

	Room 1	Room 2	Room 3	Room 4	Room 5	Room 6	Room 7	Room 8	Room 9	Room 10	
08:00	Registration					Registration					08:00
10:00	Opening (Room 1)					Opening (Room 1)					10:00
10:10	<i>Plenary</i> (Room 1, <i>Chair</i> : Ju Li, MIT, USA) Amorphous materials on the meso-scale: achieving experimental length and timescales Christopher A. Schuh , Department of Materials Science and Engineering, MIT, USA					<i>Plenary</i> (Room 1, <i>Chair</i> : Ju Li, MIT, USA) Amorphous materials on the meso-scale: achieving experimental length and timescales Christopher A. Schuh , Department of Materials Science and Engineering, MIT, USA					10:10
11:00	<i>Plenary</i> (Room 1, <i>Chair</i> : Alexey Lyulin, Technische Universiteit Eindhoven, The Netherlands) Multiscale modeling and realization of photo-responsive polymers Maenghyo Cho , School of Mechanical and Aerospace Engineering, Seoul National University, Korea					<i>Plenary</i> (Room 1, <i>Chair</i> : Alexey Lyulin, Technische Universiteit Eindhoven, The Netherlands) Multiscale modeling and realization of photo-responsive polymers Maenghyo Cho , School of Mechanical and Aerospace Engineering, Seoul National University, Korea					11:00
11:50	Lunch					Lunch					11:50
	Symposium C-1 <i>Chair</i> : Emmanuel Clouet , CEA Saclay, SRMP, France	Symposium E-1 <i>Chairs</i> : William A. Curtin , LAMMM, EPFL, Switzerland, Liang Qi , University of Michigan, United States of America	Symposium F-1 <i>Chair</i> : Yunzhi Wang , The Ohio State University, United States of America	Symposium M-1 <i>Chair</i> : Thomas Voigtmann , German Aerospace Center, Cologne, Germany	Symposium O-1 <i>Chairs</i> : Lars Pastewka , University of Freiburg, Germany, Izabela Szlufarska , University of Wisconsin, United States of America	Symposium A-1 <i>Chair</i> : Anton Van der Ven , University of California Santa Barbara, United States of America	Symposium I-1 <i>Chairs</i> : David Sroloviz , University of Pennsylvania, USA, Enrique Martinez Saez , Los Alamos National Laboratory, USA	Symposium L-1 <i>Chairs</i> : Jerome Weiss , CNRS/University of Grenoble-Alpes, France, Yinan Cui , University of California, Los Angeles, United States of America		Symposium J-1 <i>Chairs</i> : Jinghong Fan , Alfred University, United States of America, Sinan Keten , Northwestern University, United States of America	
13:30	<i>Invited</i> Kinetic Monte Carlo model of screw dislocation-solute coevolution in W-Re alloys Jaime Marian , Dept. of Materials Science and Engineering, University of California Los Angeles, United States of America	<i>Invited</i> Mechanism of enhanced ductility in Mg alloys W. Curtin , EPFL, Switzerland	<i>Invited</i> An integrated experimental and computational approach to microstructure-property relationships in structural materials Yunzhi Wang , The Ohio State University, United States of America	<i>Invited</i> Structure-property relations in sheared dense flocculated suspensions Jan Vermant , ETH Zurich, Switzerland	A numerical insight into third body flow regimes within dry contacts Guilhem Mollon , INSA Lyon - LaMCoS, France	<i>Invited</i> Atomistic to continuum: coarse-graining in and out of equilibrium Celia Reina , University of Pennsylvania, United States of America	<i>Invited</i> Grain growth at the nanoscale: the coupling of stress and grain boundary motion Peter Voorhees , Northwestern University, United States of America	<i>Invited</i> Flow and failure of (amorphous) materials - a nonequilibrium phase transition? Peter Schall , University of Amsterdam, Netherlands		<i>Invited</i> A multiscale failure analysis for layered composites with statistical account of manufacturing defects Ramesh Talreja , Texas A&M University, United States of America	13:30
13:45					A novel multiscale framework for modeling of diamond tools wear Adriana Quacquarelli , Université de Lyon, LaMCoS, INSA-Lyon, CNRS UMR5259, F-69621, France						13:45
