstitial solid solutions** Mark Asta, University of California, Berkeley, USA	(invited) **Enhanced free energy based structure prediction in materials science** Mark Tuckerman, New York University, USA	(invited) **First-principles modelling of screw dislocation mobility in Zr and Ti** Emmanuel Clouet, CEA Saclay / SRMP, France	(invited) **Local strain measurements during in situ TEM deformation with nanobeam electron diffraction** Christoph Gammer, Erich Schmid Institute of Materials Science, Austria	(invited) **Rolling, sliding and fretting contact of viscoelastic materials** Daniel Nelias, INSA Lyon, France	
11:20	**An ICME approach for additive manufacturing** Jim Belak, Lawrence Livermore National Laboratory, USA	**Active learning of interatomic potentials** Alexander Shapeev, Skolkovo Institute of Science and Technology, Russia	**Emergence of cooperativity in plasticity of soft glassy materials** Jérôme Crassous, Université Rennes 1, France	**Nb precipitation in zirconium alloys** Maeva Cottura, SRMP-CEA Saclay, France	**Cross-entropy minimization and importance sampling of rare events** Wei Zhang, Freie Universität Berlin, Germany	**Dislocation trajectory and Schmid law deviation in BCC metals** Lucile Dezerald, IJL, France	**Plasticity of Olivine Mg2SiO4: Insights from nanomechanical experiments and atomistic calculations** Srinivasan Mahendran, UMET University Lille 1, France	**Modelling viscoelastic reciprocating contacts** Giuseppe Carbone, Politecnico di Bari, Italy	
11:40	**Multiscale optimization for novel material design using a combined numerical and experimental approach** Grace Gu, MIT, USA	**QM/MM coupling for crystalline defect simulations** Christoph Ortner, University of Warwick, UK	**Microscopic origin of the yielding behaviour in metallic glasses in terms of nonaffine stress relaxation and viscous stress build-up** Alessio Zaccone, University of Cambridge, UK	**Multiscale modelling of Ti-Al-N thin film growth using DFT and kMC approaches: microstructural evolution** Cedric Mastail, Institut Pprime, France	**Comparison of minimum action and steepest descent paths in gradient systems** Grisell Diaz Leines, ICAMS - Ruhr University Bochum, Germany	**Interaction of interstitial iron with dislocations in silicon** Matous Mrovec, Fraunhofer IWM, Germany	**Dislocations in ferroelectric perovskite $KNbO_3$: Insight from theory and experiment** Pierre Hirel, UMET University Lille 1, France	**Multiscale plasticity simulation applied to an experimental scratch test on copper using smooth particle hydrodynamics** Andras Vernes, AC2T, Austria	
12:00	**Mechanical and morphological study of dental tissues** Elsa Vennat, Centrale-Supélec, France	**Mathematical modeling of incommensurate 2D materials** Mitchell Luskin, University of Minnesota, USA	**Thermal fluctuations and elastic relaxation in the compressed exponential dynamics of colloidal gels** Mehdi Bouzid, Georgetown Univeristy, USA	**Effect of interfacial structure on the heterogeneous nucleation of Pb at a Cu surface** Brian Laird, University of Kanas, USA	**Nested sampling of reaction paths** Gabor Csanyi, University of Cambridge, UK	**Stabilization of the screw dislocation hard core by interstitial solutes in body-centered cubic metals** Berengere Luthi, CEA, France	**Understanding Atomic Force Microscopy: From atomic to macroscopic scale** David Gao, University College London, UK	**Dislocation microstructure evolution during indentation and sliding in Discrete Dislocation Dynamics** Johanna Gagel, Karlsruhe Institute of Technology, Germany	
12:20	**Lunch** *Chambertin* *Followed by coffee in Foyer Bar and Hall D'Accueil*								

13:50	**A2** *R8 Mercurey* *Chair: Lorenzo Valdevit, University of California Irvine, USA*	**C2** *R3 Santenay-Chablis* *Chair: Alexei Lozinski, Université de Franche-Comté, France*	**D2** *R4 Musigny* *Chair: Jean-Louis Barrat, Université Grenoble Alpes, France*	**E2** *R2 Morey Saint Denis* *Chair: Chris Race, University of Manchester, UK*	**F2** *R9 Saint Romain* *Chair: Fabio Pietrucci, Université Pierre et Marie Curie, France*	**G2** *R1 Amphi Romanée Conti* *Chair: Benoit Devincre, LEM, CNRS-ONERA, France*	**K1** *R10 Monthelie* *Chair: Riccardo Ferrando, University of Genoa, Italy*	**M2** *R7 Givry+Savigny* *Chair: Hosni Idrissi, Université Catholique de Louvain, Belgium*	**N2** *R6 Volnay* *Chair: Kerstin Falk, Fraunhofer IWM, Germany*
	(invited) **Optimal design and advanced manufacturing of micro and nano-architected materials** Lorenzo Valdevit, University of California, Irvine, USA	(invited) **Model order reduction techniques for numerical homogenization** Assyr Abdulle, EPFL, Switzerland	(invited) **Mesoscopic modeling - specific ingredients and emergent behaviors** Kirsten Martens, Université Grenoble Alpes & CNRS, France	(invited) **Combination of atomistic simulation and phase-field modeling techniques for a texture control in steel sheets** Byeong-Joo Lee, Pohang University of Science and Technology (POSTECH), South Korea	(invited) **Energy landscape and pathways of point defects in body-centered-cubic metals** Mihai-Cosmin Marinica, CEA - Université Paris-Saclay, France	(invited) **Atomistic simulations of screw dislocations: core structure, Peierls potential, and finite temperature motion** Mark Gilbert, CCFE/Euratom, UK	(invited) **Ordering and surface segregation in miscible Nanoalloys: cases of Co-Pt, Pd-Au and Pd-Pt** Christine Mottet, CINaM - CNRS / AMU, France	(invited) **Dislocation and back stress dominated viscoplasticity in freestanding sub-micron Pd et Cu films** Thomas Pardoen, Université Catholique de Louvain (UCL), Belgium	(invited) **Adhesion between elastic solids: From single-wavelength roughness to self-affine surfaces** Martin Müser, Saarland University, Germany
14:20	**Homogenized dynamics of lattice-structured meta-materials** John Moore, Lawrence Livermore National Laboratory, USA	**Control of oscillators, temporal homogenization, and energy harvest by super-parametric resonance** Molei Tao, Georgia Institute of Technology, USA	**Elasto-plastic automata with realistic near field interactions: avalanches and diffusion** Damien Vandembroucq, ESPCI ParisTech, France	**Simulation and modeling of electromigration of C in Fe: a Molecular Dynamics approach** Patrice Chantrenne, INSA, France	**Metadynamics simulations of phase transitions in crystalline and amorphous ice** Silvio Pipolo, Université Pierre et Marie Curie, France	**Kink pair production and dislocation motion** Steve Fitzgerald, University of Oxford, UK	**Experimental and modeling comparison in atom segregation of Ag-based bimetallic clusters** Pascal Andreazza, Université d'Orléans, France	**Micro-fracture testing of tungsten: Simulation and experiment** Sabine Weygand, Karlsruhe Institute of Technology (KIT), Germany	**Cavitation of fluids between heterogeneous slipping-sticking surfaces** Daniele Savio, Fraunhofer IWM, Germany
14:40	**Crystal plasticity study of monocrystalline stochastic honeycombs under in-plane compression** Franz Roters, MPI für Eisenforschung, Germany	**Numerical homogenization based fast solver for PDEs with arbitrarily rough coefficients** Lei Zhang, Shanghai Jiao Tong University, China	**Avalanche phenomena and shear localization near the fracture limit of amorphous solids** David Fernandez-Castellanos, Institute of Materials Simulation (WW8) - FAU, Germany	**A molecular dynamics study of the effect of helium clusters on grain boundary migration in bcc iron** Aulia Tegar Wicaksono, University of British Columbia, Canada	**Nucleation and interfacial adsorption in ternary systems** Thomas Philippe, CNRS - Ecole Polytechnique, France	**Onset of plasticity in zirconium in relation with hydrides precipitation** Laurent Pizzagalli, Institut P' / CNRS, France	**Multi-scale modeling of core-shell Fe@Au nanoparticles** Magali Benoit, CEMES-CNRS, France	**Dislocation Dynamics simulations and in-situ TEM observations of interactions between dislocations and irradiation induced loops in recrystallized Zircaloy-4** Laurent Dupuy, CEA-Saclay, France	**The application of a molecular-continuum coupling strategy for the modelling of liquid lubricants** Eduardo Ramos Fernandez, Imperial College London, UK
15:00	**Disordered auxetic materials** Charlotte Petersen, Aalto University, Finland	**The local orthogonal decomposition method for problems with complex geometry** Daniel Elfverson, Umeå University, Sweden	**Reducing the gap between real particle rearrangements and idealized shear transformations in deformation models for amorphous solids** Alexandre Nicolas, CNRS & University Paris-Sud, France	**Multi-scale study of the gas-phase growth of Silicon clusters in realistic conditions** Giovanni Barcaro, CNR-IPCF, Italy	**Estimating rates of thermally activated events by sampling and unbiasing dynamically activated paths** Manuel Athènes, CEA, France	**Dislocation core transitions in disicides** Vaclav Paidar, Institute of Physics AS CR, Czech Republic	**A Cahn-Hilliard approach to modelling phase separation in bimetallic nanoparticles** Mohammad Ahmed, University of Birmingham, UK	**The effect of dimensionality and size on the nanoindentation – A combined experimental/computational multiscale study** Shyamal Roy, Israel Institute of Technology, Israel	**Molecular dynamics simulations of iron-oxide lubrication by glycerol/water solutions** Bartlomiej Czerwinski, Luleå University of Technology, Sweden
15:20	**General properties and upper bound estimates for plasticity in porous continua** Amine Benzerga, Texas A&M University, USA	**From the Newton equation to the wave equation in case of shocks** Marc Josien, ENPC, France	**Creep and onset of flow in amorphous solids** Samy Merabia, CNRS and University Lyon 1, France	**Multiscale simulation of interface-dominated structural transformations in Fe-C alloys** Xie Zhang, Max-Planck-Institut für Eisenforschung, Germany		**Multiscale modelling of dislocation loops and precipitates in irradiated metals** Arttu Lehtinen, Aalto University, Finland	**Modeling finite-size effects on phase-separation transitions in nanoalloys** Micha Polak, Ben-Gurion University of the Negev, Israel	**Toward the understanding of the brittle to ductile transition at low size in silicon: experiments and simulation** Julien Godet, Pprime Institute - University of Poitiers, France	**The area of contact for non-adhesive rough surfaces: Comparison between md and persson's model** Soheil Solhjoo, University of Groningen, Netherlands
15:40	**Coffee break** *Foyer Bar and Hall D'Accueil*								