14:00	Thermally activated solute-drag strengthening by interstitial impurities in BCC Cr Christian Brandl , Karlsruhe Institute of Technology, Germany	<i>Invited</i> Interaction of screw dislocations with interfaces during multiaxial loading: large scale 3D simulations Maxime Dupraz , PEM-LSC-PSD, Paul Scherrer Institute, Villigen, Switzerland	Development of a multiscale simulation system based on microstructure of fine-grained aluminum Atsushi Sagara , Dept. of Finemechanics, Tohoku Univ., Japan	<i>Invited</i> Soft deformable colloids make strong liquids with stress-driven relaxation Emanuela Zaccarelli , CNR Institute for Complex Systems, Rome, Italy	Thermodynamics of sliding contact: Joule-Thomson effect Vera Deeva , Tomsk Polytechnic University, Russia	Finite-temperature localized stress and strain for atomic models Ranganathan Parthasarathy , Tennessee State University, United States of America	Verification of grain growth models by time-resolved 3D experiments in pure iron Jin Zhang , Northwestern University, United States of America	<i>Invited</i> Reversibility and criticality in amorphous and crystalline solids Charles Reichhardt , Los Alamos National Laboratory, United States of America		<i>Invited</i> Multiscale modeling of fiber reinforced materials for future aerospace structures Anthony M Waas , U., Washington, Seattle, WA 98195; also Univ. of Michigan, Aerospace Engineering, Ann Arbor, MI 48109, United States of America	14:00
14:15	Generalized yield criterion in BCC metals from first principles Antoine Kravch , Institut Lumière Matière, Université Lyon 1, France		Image-based crystal plasticity analysis on the activities of slip systems in polycrystal alpha-Ti Yoshiki Kawano , Kitami Institute of Technology, Japan		Molecular simulation of adsorption process of anti-corrosion additives Kohei Nishikawa , University of Hyogo, Japan	Uncertainty quantification for classical effective potentials Sarah Longbottom , School of Engineering, University of Warwick, UK	Coarse-grained, three-dimensional modeling of defects at low-angle grain boundaries with the amplitude expansion of the phase field crystal model Marco Salvalaglio , Technische Universität Dresden, Germany				14:15
14:30	Dislocation motion in high entropy alloys Luchan Zhang , National University of Singapore, Singapore	The Multiscale calculations on the behaviors of some nuclear fuels and cladding materials Shiyu Du , Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, China	Micro structure-based crystal plasticity modeling of duplex titanium alloy during hot deformation Jun Zhang , Institute of Systems Engineering, China Academy of Engineering Physics, China	Linear viscoelasticity on matter out of equilibrium Leticia Lopez-Flores , Universidad Autonoma de San Luis Potosi, Mexico	The adhesive behavior of elastic contacts in the presence of interfacial shear stresses Giuseppe Carbone , Department of Mechanics, Mathematics and Management - Polytechnic University of Bari, Italy	The role of null-lagrangians in the continuum interpolation of the linear chain with hyper-pre-stress Alexandre Danescu , Ecole Centrale de Lyon, France	Estimation of grain boundary anisotropy using multi-phase-field model based on the ensemble Kalman filter Akinori Yamanaka , Tokyo University of Agriculture and Technology, Japan	<i>Invited</i> Exploring crystal-plastic constitutive rules with the OOF tool Andrew Reid , NIST, United States of America		<i>Invited</i> A-DISC (Adaptive Discrete-Smeared Crack) model for multi-scale progressive damage analysis of composite structures Tong-Earn Tay , National University of Singapore, Singapore	14:30
14:45	Modeling the climb-assisted glide of edge dislocations through a random distribution of nanosized vacancy clusters Marie Landeiro Dos Reis , SRMP-CEA Saclay, France	The connection between ideal strengths and deformation mechanisms in BCC refractory metals Liang Qi , University of Michigan, United States of America	Nonlocal multiscale modeling of deformation behavior of polycrystalline copper by second-order homogenization method Makoto Uchida , Osaka City Univ., Japan	Memory effects in functional polymers: The interplay between entropic elasticity and kinetic arrest Fathollah Vamik , Ruhr-University Bochum, Germany	Soft matter mechanics: numerical and experimental methodologies for dry and lubricated tribological problems Camille Putignano , Polytechnic University of Bari, Italy	Practical time averaging of nonlinear dynamics Amit Acharya , Carnegie Mellon University, United States of America	<i>Invited</i> Multiscale modelling of graphene from nano to micron scales Tapio Ala-Nissila , Aalto and Loughborough University, Finland				14:45