16:10	**A3** *R8 Mercurey* *Chair: Nathan Barton, Lawrence Livermore National Laboratory, USA*	**C3** *R3 Santenay-Chablis* *Chair: Katie Newhall, UNC Chapel Hill, USA*	**D3** *R4 Musigny* *Chair: Emanuela del Gado, Georgetown University, USA*	**E3** *R2 Morey Saint Denis* *Chair: John Ågren, KTH, Sweden*	**F3** *R9 Saint Romain* *Chair: Rodolphe Vuilleumier, Ecole Normale Supérieure - CNRS - UPMC, France*	**G3** *R1 Amphi Romanée Conti* *Chair: Laurent Pizzagalli, Institut P' / CNRS, France*	**J1** *R5 Pommard* *Chair: Nicolas Combe, Cemes, CNRS UP 8011 and Univ Paul Sabatier, France*	**K2** *R10 Monthelie* *Chair: Nils Warnken, University of Birmingham, UK*	**N3** *R6 Volnay* *Chair: Daniele Savio, Fraunhofer IWM, Germany*
	(invited) **Poisson's function of single-wire entangled materials: from below 0 in tension to above 0.5 in compression** David Rodney, University of Lyon, France	(invited) **Kinetic Modeling of Materials Coarsening: from individual grains to network statistics** Maria Emelianenko, George Mason University, USA	(invited) **Stress state effects on non-affine displacements and strain hardening of a metallic glass** Todd Hufnagel, Johns Hopkins University, USA	(invited) **Microstructural pattern formation during liquid metal dealloying** Alain Karma, Northeastern University, USA	(invited) **Hierarchical dynamics of biomolecular processes** Gerhard Stock, University of Freiburg, Germany	(invited) **Direct atomistic simulations of bulk crystal plasticity** Vasily Bulatov, Lawrence Livermore National Laboratory, USA	(invited) **Shear-coupled grain boundary motion: Atomistics to continuum** Yuri Mishin, George Mason University, USA	(invited) **Experimental atomic arrangements in size-selected clusters - a benchmark for nanoscale modelling** Richard Palmer, University of Birmingham, UK	(invited) **Tight-binding quantum chemical molecular dynamics simulations on tribochemical reaction dynamics of diamond-like carbon thin films** Momoji Kubo, Tohoku University, Japan
16:40	**Microstructure modeling of porous electrodes for solid oxide fuel cells (SOFCs)** Jochen Joos, Karlsruhe Institute of Technology (KIT), Germany	**Stochastic model for dislocation climb** Xiaohua Niu, Hong Kong University of Science and Technology, Hong Kong	**Metadynamics of Slow Deformation and Flow: Time-dependent amorphous plasticity (creep)** Penghui Cao, MIT, USA	**Diffuse interface modelling of microstructure evolution in the presence of flow: Hydrodynamics equations** Amol Subhedar, ICAMS - Ruhr-Universität Bochum, Germany	**Long-time atomistic simulations with Parallel Trajectory Splicing** Danny Perez, Los Alamos National Laboratory, USA	**Molecular dynamics investigation of dislocation-dislocation interaction at Ag precipitate interface embedded in Cu matrix** Dennis Rapp, IMWF - Universität Stuttgart, Germany	**Atomistic migration mechanisms of grain boundaries deviated from the symmetric tilt orientation** Sherri Hadian, Max-Planck Institute, Germany	**Ageing of nanoalloys: Formation and dissolution of the onion-like nanostructure** Fabienne Berthier, CNRS-University Paris Sud, France	**On the solid lubrication processes of silicon oxide containing hydrogenated amorphous carbon coatings** Julien Fontaine, Ecole Centrale de Lyon, France
17:00	**Size effects and irregularity in open cellular foams** Stefan Liebenstein, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany	**On the temporal coarse graining in dislocation dynamics** Anter El-Azab, Purdue University, USA	**Shear bands and energy dissipation in metallic and network-forming glasses** Richard Jana, Karlsruhe Institute of Technology, Germany	**Modeling pattern formation in multi-component fluids on the mescoscale: a phase-field approach** Gyula Toth, University of Bergen, Norway	**Error estimates for transport coefficients in molecular dynamics** Gabriel Stoltz, Ecole des Ponts, France	**Evolution of dislocations during nanoindentation and nanoscratching of HCP metals: Molecular dynamics study** Iyad Alabd Alhafez, University Kaiserslautern, Germany	**Examining the interplay of tension and shear for a metal grain boundary through atomistic ab initio computational studies** Flemming Ehlers, Université Paris Diderot, France	**Investigating structural transitions in metallic nanoalloys via Metadynamics** Kevin Rossi, King's College London, UK	**Mechanochemical breaking of C-C bonds at the tribological interface between diamond and silica** Gianpietro Moras, Fraunhofer Institute for Mechanics of Materials IWM, Germany
17:20	**Elaboration of BN membrane using a new elegant approach** Catherine Marichy, Laboratory of Multimaterial and Interfaces - UMR 5615, France	**Generic adaptive resolution approach to reverse mapping of polymer melts** Jakub Krajniak, KU Leuven, Belgium	**Yield cirteria developed using atomic scale simulations** Gergely Molnar, Ecole des Mines de Saint Etienne, France	**Metal droplet entrainment by solid particles in slags: a combined phase field – experimental approach** Inge Bellemans, Ghent University, Belgium		**Molecular dynamics simulations of intrusions and extrusions in iron, copper and nickel during cyclic loading** Youssef Maniar, Robert Bosch GmbH, Germany	**Effect of a normal stress on the shear-coupled grain boundary migration** Nicolas Combe, CNRS UP 8011 and Univ Paul Sabatier, France	**New designed synthesis of metallic nanoparticles and nanoalloys** Christophe Petit, MONARIS UPMC, France	**Tribochemistry of steel lubrication by graphene** Paolo Restuccia, Universita' degli Studi di Modena e Reggio Emilia, Italy
17:40		**Flash posters C** *R3 Santenay-Chablis*			**Flash posters F** *R9 Saint Romain*				
18:10 - 20:00	**Exhibitor and poster session 1 - Wine & cheese party** *Grands Echézeaux Hall*								

Tuesday October 11th, 2016

MMM 2016

Plenary session 2
R1 Amphi Romanée Conti
Chair: Vasily Bulatov, Lawrence Livermore National Laboratory, USA

08:30 (plenary) **Can a simulation be reality? Does it matter?**
Helena Van Swygenhoven-Moens, Paul Scherrer Institut, Switzerland

09:20 (plenary) **Reaching experimental times at the atomic scale in complex materials: the kinetic activation-relaxation technique**
Normand Mousseau, Université de Montréal, Canada

10:10 **Presentation of poster prizes (poster session 1)**

10:20 **Coffee break**
Foyer Bar and Hall D'Accueil

10:50	**A4** *R8 Mercurey* *Chair: Jim Belak, Lawrence Livermore National Laboratory, USA*	**C4 + F4** *R3 Santenay-Chablis* *Chair: TBC*	**D4** *R4 Musigny* *Chair: Kirsten Martens, University Grenoble Alpes & CNRS, France*	**E4** *R2 Morey Saint Denis* *Chair: Alain Karma, Northeastern University Physics Department, USA*	**G4** *R1 Amphi Romanée Conti* *Chair: Daniel Caillard, CEMES-CNRS, France*	**J2** *R5 Pommard* *Chair: Rebecca Janisch, ICAMS, Germany*	**K3** *R10 Monthelie* *Chair: Christophe Petit, MONARIS UPMC, France*	**M3** *R7 Givry+Savigny* *Chair: Ricardo Lebensohn, Los Alamos National Laboratory, USA*	**N4** *R6 Volnay* *Chair: Matous Mrovec, ICAMS, Ruhr University Bochum, Germany*
	(invited) **Structural and mechanical inhomogeneities in cement paste** Katerina Ioannidou, MIT, USA	(invited) **Continuum modeling of heteroepitaxial growth in semiconductors** Francesco Montalenti, Università di Milano-Bicocca, Italy	(invited) **Universality of avalanche exponents in amorphous plasiticity** Zoe Budrikis, ISI Foundation, Italy	(invited) **Multiscale modelling of structure evolution in industrial materials** John Ågren, KTH, Sweden	(invited) **Recent progress in dislocation dynamics simulation and its contribution to crystal plasticity modeling** Benoit Devincre, LEM CNRS-ONERA, France	(invited) **From random-walk to stress-driven grain boundary motion in pure FCC metals** Christian Brandl, Karlsruhe Institute of Technology, Germany	(invited) **Computational design of nanoalloys using DFT calculations, genetic algorithms and machine learning** Tejs Vegge, Technical University of Denmark, Denmark	(invited) **Using FFT-based simulations to incorporate local twinning features into Polycrystal Plasticity modeling** Carlos Tome, Lawrence Berkeley National Laboratory, USA	(invited) **Thermodynamics of the Aubry superlubric-pinned transition in D=2 dimensions** Erio Tosatti, SISSA / ICTP / CNR-IOM Democritos, Italy
11:20	**Kinetic Monte Carlo simulations of nanoparticle precipitation: the early hydration rate of cement** Enrico Masoero, Newcastle University, UK	**Elementary mechanisms of shear-coupled grain boundary migration** Nicolas Combe, CEMES/CNRS UP 8011 and Univ Paul Sabatier, France	**Avalanche statistics when approaching (or leaving) the yielding transition of amorphous solids** Ezequiel Ferrero, Universite Grenoble Alpes, France	**Modelling microstructure evolution in metallic alloys: elasticity and plasticity** Yann Le Bouar, CNRS/ONERA, France	**The interaction strengths between slip systems revisited** Ronan Madec, CEA / DAM / DIF, France	**Atomistic shear deformation mechanisms of interfaces in TiAl** Rebecca Janisch, ICAMS Ruhr-Universitaet Bochum, Germany	**Modeling of complex metal alloys and nanoparticles via multiscale first-principles methods** Kari Laasonen, Aalto University, Finland	**Multiscale modeling of IN718 superalloy based on micropillar compression and computational homogenization** Javier Llorca, Polytechnic University of Madrid & IMDEA Materials Institute, Spain	**Thermal effects on nanoscale van der Waals adhesion and sliding** Mircea Rastei, IPCMS, France
11:40	**Linear pore size dependence of water diffusion in nanoconfinement as assessed by noninvasive relaxometry method** Dominique Petit, CNRS/Université de Montpellier, France	**Multiscale modelling of materials chemomechanics** James Kermode, University of Warwick, UK	**Role of inertia in the rheology of amorphous systems: a finite element based elasto plastic model** Kamran Karimi, University of Grenoble, France	**Optimize material parameters with 4D experiments and phase-field simulations** Jin Zhang, DTU, Denmark	**Plastic zone properties at a crack tip investigated with the Discrete-Continuous Model** Laurent Korzeczek, ONERA, France	**Modelling plastic deformation in interface dominated microstructures using a dislocation based continuum formulation** Markus Sudmanns, Karlsruhe Institute of Technology, Germany	**Structural optimization of Au-Co nanoalloys** Emanuele Panizon, University of Genoa Italy	**Lattice strain evolution during biaxial loading of 316L stainless steel cruciform samples using an FE-FFT approach** Manas Upadhyay, Paul Scherrer Institute, Switzerland	**Viscosity and diffusivity of hydrocarbon lubricants under tribological conditions** Kerstin Falk, Fraunhofer IWM, Germany
12:00	**Effect of the curing temperature on the C-S-H composition and density in a Class G cement paste** Sara Bahafid, Université Paris Est, France	**Uncertainty quantification across the DFT/MD scale boundary in sequential multiscale simulations** Peter Brommer, University of Warwick, UK	**Universality of slip avalanches in flowing granular matter** Dmitry Denisov, University of Amsterdam, Netherlands	**Effects of fcc/fcc grain boundaries on the formation of bcc phase in pure iron by molecular dynamics simulation** Xiaoqin Ou, Delft University of Technology, Netherlands	**Modeling the Bauschinger effect and cyclic hardening in single crystals from dislocation dynamics simulations** Sylvain Queyreau, LSPM CNRS - Univ. Paris XIII, France	**Effects of interfaces on deformation mechanisms and their optimization in TiAl intermetallic alloys** Dongsheng Xu, Institute of Metal Research - Chinese Academy of Sciences, China	**Modelling nanoalloy catalysts: From free to oxide-supported particles** Roy Johnston, University of Birmingham, UK	**Quaternion correlation for tracking crystal motions** Qiwei Shi, EDF R&D, France	**Theoretical modeling and experimental validation of film forming mechanisms under deceleration** Juliette Cayer-Barrioz, LTDS - CNRS - Ecole Centrale de Lyon, France

12:20 **Lunch**
Chambertin
Followed by coffee in Foyer Bar and Hall D'Accueil

13:50	**A5** *R8 Mercurey* *Chair: David Jauffres, SIMAP / University of Grenoble Alpes, France*	**C5** *R3 Santenay-Chablis* *Chair: Christoph Ortner, University of Warwick, UK*	**D5** *R4 Musigny* *Chair: Luca Cipelletti, L2C University Montpellier and CNRS, France*	**E5** *R2 Morey Saint Denis* *Chair: Maria Emelianenko, George Mason University, USA*	**G5** *R1 Amphi Romanée Conti* *Chair: Sylvain Queyreau, LSPM CNRS - Univ. Paris XIII, France*	**H1** *R6 Volnay* *Chair: Pär Olsson, KTH Royal Institute of Technology, Sweden*	**J3** *R5 Pommard* *Chair: Remi Dingreville, Sandia National Laboratories, USA*	**K4** *R10 Monthelie* *Chair: Roy Johnston, University of Birmingham, UK*	**M4** *R7 Givry+Savigny* *Chair: Stefan Sandfeld, University of Erlangen-Nürnberg, Germany*
	(invited) **3D image-based multiscale modeling of hierarchical porous electrodes: mechanical strength and effective conductivity** David Jauffres, SIMAP / University of Grenoble Alpes, France	(invited) **Large-scale real-space electronic structure calculations** Vikram Gavini, University of Michigan, USA	(invited) **Making a jammed emulsion flow: local rearrangements and correlated motion** Emanuela Del Gado, Georgetown University, USA	(invited) **The role of the mesoscale in grain boundary migration** Chris Race, University of Manchester, UK	(invited) **Large scale dislocation dynamics simulations of plasticity and point defect evolution in persistent slip bands** Jaafar El-Awady, Johns Hopkins University, USA	(invited) **Direct HRTEM Observation of the Clustering Process of Self-Interstitial Atoms in Iron** Kazuto Arakawa, Shimane University, Japan	(invited) **Atomistic study of mechanism transition of grain boundary motion and dislocation nucleation from grain boundary** Shigenobu Ogata, Osaka University, Japan	(invited) **Tight-binding strategy to model the energetics of magnetic alloys and nanoalloys** Christine Goyhenex, IPCMS, CNRS-Université de Strasbourg, France	(invited) **Coupling microstructure-sensitive modeling and in situ experiments to improve fatigue life predictions** Michael Sangid, Purdue University, USA
14:20	**Enhanced resilience of architected materials with hierarchical microstructures** Paolo Moretti, Friedrich-Alexander-University Erlangen-Nuremberg, Germany	**Automating diffusivity calculations for interstitial and solute diffusion from first-principles** Dallas Trinkle, University Illinois, Urbana-Champaign, USA	**Vibrational properties of amorphous materials, and application to nanocomposites** Anne Tanguy, INSA, France	**Linking design of materials and technological process parameters for tailored integration in Microelectronics field: climbing the scales** Anne Hemeryck, LAAS-CNRS, France	**Strain bursts and dislocation avalanches in irradiated micropillars** Nasr M Ghoniem, University of California, Los Angeles, USA	**Effect of irradiation on chromium precipitation in ferritic steels** Frederic Soisson, CEA Saclay, France	**Influence of hydrogen on grain boundary cohesion in nickel** Matous Mrovec, ICAMS, Ruhr University Bochum, Germany	**Molecular dynamics simulations of self-propagating reactions in Ni-Al multilayer nanofoils** Olivier Politano, Laboratoire ICB - Univ. Bourgogne, France	**Unravelling dislocation collective properties with dislocation dynamics simulations for continuous modeling** Vanessa Verbeke, CNRS - ONERA, France
14:40	**Massively parallel FFT-based simulations to analyze the behavior of architected SiC/SiC composite tubes from synchrotron X-ray tomography** Yang Chen, CEA - Saclay, France	**The flexibility of daubechies wavelets for electronic structure calculations** Thierry Deutsch, Univ. Grenoble Alpes / CEA / INAC, France	**Confinement effects on the correlations of plasticity** Fathollah Varnik, Ruhr-Universität Bochum, Germany	**Size-effects on grain growth by MD-simulations** Luis Barrales Mora, IMM, Germany	**DD simulations of interactions between gliding dislocations and radiation-induced loops in α-iron: bridging the atomic and the crystalline scales** Xiangjun Shi, Université Paris 13, France	**Numerical and experimental determination of the formation and properties of nanometric-sized helium-filled bubbles in semiconductors** Laurent Pizzagalli, Institut P' / CNRS, France	**Strength of interfaces with segregated impurities from first principles** Miroslav Cerny, Academy of Sciences of the Czech Republic, Czech Republic	**Nanoalloys as catalysts for fuel cell application: Multiscale simulation and experimental study** Daojian Cheng, Beijing University of Chemical Technology, China	**Analysis and data mining of discrete dislocation data with the D2C framework** Dominik Steinberger, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
15:00	**Generation, compaction and strength of nanostructured silica aggregates using the discrete element method** Étienne Guesnet, SIMAP / University of Grenoble Alpes, France	**Wavefunction in DFT embedding for Materials Design** Stuart Bogatko, Imperial College London, UK	**Rheology of weakly attractive systems: the role of energy dissipation** Ehsan Irani, University of Goettingen, Germany	**Influence of precipitation kinetics on static recrystallization during hot deformation of a 2xxx aluminium alloy** Evgeniya Kabliman, LKR Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria	**The effect of temperature and dislocation mobility on the attenuation of the dynamic yield point in shocks** Benat Gurrutxaga-Lerma, Imperial College London, UK	**Artificial Neural Network based cohesive model from ab initio: principles and applications to single point-defect migration in binary Fe-based alloys** Nicolas Castin, SCK-CEN, Belgium	**Hydrogen induced grain boundary decohesion in nickel extracted from molecular dynamics simulations** Douglas Spearot, University of Florida, USA	**Metallic nanoclusters on graphene/Ir(111): insights from ab-initio calculations and experiments** Maria Peressi, University of Trieste, Italy	(invited) **Dislocation transfer through twin-boundaries analyzed by x-ray µLaue diffraction** Christoph Kirchlechner, Max-Planck-Institute für Eisenforschung GmbH, Germany
15:20	**Assessing the fracture strength of geological and related materials via an atomistically based J-integral** Reese Jones, Sandia, USA	**Green's functions for seamless elastic boundaries in atomic-scale calculations** Lars Pastewka, Karlsruhe Institute of Technology, Germany	**From kinetics to rheology in inertial granular flows** Eric DeGiuli, Ecole Polytechnique Federale de Lausanne, Switzerland		**A discrete dislocation dynamics description of grain boundary sliding and its contribution to plastic deformation in polycrystalline materials** Siu Sin Quek, Institute of High Performance Computing Singapore, Singapore	**Modeling the pressure vessel steel microstructure evolution under neutron irradiation - input from ab initio calculations in Fe multi component alloys** Christophe Domain, EDF R&D, France	**Hydrogen segregation to grain boundaries in nickel** Remi Dingreville, Sandia National Laboratories, USA	**Instability of (100) facets in monolayer-thick core@shell nanoalloys: The emergence of pyritohedral and chiral symmetries** Riccardo Ferrando, University of Genoa, Italy	
15:40	**Coffee break** *Foyer Bar and Hall D'Accueil*								