15:00		Nanoscaled matrix-inclusions-composites Konrad Schneider , Institute of Continuum and Material Mechanics, Hamburg University of Technology, Germany	Residual stress prediction for turning of Ti-6Al-4V considering the microstructure evolution Donald S Shih , Magnesium Research Center, Kumamoto University, Japan	Modelling and experimental verified coupled visco hyper electro-elastic behaviour of dielectric elastomer circular actuator Arpit Srivastava , IIT KANPUR, INDIA - 208016, India	Two simple models for pull-off decay of self-affine rough surfaces Antonio Papangelo , Politecnico di Bari, Italy			Objective fusion of multiscale experiments and multiscale models using Bayesian inference Surya Raju Kalidindi , Georgia Tech, United States of America		Analysis for the plane problem of layered magnetoelectric composite with collinear interfacial cracks Wenxiang Tian , School of Aerospace Engineering and Applied Mechanics, Tongji Univ, China	15:00
15:15	Coffee Break					Coffee Break					15:15

	Room 1	Room 2	Room 3	Room 4	Room 5	Room 6	Room 7	Room 8	Room 9	Room 10		
	Symposium C-2 <i>Chair: Stefan Sandfeld</i> , Chair of Micromechanical Materials Modelling, TU Bergakademie Freiberg, Germany	Symposium E-2 <i>Chairs: Ya-Fang Guo</i> , Beijing Jiaotong University, China. <i>Flemming JH Ehlers</i> , University Paris Diderot, France	Symposium F-2 <i>Chair: Selim Esedoglu</i> , University of Michigan, United States of America	Symposium M-2 <i>Chair: Emanuela Zaccarelli</i> , University of Rome I, Italy	Symposium O-2 <i>Chairs: Mark Owen Robbins</i> , Johns Hopkins University, United States of America. <i>Tasuku Onodera</i> , Hitachi, Ltd., Japan	Symposium A-2 <i>Chair: Kenjiro Sugio</i> , Hiroshima Univ., Japan	Symposium I-2 <i>Chair: Elizabeth Holm</i> , Carnegie Mellon University, United States of America	Symposium L-2 <i>Chairs: Charles Reichhardt</i> , Los Alamos National Laboratory, United States of America. <i>Peter Schall</i> , University of Amsterdam, Netherlands		Symposium J-2 <i>Chairs: Anthony M Waas</i> , University of Washington, United States of America. <i>Jungian Zhang</i> , Shanghai University, China		
15:45	<i>Invited</i> Finite deformation mesoscale field dislocation mechanics <i>Amit Acharya</i> , Carnegie Mellon University, United States of America	Using IM3D to simulate nano-beam and nano-target effects in ion radiation <i>Ju Li</i> , Massachusetts Institute of Technology, United States of America	<i>Invited</i> New algorithms for simulating grain boundary motion <i>Selim Esedoglu</i> , University of Michigan, United States of America	MMM in aircraft industries: use cases for simulation of additive manufacturing <i>Annett Seide</i> , MTU Aero Engines AG, Germany	Droplet spreading on a surface exhibiting solid-liquid interfacial premelting <i>Yang Yang</i> , East China Normal University, China	<i>Invited</i> Bridging the chasm between phenomenological theories and electronic structure <i>Anton Van der Van</i> , University of California Santa Barbara, United States of America	<i>Invited</i> Energy and dynamics of grain boundaries based on underlying microstructure <i>Yang Xiang</i> , Hong Kong University of Science and Technology, Hong Kong	<i>Invited</i> The role of system size, internal disorder, and dislocation patterning on the nature of plastic fluctuations <i>Jerome Weiss</i> , CNRS/University of Grenoble-Alpes, France		<i>Invited</i> Simulation-based design of bioinspired impact-resistant nanocellulose films with bouligand microstructure <i>Sinan Keten</i> , Northwestern University, United States of America	15:45	