16:10	**A6** *R8 Mercurey* *Chair: Emanuela Del Gado, Georgetown University, USA*	**C6** *R3 Santenay-Chablis* *Chair: Frederic Legoll, Ecole des Ponts and INRIA, France*	**D6** *R4 Musigny* *Chair: Alexandre Nicolas, CNRS & Univ. Paris-Sud, France*	**E6** *R2 Morey Saint Denis* *Chair: Tom Arsenlis, Lawrence Livermore, National University, USA*	**G6** *R1 Amphi Romanée Conti* *Chair: Steve Fitzgerald, University of Oxford, UK*	**H2** *R6 Volnay* *Chair: Kazuto Arakawa, Shimane University, Japan*	**J4** *R5 Pommard* *Chair: Douglas Medlin, Sandia National Laboratories, USA*	**L1** *R10 Monthelie* *Chair: Patrice Turchi, Lawrence Livermore National Laboratory, USA*	**M5** *R7 Givry+Savigny* *Chair: Ruth Schwaiger, KIT, Germany*
	(invited) **Role of mesoscale structure in the mechanical behavior of self-standing thin clay films** Matthieu Vandamme, Ecole des Ponts ParisTech, France	(invited) **A parallel implementation of the mixed multiscale finite element method for the simulation of two-phase flows in porous media** Guillaume Enchéry, IFPEN, France	(invited) **Microscopic dynamics and macroscopic rheology in a semi-crystalline polymer** Luca Cipelletti, L2C University Montpellier and CNRS, France	(invited) **Growth and ripening under mechanochemical coupling** Reza Darvishi Kamachali, ICAMS - Ruhr-Uni-Bochum, Germany	(invited) **Continuum dislocation modeling of wedge indentation** Giacomo Po, University of California, Los Angeles, USA	(invited) **Impurity flux coupling and anomalous swelling in iron** Pär Olsson, KTH Royal Institute of Technology, Sweden	(invited) **Effect of bi-phase interfaces on texture evolution in HCP/BCC nanolaminates fabricated by severe plastic deformation** Irene Beyerlein, University of California at Santa Barbara, USA	(invited) **Modelling and validation of rapidly solidified alloy structures** Hani Henein, University of Alberta, Canada	(invited) **Modelling plastic deformation in micro- and nano-samples using the Discrete-Continuum Model** Riccardo Gatti, LEM / UMR 104 CNRS-ONERA, France
16:40	**Small-angle scattering analysis of empty or loaded hierarchical porous materials** Cedric Gommes, University of Liege, Belgium	**Asymptotic Preserving numerical schemes for multiscale parabolic problems** Gilles Vilmart, University of Geneva, Switzerland	**Influence of deformation induced topological anisotropy on mechanical properties of Silica Glass: An atomistic study** Erik Bitzek, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany	**Ab initio study of the influence of hydrogen and iron on the nucleation of prismatic loops in Zr alloys submitted to irradiation** Benjamin Christiaen, Electricité de France (EDF), France		**Scaling laws for formation energy of large interstitial clusters in V, W and Fe from ab-intio simulations** Mihai-Cosmin Marinica, CEA, DEN, Service de Recherches de Metallurgie Physique, France	**Multi-scale simulation of mechanical properties of carbide-metal interfaces from first-principles calculations** Elric Barbé, CEA Saclay DEN/DMN/SRMP, France	**Combining numerical modeling and ultra-fast In-situ TEM for quantitative studies of rapid solidification microstructure evolution dynamics** Jorg Wiezorek, University of Pittsburgh, USA	**Incorporating the nudged elastic band method into dislocation dynamics to investigate thermally activated plastic events** Pierre-Antoine Geslin, Université Lyon 1-CNRS, France
17:00	**Combined experimental-modeling approach towards better predictions of fruit tissue dehydration** Kevin Prawiranto, ETH Zürich / Empa, Switzerland	**A generalized finite element method for linear thermoelasticity** Anna Persson, Chalmers University of Technology, Sweden	**Small-scale mechanical response and dynamical behaviour of a model amorphous silicon solid** Anne Tanguy, INSA, France	**Modelling recrystallization and massive α/γ transformation during intercritical heating of a Dual Phase steel** Mélanie Ollat, MATEIS INSA Lyon Lab, France	**Phase-field modeling of dislocations in face-centered cubic materials involving micropores** Antoine Ruffini, CNRS - ONERA, France	**DFT study on the contribution of phonon and electron excitations to the free energy of embedded defect clusters** Matthias Posselt, Helmholtz-Zentrum Dresden-Rossendorf, Germany	**Elastic-perfect plastic behavior in elongated Au-Si core-shell nanowires due to the confinement of the dislocations by a hard amorphous shell** Julien Godet, Pprime Institute University of Poitiers, France	**Solidification cracking during Selective Laser Melting of Inconel 738LC: origins and remedy** Eric Jaegle, Max-Planck-Institut fuer Eisenforschung, Germany	**Investigation of plasticity/fatigue mechanisms at interfaces in Ni using ex-situ and in-situ SEM/TEM micro/nano-mechanical testing** Vahid Samaeeaghmiyoni, University of Antwerp, Belgium
17:20	**Modeling the transport of water and ions tracers in a micrometric sample of clay** Pauline Bacle, PHENIX / Université Pierre et Marie Curie, France	**Exploiting local macroscopic quasi-homogeneities to accelerate multi-scale microstructure simulations** Md Khairullah, KU Leuven, Belgium	**Mapping between atomistic simulations and Eshelby inclusions in the shear deformation of amorphous Silicon** Francesca Boioli, University of Lyon1, France	**Phase field modeling of abnormal grain growth** Ying Liu, University of British Columbia, Canada	**Atomistic simulation of face-centered cubic metallic nanospheres under uniaxial compression** Selim Bel Haj Salah, Institut Pprime, France	**Anomalous vacancy-assisted chromium segregation in FeCr alloys** Mikhail Lavrentiev, Culham Centre for Fusion Energy, UK	**Multiscale modeling of heterophase interfaces between alpha zirconium and gamma-ZrH hydrides** Marc-Antoine Louchez, UMET, France	**Numerical investigation of the columnar-to-equiaxed transition using a 2D needle network model** Pierre-Antoine Geslin, Université Lyon 1-CNRS, France	**Modelling of internal stresses in deformation-induced dislocation microstructures and comparison with experimental data** Maxime Sauzay, CEA Saclay, France
17:40									**Flash posters M** *R7 Givry+Savigny*
18:10 - 20:00	**Exhibitor and poster session 2 - Wine & cheese party** *Grands Echézeaux Hall*								

Wednesday October 12th, 2016

08:30	**B1 + E7** *R2 Morey Saint Denis* *Chair: Christian Elsässer, Fraunhofer IWM, Germany*	**C7** *R3 Santenay-Chablis* *Chair: Mitchell Luskin, University of Minnesota, USA*	**D7** *R4 Musigny* *Chair: M. Carmen Miguel, University of Barcelona, Spain*	**G7** *R1 Amphi Romanée Conti* *Chair: Tom Arsenlis, Lawrence Livermore, National University, USA*	**H3** *R6 Volnay* *Chair: Maylise Nastar, CEA, France*	**I1** *R8 Mercurey* *Chair: Marcus Müller, Georg-August University, Germany*	**J5** *R5 Pommard* *Chair: Doug Spearot, University of Florida, UK*	**L2** *R10 Monthelie* *Chair: Markus Rettenmayr, Friedrich Schiller University Jena, OSIM, Germany*	**M6** *R7 Givry+Savigny* *Chair: Manas Upadhyay, Paul Scherrer Institute, Switzerland*
	(invited) **Strategies and algorithms for the automated parallel data mining of annealing microstructure evolution pathways** Markus Kühbach, RWTH Aachen University, Germany	(invited) **Error estimators for first-principle molecular simulation** Eric Cancès, CERMICS - Ecole des Ponts and INRIA, France	(invited) **Avalanche phenomena in a sheared granular layer coupled to soft elastic plates** Robert Ecke, Los Alamos National Laboratory, USA	(invited) **Continuum dislocation dynamics: From dislocation kinematics to work hardening** Michael Zaiser, FAU Universität Erlangen-Nürnberg, Germany	(invited) **MMM and the challenge of driven materials** Georges Martin	(invited) **Multi scale modeling of block polymers for applications in patterning** Juan de Pablo, University of Chicago, USA	(invited) **Chemo-thermo-mechanical framework for the prediction of stress evolution during metal oxidation** Amine Benzerga, Texas A&M University, USA	(invited) **Multiscale modeling of hot-tearing** Michel Rappaz, EPFL, Switzerland	(invited) **Predictive Metallurgy: from Quantum to Continuum** William A Curtin, École Polytechnique Fédérale de Lausanne, Switzerland
09:00	**Coupled microstructural and mechanical models for non-isothermal treatments of a 6061 aluminum alloy** Daniel Nelias, INSA Lyon, France	**Foundations of kinetic Monte Carlo models and the accelerated dynamics techniques** Tony Lelievre, Ecole des Ponts ParisTech, France	**Yielding and flow properties of vibrated granular media** Olivier Dauchot, UMR Gulliver / CNRS / ESPCI, France	**Modeling the creep properties of olivine in the lithospheric mantle from dislocation dynamics models** Karine Gouriet, Unité Matériaux et Transformations / CNRS UMR 8207, France	**Segregation and precipitation on defect clusters: A phase field approach** Pascal Bellon, University of Illinois, USA	**Molecular mechanisms of plastic deformation in sphere-forming thermoplastic elastomers** Joerg Rottler, University of British Columbia, Canada	**Phase field modelling of growth and failure of oxide intrusions along grain boundaries** Victor de Rancourt, CEA, France	**Upscaling from mesoscopic to macroscopic solidification models by volume averaging** Miha Založnik, Institut Jean Lamour, France	**Flaw insensitivity of defect-scarce nanowires: Atomistic simulations and experiments** Christian Brandl, Karlsruhe Institute of Technology, Germany
09:20	**Revealing the mechanism of Z phase-formation in 12% Cr ferritic-martensitic steels** Daniel Urban, Fraunhofer IWM, Germany	**Stochastic processes and diffusive molecular dynamics** Gideon Simpson, Drexel University, USA	**Mechanical instabilities in granular media induced by non-linear acoustic waves** Julien Leopoldes, ESPCI, France	**An accurate and efficient elastic force computation for discrete dislocations in anistropic polycrystals** Tom Arsenlis, Lawrence Livermore National University, USA	**Coupling radiation damage from binary collision Monte Carlo to phase field microstructure evolution** Daniel Schwen, Idaho National Laboratory, USA	**Modelling polymer deformation during 3D printing** Claire McIlroy, Georgetown University, USA	**Material parameter identification by using atomistic-to-continuum homogenization for thermo-mechanically coupled problems** Christian Sievers, TU Dortmund, Germany	**Multiscale modeling of dendritic microstructure** Charles-Andre Gandin, MINES ParisTech CEMEF UMR CNRS 7635, France	**MgO nanoparticle deformation at room temperature: insights from MD simulations and in situ TEM** Jonathan Amodeo, INSA-Lyon, France
09:40	**Mesoscale model of stacked organic light emitting diodes** Alison Walker, University of Bath, UK	**Assessment of phase-field-crystal concepts using long-time molecular dynamics** William A Curtin, École Polytechnique Fédérale de Lausanne, Switzerland	**Suppression of the threshold of a granular solid by mechanical fluctuations** Axelle Amon, Université Rennes 1, France	**Atomistically based discrete dislocation dynamics simulations of plastic deformation in Magnesium** Jaafar El-Awady, Johns Hopkins University, USA	**Design of radiation-resistant alloys** Thomas Schuler, University of Illinois Urbana-Champaign, USA	**Bridging the gap between molecular and macroscopic models of the mechanics and dynamics of anisotropic fluids** Patrick Ilg, University of Reading, UK	**A thermodynamically consistent diffuse interface crystal plasticity model to study grain growth during dynamic recrystallization** Nikhil Chandra Admal, University of California Los Angeles, USA	**Mesoscopic envelope model and phase field simulations of columnar and equiaxed dendritic growth** Alexandre Viardin, ACCESS e.V., Germany	**Multiscale description of the formation of spatially self-confined quasi-one-dimensional nano-phases around dislocations** Gerard Paul Leyson, Max-Planck-Institut fur Eisenforschung, Germany
10:00	**Gathering materials properties from literature for the design of new materials** Lothar Kunz, Robert Bosch GmbH, Germany	**Predicting solute segregation kinetics and properties in binary alloys from a dynamical variational gaussian model** Chad Sinclair, University of British Columbia, Canada	**Shear cessation in Brownian-dynamics simulation for 2D hard disks** Sebastian Fritschi, University of Konstanz, Germany	**Parametric model of double cross-slip treated by mathematical theory of evolving curves** Miroslav Kolář, FJFI CVUT v Praze, Czech Republic	**Modeling of radiation-induced precipitation in an under-saturated solute solution** Duc Nguyen-Manh, Culham Centre for Fusion Energy, UK	**Coarse-grained molecular dynamics simulation of amorphous polymers under multiaxial loading** Yoshitaka Umeno, University of Tokyo, Japan	**Collective influence of texture, grain shape, size and dislocation density on the plasticity of polycrystalline metallic thin films** Hareesh Tummala, INP Grenoble and UCL, Belgium	**Multi-scale modeling of dendritic solidification and the effect of convection on microstructure selection in alloys** Damien Tourret, Los Alamos National Laboratory, USA	**Solute interaction with the bcc-fcc interface in iron** Matthias Militzer, University of British Columbia, Canada
10:20	**Coffee break** *Foyer Bar and Hall D'Accueil*								
Plenary session 3 *R1 Amphi Romanée Conti* *Chair: Anter El-Azab, Purdue University, USA*									
10:50	(plenary) **Data-driven materials research: Novel routes to new insight and predictions** Claudia Draxl, Humboldt University, Germany								
11:40	(plenary) **Computational Mechanics Approaches for Addressing the Integrated Computational Materials Engineering (ICME) Initiative** Somnath Ghosh, Johns Hopkins University, USA								
12:30	**Presentation of poster prizes (poster session 2)**								
12:40	**Lunch** *Chambertin* *Followed by coffee in Foyer Bar and Hall D'Accueil*								
14:00 - 19:00	**Excursions to Beaune or Dijon** ***(pre-booked participants only)***								

Plenary session 4
R1 Amphi Romanée Conti
Chair: Erik Van der Giessen, Zernike Institute for Advanced Materials, Netherlands