16:00		First principles studies of H interaction with the face-centred cubic Al Z5 [100] twist grain boundary during a uniaxial tensile test <i>Sylvain Quevreau</i> , Universite Paris XIII, LSPM UPR 3407, France		Viscoelastic behaviour of heterogeneous materials studied thanks to an extension of craft software in harmonic regime <i>Julien Boisse</i> , University of Lorraine, France, France	Comparative study on the adsorption of volatile organic compounds on the surfaces of two-dimensional materials: toward the early lung cancer detection <i>Van An Dinh</i> , Nanotechnology Program, Vietnam Japan University, Viet Nam						16:00	
16:15	Anisotropic and non-symmetric continuum dislocation dynamics <i>Thomas Hochrainer</i> , TU Graz, Austria	Investigation of the {10-11} twin boundary migration in Magnesium <i>Ya-Fang Guo</i> , Institute of Engineering Mechanics, Beijing Jiaotong University, China	The role of grain shape in discrete element modeling of snow mechanics <i>Carolin Willibald</i> , Institute for Snow and Avalanche Research (SLF, ETH), Switzerland	Multi-scale modelling of Zener pinning during the solid solution treatment of a nickel-based superalloy <i>Magnus Jack Anderson</i> , The University of Birmingham, UK	Adsorption of the volatile organic compounds on graphene including van de Waals interaction <i>Thi Viet Bac Phung</i> , Nanotechnology Program, Vietnam Japan University – Vietnam National University, Viet Nam	Two-component Dirac-Kohn-Sham calculation for multiscale modeling of materials <i>Koichi Nakamura</i> , Kyoto Univ. Japan	Grain growth in ultrafine-grained thin films: a 3D problem <i>Ahu Oencue</i> , Institute of Experimental Physics, Otto-von-Guericke University, Germany	Dislocations associated with stick-slip friction of lubricants in boundary lubrication <i>Yongsheng Leng</i> , George Washington Univ, United States of America		<i>Invited</i> Amelogenesis: Nature's 3D printing system for multi-scale laminates <i>Brian Cox</i> , Arachne Consulting, United States of America	16:15	
16:30	Numerical simulation of model problems in plasticity based on field dislocation mechanics <i>Leo Morin</i> , PIMM, Arts et Métiers-ParisTech, CNAM, CNRS, UMR 8006, 151 bd de l'Hopital, 75013 Paris, France	Effect of twins on mechanical properties of silicon nanowires <i>Zheng Qin</i> , Tianjin Univ., China	Experimental-computational analysis of primary static recrystallization in DC04 steel <i>Martin Diehl</i> , Max-Planck-Institut fuer Eisenforschung GmbH, Germany	Assessment of residual stresses in welds made of multiphase alloys <i>Victor De rancourt</i> , Commissariat a l'energie atomique, France	Diffusion of a Cu nanodroplet on an amorphous carbon surface <i>Yu-Chen Chiu</i> , National Chiao Tung University, Taiwan	Combination of kinetic Monte Carlo method and first principles calculation to explore stable structure of solute cluster in Al-Si based alloys <i>Kenjiro Sugio</i> , Hiroshima Univ., Japan	The kinetics of ideal grain growth: a large scale monte carlo simulation <i>Xiangge Qin</i> , School of Materials Science and Engineering, Jiamusi University, China	Comparison of surface-indentation and pillar-compression at the nanoscale of FCC metals: Unification of size effects using 3D discrete dislocation dynamics <i>Hanxu Song</i> , west virginia university, United States of America			16:30	
16:45	Direct computation of the stress field due to geometrically necessary dislocation densities <i>Yichao Zhu</i> , Dalian University of Technology, China	Intrinsic ductility of alloys from nonlinear elasticity <i>Ian Winler</i> , University of California, Berkeley, United States of America	Large scale phase-field simulations of solid state sintering <i>Johannes Hoetzer</i> , Karlsruhe University of Applied Sciences, Germany	Atomic analysis of crystalline nucleation and growth in the supercooled liquid of glass-forming binary alloy <i>Masato Wakeda</i> , Research Center for Structural Materials, National Institute for Materials Science, Japan	First principal modeling of oxygen and carbon adsorption on Fe (110) surface with symmetrical tilt Sigma3(111) grain boundary <i>Ivan Lobzenko</i> , Toyota Technological Institute, Japan	Electronic structure analysis of Fermi level instability in Fe-rich Si alloy <i>Chen Ying</i> , School of Engineering, Tohoku University, Japan	Understanding the energetics of grain boundary motion in terms of compatible transformations and optimal transport theory <i>Ian W Chesser</i> , Carnegie Mellon University, United States of America	Statistical models for cross slip and reaction rate processes in continuum dislocation dynamics <i>Vignesh Vivekanandan</i> , Purdue University, United States of America		Role of geometrical features on mechanical properties in bio-inspired staggered composites <i>Siladitya Pal</i> , Indian Institute of Technology Roorkee, India	16:45	