08:30 (plenary) **Crystallography in Curved Space - the Interplay of Crystalline Order, Geometry and Topology**
Axel Voigt, Technische Universität Dresden, Germany

09:20 (plenary) **A new simulator for real-scale dislocation plasticity based on dynamics of dislocation-density functions**
Alfonso H W Ngan, University of Hong Kong, Hong Kong

10:10 **Results of the Image Art Competition**

10:20 **Coffee break**
Foyer Bar and Hall D'Accueil

	B2 *R9 Saint Romain* *Chair: Jörg Neugebauer, Max-Planck-Institut für Eisenforschung GmbH, Germany and Daniel Urban, Fraunhofer IWM, Germany*	**C8** *R3 Santenay-Chablis* *Chair: Frederic Legoll, Ecole des Ponts and INRIA, France*	**D8** *R4 Musigny* *Chair: Damien Vandembroucq, CNRS/ESPCI Paris, France*	**E8** *R2 Morey Saint Denis* *Chair: Luis Barrales-Mora, Institute of Physical Metallurgy and Metal Physics, Germany*	**G8** *R1 Amphi Romanée Conti* *Chair: Javier Gil Sevillano, University of Navarra, Spain*	**H4** *R6 Volnay* *Chair: Blas Uberuaga, Los Alamos National Laboratory, USA*	**I2** *R8 Mercurey* *Chair: Jay Schieber, Illinois Institute of Technology, USA*	**J6** *R5 Pommard* *Chair: Timothy Germann, Los Alamos National Laboratory, USA*	**M7** *R7 Givry+Savigny* *Chair: Chad Sinclair, University of British Columbia, Canada*
10:50	(invited) **Harnessing electronic structure for engineering alloy design through big data** Krishna Rajan, University at Buffalo-the State University of New York, USA	(invited) **Multiscale computations with MsFEM: a posteriori error estimation, adaptive strategy, and coupling with PGD model reduction** Ludovic Chamoin, ENS Cachan - INRIA, France	(invited) **Cooperative phenomena in the mechanical behavior of filamentous materials with molecular motors** M. Carmen Miguel, University of Barcelona, Spain	(invited) **Multiscale modeling of the recrystallization** Marc Bernacki, Mines ParisTech, France	(invited) **Solid solution hardening in Fe-X alloys (X = Si, Ni, Al, Cr)** Daniel Caillard, CEMES-CNRS, France	(invited) **Multiscale modeling of the influence of semi-coherent interfaces on point defect concentrations and point defect clustering** Thomas Jourdan, CEA Saclay, France	(invited) **Simulating mechanical properties of nanostructured polymers with coarse grained models** Jean-Louis Barrat, Université Grenoble Alpes, France	(invited) **Large scale atomistic simulations of the interaction of single arm sources with grain boundaries in FCC bipillars** Satish Rao, EPFL, Switzerland	(invited) **Analysis of experimental grain scale data in a crystal plasticity framework** Grethe Winther, Technical University of Denmark, Denmark
11:20	**High-Throughput approach for the discovery of novel hardmagnetic phases** Georg Krugel, Fraunhofer IWM, Germany	**Localized adaptive model reduction for multi-scale problems** Felix Schindler, University of Muenster, Germany	**Delocalized plastic flow in proton-irradiated monolithic metallic glasses** Seunghwa Ryu, KAIST, South Korea	**Simulation of sub-grain growth utilizing a computationally efficient level-set model** Christian Mießen, RWTH Aachen University, Germany	**Cross-slip in FCC solid solutions** Wolfram Nöhring, École Polytechnique Fédérale de Lausanne, Switzerland	**Modeling of one-dimensional migration of interstitial clusters and their growth behavior in alpha-iron under electron irradiation** Yosuke Abe, Japan Atomic Energy Agency, Japan	**Effect of network structure on fracture process of double-network gels by coarse-grained molecular dynamics simulation** Keisuke Saito, Tohoku University, Japan	**Critical intergranular porosity for a transition from intrinsinc ductility to brittleness** Döme Tanguy, CNRS-Lyon1, France	**Investigation of nonmetallic inclusion-driven failures** Diwakar Naragani, Purdue University, USA
11:40	**Interstitial solution enthalpies derived from first-principles: Knowledge discovery using high-throughput databases** Tilmann Hickel, Max-Planck-Institut für Eisenforschung GmbH, Germany	**Numerical upscaling by a localized orthogonal decomposition** Patrick Henning, KTH Royal Institute of Technology, Sweden	**Combining continuum mechanics with microscopic descriptions of nonlinear glassy rheology: Hybrid-lattice Boltzmann simulations** Thomas Voigtmann, German Aerospace Center, Germany	**Investigation of nanoscale field emitters on copper surfaces under high electric field** Vahur Zadin, University of Tartu, Estonia	**A unified model for solid solution strengthening in high-entropy BCC alloys** Francesco Maresca, École Polytechnique Fédérale de Lausanne, Switzerland	**Point defects in materials: measurement of elastic dipoles and polarisability effects** Celine Varvenne, CNRS - CINaM, France	**Inter-particle forces beyond the classical DLVO theory** Christophe Labbez, ICB UMR 6303 CNRS, France	**Atomic scale study of twinning in Zirconium** Olivier Mackain, CEA, France	**Towards an experimentally informed multiscale model of FIB-induced irradiation damage** Julien Guénolé, FAU Erlangen-Nürnberg, Germany
12:00	**Three-parameter crystal-structure prediction for sp-d valent compounds** Thomas Hammerschmidt, ICAMS / Ruhr-Universität Bochum, Germany	**An embedded corrector problem for stochastic homogenization** Virginie Ehrlacher, CERMICS - Ecole des Ponts Paristech & INRIA, France	**Fragility in shear-jammed suspensions** Romain Mari, University of Cambridge, UK	**Comparison of dislocation-based model of recovery and cross-correlation based EBSD measurements in single crystals** Szilvia Kalácska, Eötvös Loránd University (ELTE), Hungary	**Dislocation multiplication and cross-slip in continuum dislocation dynamics** Thomas Hochrainer, Universität Bremen, Germany	**Absorption rates for cluster-dynamics modelling of mixed 1D-3D mobile species** Gilles Adjanor, EDF R&D, France	**Continuous-discontinuous long fiber-reinforced polymer structures: Modeling, characterization and validation** Kay André Weidenmann, Karlsruhe Institute of Technology, Germany	**The role of interfaces in nucleation of dynamic damage in FCC and BCC materials** Tim Germann, Los Alamos National Laboratory, USA	**Combined molecular dynamics/experimental study of the strength of Cu|Au multilayer nanopillar systems** Adrien Gola, KIT / IAM-CMS, Germany

12:20 **Lunch**
Chambertin
Followed by coffee in Foyer Bar and Hall D'Accueil

	B3 *R9 Saint Romain* *Chair: Isao Tanaka, Kyoto University, Japan and Lothar Kunz, Robert Bosch GmbH, Germany*	C9 *R3 Santenay-Chablis* *Chair: William Curtin, École Polytechnique Fédérale de Lausanne, Switzerland*	E9 *R2 Morey Saint Denis* *Chair: Anter El-Azab, Purdue University, USA*	G9 *R1 Amphi Romanée Conti* *Chair: Thomas Hochrainer, Universität Bremen, Germany*	H5 *R6 Volnay* *Chair: Mira Todorova, Max-Planck-Institut fuer Eisenforschung, Germany*	I3 *R8 Mercurey* *Chair: Mikko Kartunnen, Eindhoven University of Technology, Netherlands*	J7 *R4 Musigny + R5 Pommard* *Chair: Remi Dingreville, Sandia National Laboratories, USA*	L3 *R10 Monthelie* *Chair: Aurelien Perron, Lawrence Livermore National Laboratory, USA*	N5 *R7 Givry+Savigny* *Chair: Julien Fontaine, Ecole Centrale de Lyon, France*
13:50	(invited) **First-principles materials exploration of piezoelectrics** Tamio Oguchi, Osaka University, Japan	(invited) **Speculatively parallel temperature accelerated dynamics** Arthur Voter, Los Alamos National Laboratory, USA	(invited) **Plasticity at the microscale: a discrete dislocation dynamics study of the role of interfaces and strain gradients on the effective plastic slip distribution** Daniel Weygand, Karlsruhe Institute of Technology, Germany	(invited) **Crystal Plasticity simulations of the mechanical behavior of Mg alloys** Javier Segurado, Polytechnic University of Madrid, Spain	(invited) **Mesoscale modeling of laser-induced crystallization of amorphous Ge** Jaime Marian, University of California Los Angeles, USA	(invited) **Multiscale modelling approach to the rheological behaviour of polymer nanocomposites: Nonequilibrium thermodynamics modeling coupled with NEMD simulations** Pavlos Stephanou, ETH Zurich, Switzerland	(invited) **Boundary layer formation in continuum dislocation dynamics** Philip Eisenlohr, Michigan State University, USA	(invited) **Crystal-melt interfacial fields: Determinism in pattern dynamics** Martin Glicksman, Florida Institute of Technology, USA	(invited) **Friction is Fracture: Classical shear cracks drive the onset of frictional motion** Jay Fineberg, Hebrew University of Jerusalem, Israel
14:20	**Synthetic screening of electrolytes for Li-Air batteries** Reese Jones, Sandia, USA	**Coupled atomistic/discrete-dislocation method in 3d** Max Hodapp, Ecole Polytechnique Fédérale de Lausanne, Switzerland	**A crystal plasticity formulation for HCP metals informed by dislocation dynamics** Nathan Barton, Lawrence Livermore National Laboratory, USA	**Intrinsic scale effects in the deformation of structural materials** Christopher Woodward, Air Force Research Laboartory, USA	**Alloying effects on the formation of C15 interstitial clusters in iron** Luca Messina, CEA, DEN, Service de Recherches de Métallurgie Physique, France	**Simulation of viscoelastic flows via Smoothed Particle Hydrodynamics combined with the Discrete Slip-Link Model** Jay D Schieber, Illinois Institute of Technology, USA	**Interface controlled devitrification kinetics in a binary Fe-C glass** Chad Sinclair, University of British Columbia, Canada	**Simulating rapid solidification by a self-consistent sharp-interface model** Klemens Reuther, Friedrich Schiller University Jena, Germany	**Molecular modeling of liquid/solid friction for nanofluidic applications** Laurent Joly, Institut Lumière Matière, Université Lyon 1, France
14:40	**Tight-binding quantum chemical molecular dynamics simulation on chemical reaction between organic carbonate and Li anode in Li-air battery** Keita Watanabe, Tohoku University, Japan	**Using embedding into a polarizable solid to study defects in insulators** David Gao, University College London, UK	**Dislocation multiplication by glissile junction formation in discrete dislocation dynamics and crystal plasticity** Markus Stricker, KIT-IAM Karlsruhe Institute of Technology - Institute for Applied Materials, Germany	**A multi-scale model of dislocation creep in MgSiO3 perovskite** Philippe Carrez, University of Lille 1, France	**Multiscale study of plasma induced trapping of hydrogen isotopes in tungsten** Petr Grigorev, SCK-CEN, Belgium	**Multiscale modelling of buckling in thin polymer films and characterization by molecular dynamics** Fabrice Detrez, Université Paris Est, Laboratoire MSME, France	**From atomistic simulations towards a mesoscale representation of the absorption of dislocations in grain boundaries** Julien Guénolé, FAU Erlangen-Nürnberg, Germany	**Crystallographic effects on lamellar eutectic growth patterns** Silvere Akamatsu, CNRS - UPMC, France	**Contact mechanics of polymer composites; a decoupled multi-level approach** Lambert van Breemen, Eindhoven University of Technology, Netherlands
15:00	**Investigating the relation of molecular conductance and structure for thousands of junction geometries** Hector Vazquez, Czech Academy of Sciences, Czech Republic	**A study of conditions for dislocation nucleation in coarser-than-atomistic scale models** Akanksha Garg, FM Global, USA	**Predictions on the influence of microstructure variations on property scatter in additive manufacturing** Chinnapat Panwisawas, University of Birmingham, UK	**The role of climb in the plastic deformation of Earth's materials: recovery process and viable strain producing mechanism** Francesca Boioli, Institut Lumière Matière, University of Lyon1, France	**Shock induced phase transition in polycrystalline iron** Nina Gunkelmann, Friedrich-Alexander-University Erlangen-Nürnberg, Germany	**Minimalist two-scale model for the viscoelastic behavior of elastomers filled with hard nano-particles** Markus Hütter, Eindhoven University of Technology, Netherlands		**Theoretical and numerical study of eutectic growth kinetics of NiZr-NiZr2 alloy at low undercoolings** Sumanth Nani Enugala, IAM-CMS, Karlsruhe Institute of Technology, Germany	**Towards a full picture of a lubricant behavior under severe conditions** Laetitia Martinie, INSAVALOR, France
15:20	**Atomic-Green's-Function approach to phonon scattering by extended defects in silicon** Tao Wang, Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Germany	**Using Zwanzig's technique to investigate stochastic defect motion over small and large barriers** Thomas Swinburne, Culham Centre For Fusion Energy, UK	**Rafting of single crystal Ni-based superalloys: results from a coupled phase-field and continuum dislocation dynamics model including climb** Ronghai Wu, University of Erlangen-Nuremberg, Germany	**Unraveling the temperature dependence of the yield strength of tungsten single crystals using atomistically-informed crystal plasticity** Jaime Marian, University of California Los Angeles, USA	**Modeling of out-of-local equilibrium flux couplings in dilute aluminum alloys** Maylise Nastar, CEA, France			**Transition path sampling simulations of nucleation during solidification in nickel** Grisell Diaz Leines Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr University Bochum, Germany	**Capturing the small and large scales effect when modelling mixed lubrication** Noel Brunetiere, Institut Pprime - CNRS, France
15:40	**Coffee break** *Foyer Bar and Hall D'Accueil*								

16:10	**B4** *R9 Saint Romain* *Chair: Alison Walker, University of Bath, UK and Tilmann Hickel, Max-Planck-Institut für Eisenforschung GmbH, Germany*	**C10** *R3 Santenay-Chablis* *Chair: Alexei Lozinski, Laboratoire de Mathématiques de Besançon, France*	**E10** *R2 Morey Saint Denis* *Chair: Daniel Weygand, Karlsruhe Institute of Technology, Germany*	**G10** *R1 Amphi Romanée Conti* *Chair: Javier Segurado Escudero, Polytechnic University of Madrid, Spain*	**H6** *R6 Volnay* *Chair: Thomas Jourdan, CEA Saclay, France*	**I4** *R8 Mercurey* *Chair: Lambèrt van Breemen, Eindhoven University of Technology, Netherlands*	**J8** *R4 Musigny + R5 Pommard* *Chair: Ricardo A Lebensohn, Los Almos National Laboratory, USA*	**L4** *R10 Monthelie* *Chair: Patrice Turchi, Lawrence Livermore National Laboratory, USA*	**N6** *R7 Givry+Savigny* *Chair: Guiseppe Carbone, Politecnico di Bari, Italy*
	(invited) **Optimization of nanostructured materials for thermoelectric and electrothermal applications** Ali Shakouri, Purdue University, USA	(invited) **Adaptive GMsFEM and its applications** Eric Chung, The Chinese University of Hong Kong, Hong Kong	(invited) **Computational modeling of dislocations microstructure in deformed crystals and comparison with 3D X-ray microscopy** Anter El-Azab, Purdue University, USA	(invited) **Elasto-plastic behaviour of nanostructured bcc iron columnar structures** Javier Gil Sevillano, University of Navarra, Spain	(invited) **Formation and dissolution of protective oxide layers in a wet electrochemical environment** Mira Todorova, Max-Planck-Institut fuer Eisenforschung, Germany	(invited) **Micromechanics of semicrystalline polymers: towards quantitative predictions** Hans van Dommelen, Eindhoven University of Technology, Netherlands	(invited) **Continuous modeling of grain boundary structure in a field theory of dislocations and generalized disclinations** Claude Fressengeas, LEM3 CNRS, France	(invited) **Solidification in 4D: from Dendrites to Eutectics** Peter Voorhees, Northwestern University, USA	(invited) **An adhesive wear map for rough surfaces in dry sliding contact** Jean-Francois Molinari, EPFL, Switzerland
16:40	**Ab-initio modeling of thermal transport beyond the single crystal: effects of size, defects, dimensionality, and soft modes** Natalio Mingo, CEA-Grenoble, France	**Analysis and numerical simulation of patterns in incommensurate 2D layered materials** Paul Cazeaux, University of Minnesota, USA	**Multiple-slip continuum dislocation dynamics simulation of dislocation evolution in micro-beams** Alireza Ebrahimi, Universität Bremen, Germany	**Heterogeneous deformation in ductile FCC single crystals in biaxial stretching: the influence of slip system interactions** Jean-Lin Dequiedt, CEA, DAM, DIF, France	**Hydrogen influence on diffusion in nickel from first-principles calculations** Döme Tanguy, CNRS-Lyon1, France	**Tensile deformation of amorphous and semicrystalline polymers** Sara Jabbari-Farouji, University of Mainz, Germany	**A FFT based-method for continuum dislocation and generalized disclination mechanics** Stephane Berbenni, CNRS, LEM3 UMR 7239, France	**Critical role of crystal orientation in the large-scale long-time spatiotemporal evolution of array patterns in directional solidification** Alain Karma, Northeastern University, USA	**Simulation of dry friction and wear at mesoscale using a multibody approach** Guilhem Mollon, INSA Lyon, France
17:00	**Thermoelectric properties of half-Heusler heterostructures from first-principles calculations** Peter Kratzer, University Duisburg-Essen, Germany	**Multiscale Finite Element type approaches for convection-dominated problems in heterogeneous media** Frédéric Legoll, Ecole des Ponts and INRIA, France	**Impact of atomic scale segregation effects on microstructural evolution in binary magnesium-rare earth alloys** Christian Mießen, RWTH Aachen University, Germany	**Multiscale investigation of strain aging phenomena of pure alpha titanium** Arina Marchenko, EDF R&D, France	**Field modified diffusion in a hexagonal cell structure** Markus Tautschnig, Imperial College London, UK	**Polymer mechanical spectroscopy using coarse-grained molecular dynamics** Morgane Mahaud, Mateis, France	**Role of lattice curvatures on mechanical response of nanocrystalline materials using a couple stress elasto-viscoplastic fast Fourier transform framework** Manas Upadhyay, Paul Scherrer Institute, Switzerland	**Phase-field simulations and geometrical analysis of cellular solidification fronts** Mathis Plapp, CNRS/Ecole Polytechnique, France	**Thermostatting effects on microstructure evolution and material removal during grinding of a polycrystalline Fe surface - A molecular dynamics analysis** Stefan J Eder, AC2T Research GmbH, Austria
17:20	**Ab initio calculations of the lattice thermal conductivity and the discovery of new thermoelectric materials** Laurent Chaput, Université de Lorraine, France	**Long-range electrostatic energies and forces for fragmentation methods** Frederik Heber, Universität des Saarlandes, Germany	**Multiscale modeling of a-boron and boron carbide** Pavel Pokatashkin, Dukhov Research Institute of Automatics, Russia	**Atomistically-informed crystal plasticity in MgO polycrystals under pressure** Jonathan Amodeo, MATEIS Laboratory, INSA-Lyon, France	**Multiscale thermo-chemo-magneto-mechanical modeling of polycrystalline magnetic shape memory alloys** Olivier Hubert, LMT-Cachan, France		**Grain boundaries in Field Dislocation Mechanics: a thermodynamic formulation for the tangeantial continuity condition of distortion at the interface** Laurent Capolungo, MST-8, Los Alamos National Laboratory, USA	**Mushy zone solidification and Temperature Gradient Zone Melting** Guillaume Boussinot, ACCESS, Germany	**Lattice defects evolving in subsurface zones during grinding processes of polycrystalline ferritic iron** Ulrike Cihak-Bayr, AC2T Research GmbH, Austria
17:40	**Calculating thermal conductivity using the quasi-harmonic approximation** Georg Madsen, Ruhr-Universität Bochum, Germany	**From atoms to models of aging in metal tritides** Peter Schultz, Sandia National Laboratories, USA	**Microstructure formation during alloying reactions in nanofoils** Vladyslav Turlo, Universite de Bourgogne, France	**Dislocation based modeling for nuclear ceramics viscoplastic behavior** Luc Portelette, CEA, France			**Effects of interfaces and grain-to-grain interactions on shear banding in Al-Cu-Li rolled sheets** Vincent Taupin, LEM3, France	**Coupling CALPHAD to phase-field modeling for prediction of microstructure evolution during solidification** Aurelien Perron, Lawrence Livermore National Laboratory, USA	**Effect of the metallic counterface material on tribochemical wear of DLC coatings** Julien Fontaine, Laboratoire de Tribologie et Dynamique des Systèmes, France
18:00	**Break**								
19:00 - 23:00	**Conference dinner** ***(pre-booked participants only)*** *Château de Marsannay*								

Friday October 14th, 2016

	B5	C11	E11	G11	H7	I5	J9	N7	
08:30	*R9 Saint Romain* *Chair: Thomas Eckl, Robert Bosch GmbH, Germany and Christian Elsässer, Fraunhofer IWM, Germany*	*R3 Santenay-Chablis* *Chair: Frederic Legoll, Ecole des Ponts and INRIA, France*	*R2 Morey Saint Denis* *Chair: Franz Roters, MPI für Eisenforschung, Germany*	*R1 Amphi Romanée Conti* *Chair: Akiyoshi Nomoto, Central Research Institute of Electric Power Industry, Japan*	*R6 Volnay* *Chair: Jaime Marian, University of California Los Angeles, USA*	*R8 Mercurey* *Chair: Markus Hütter, Eindhoven University of Technology, Netherlands*	*R4 Musigny + R5 Pommard* *Chair: Stéphane Berbenni, Université de Lorraine, France*	*R7 Givry+Savigny* *Chair: Laetitia Martinie, INSAVALOR, France*	
	(invited) **Intermediate models for bridging from high-throughput data to materials properties** Ralf Drautz, ICAMS, Germany	(invited) **Reversal-time scaling in low-damping ferromagnetic models** Katie Newhall, UNC Chapel Hill, USA	(invited) **Multiscale modelling of microstructure evolution in polycrystalline materials: physical and numerical challenges** Ricardo Lebensohn, Los Alamos National Laboratory, USA	(invited) **Time evolution of the velocity distribution of dislocations** Istvan Groma, Eötvös University, Hungary	(invited) **Correlating disordering energetics and amorphization resistance in complex oxides** Blas Uberuaga, Los Alamos National Laboratory, USA	(invited) **Fluid flow and percolation in elastic contacts** Martin Müser, Saarland University, Germany	(invited) **Grain boundary plane structure-property relationships and fundamental zones** Eric Homer, Brigham Young University, USA	(invited) **The impact of coulombic interactions among polar molecules and metal substrates on lubrication properties** Konstantinos Gkagkas, Toyota Motor Europe NV/SA, Belgium	
09:00	**Combining the many-body GW and bethe-salpeter formalisms with polarizable continuum or discrete models** Xavier Blase, Institut Néel / CNRS, France	**Ab initio trained neural-network driven kinetic Monte Carlo simulations of microstructure evolution of irradiated iron alloys** Luca Messina, CEA, DEN, Service de Recherches de Métallurgie Physique, France		**Mesoscale Theory of Dislocations: from the discrete to the continuum** Alphonse Finel, LEM (ONERA/CNRS), France	**Microstructural evolution of graphite under irradiation: large scale molecular dynamics simulations** Alain Chartier, CEA, France	**Multiscale phenomena in filament networks: What is common with buckypaper and cell division** Mikko Karttunen, Eindhoven University of Technology, Netherlands	**Continuous modeling of a grain boundary in MgO and its disclination induced grain-boundary migration mechanism** Xiaoyu Sun, Université Lille 1, France	**Understanding the tribological behavior of industrial additives in ACH/ACH systems using Tight-Biding Quantum Chemicamethod** Estelle Deguillard, Total, Japan	
09:20	**Materials design of a room-temperature maser** Stuart Bogatko, Imperial College London, UK	**Stochastic approach to cluster dynamics method** Pierre Terrier, Université Paris-Est, CERMICS (ENPC) & CEA, DEN/SRMP, France	**Heterogeneous deformation in nickel-based superalloys** Hector Basoalto, University of Birmingham, UK	**The role of weakest links and system size scaling in multiscale modeling of stochastic plasticity** Péter Dusán Ispánovity, Eötvös University, Hungary	**Large scale simulations of monazite-type ceramic nuclear waste forms** Yaqi Ji, Forschungszentrum Juelich, Germany	**Chemo-mechanical coupling in shape memory polymers: Theory versus experiment** Fathollah Varnik, Ruhr-Universität Bochum, Germany	**Investigating the interplay between grain boundary facet junctions and interfacial dislocations** Douglas Medlin, Sandia National Laboratories, USA	**Effect of graft density on the wear of polymer brush by coarse-grained molecular dynamics simulation** Ryo Takakuwa, Tohoku University, Japan	
09:40	**Molecular origin of the charge carrier mobility in small molecule organic semiconductors** Pascal Friederich, Karlsruhe Institute of Technology, Germany	**A numerical study of non-linear polycrystalline materials through a homogenization technique** Thiago Schlittler, Laboratoire MSSMat - CentraleSupelec, France	**A spectral method to solve multi-physics coupled elasto-viscoplastic boundary value problems** Pratheek Shanthraj, Max Planck Institut für Eisenforschung, Germany	**Investigation of creep and load shedding in polycrystalline titanium alloys using discrete dislocation plasticity** Zebang Zheng, Imperial College London, UK	**Multi-scale simulation of the experimental response of ion-irradiated zirconium carbide: role of the diffusion driven clustering of interstitials** Jean-Paul Crocombette, CEA Saclay, France	**A FFT-based numerical homogenization tool for the study of the thermal expansion of a TATB-based pressed explosive** Jean-Baptiste Gasnier, MINES ParisTech, France	**Connecting radiation damage evolution and grain boundary structure** Blas Uberuaga, Los Alamos National Laboratory, USA	**Ionic liquids as lubricants: a multi-parameter and multi-scale puzzle** Nicolas Voeltzel, LaMCoS - INSA Lyon, France	
10:00	**Coffee break** *Foyer Bar and Hall D'Accueil*								

Plenary session 5
R1 Amphi Romanée Conti
Chair: Carmen Miguel, University of Barcelona, Spain

10:30	(plenary) **Size effects in fracture and plasticity** Stefano Zapperi, University of Milan, Italy
11:20	(plenary) **Programming shape** L Mahadevan, Harvard University, USA
12:10	**Closing remarks** François Willaime, CEA, France
12:20	**Lunch** ***(pre-booked participants only)*** *Chambertin* *Followed by coffee in Foyer Bar and Hall D'Accueil*
14:00	End of conference