17:00	Meshfree analysis for kink band formation in Mg-based LPSO phase based on crystal plasticity Cosserat model considering disclination density <i>Yuichi Kimura</i> , Grad. School of Science and Technology, Keio Univ., Japan	Tailoring the stability of {10-12} twin in magnesium with solute segregation at the twin boundary and strain path control <i>Ziran Liu</i> , Dept. of Physics, Hunan Normal University, Changsha, Hunan, China	Phase-field simulations of coupled dendritic-eutectic growth <i>Marco Seiz</i> , Institute of Applied Materials - Computational Materials Science, Karlsruhe Institute of Technology, Germany	Crystal growth in fluid flow: nonlinear response effects <i>Hailong Peng</i> , German Aerospace Center, Germany	Theoretical study of the effects of boron doping on the electronic structure of g-C₃N₄/TiO₂(001) heterojunction <i>Jianhong Dai</i> , Harbin Institute of Technology at weihai, China	From first-principles defect chemistry to device damage models of radiation effects in III-V semiconductors <i>Peter A Schultz</i> , Sandia National Laboratories, United States of America	<i>Invited</i> Microstructure stabilization and the herring condition <i>Jeremy K Mason</i> , University of California, Davis, United States of America	Designing Interfaces: a combinatorial approach to geometrical manipulation of interfaces <i>Hakan Yavas</i> , Czech Technical University, Czech Republic		Dynamic homogenization for acoustic metamaterials <i>Celia Reina</i> , University of Pennsylvania, United States of America	17:00	
17:15	Dynamic recrystallization model for Mg/LPSO alloys coupling phase-field model and dislocation-based crystal plasticity model <i>Sho Kuirai</i> , Grad. School of Science and Technology, Keio Univ., Japan	Contribution of defects on the anisotropic diffusion behaviour of hydrogen in nickel single crystals <i>Arnaud Metsue</i> , LaSIE UMR 7356 CNRS, France	The use of thermodynamic tensor models for phase-field simulations of spinodal decomposition in quaternary alloys coupled with CALPHAD data <i>Yuri Amorim</i> , Coulinho, Dept. of Materials Engineering, KU Leuven, Belgium	<i>Invited</i> Time-dependent active microrheology in dilute colloidal suspensions <i>Thomas Franosch</i> , Innsbruck Univ., Austria	<i>Invited</i> Atomistic simulations that reach anthropological timescale and beyond <i>Ju Li</i> , Massachusetts Institute of Technology, United States of America	How to model ordering processes in metallic hydrides? A Tight-Binding Ising modeling proposal and its application to Zr-H <i>Fabienne Ribeiro</i> , Institut de Radioprotection et de Sûreté Nucléaire/PSN-RES/SEMIA/LPTM, France				Cracking behavior of ferrite-pearlite pipeline steel with hierarchical and concurrent multiscale modeling schemes <i>Taolong Xu</i> , Southwest Petroleum University of China, China	17:15	
17:30		Development of simplified model for one-sided mechanical joining of dissimilar materials <i>Jaehyo Kim</i> , Dept. of Mechanical Engineering, Sogang Univ, Korea									17:30	
17:45 - 20:00	Poster session 1 - Wine & cheese party					Poster session 1 - Wine & cheese party					17:45 - 20:00	

	Room 1	Room 2	Room 3	Room 4	0120abc	Room 6	Room 7	Room 8	Room 9	Room 10	
08:00	Registration					Registration					08:00
08:30	<i>Plenary (Room 1, Chair: William Curtin, EPFL, Switzerland) Plasticity in crystals and glasses: from the atoms up</i> David Rodney, Institut Lumière Matière, University of Lyon, France					<i>Plenary (Room 1, Chair: William Curtin, EPFL, Switzerland) Plasticity in crystals and glasses: from the atoms up</i> David Rodney, Institut Lumière Matière, University of Lyon, France					08:30
09:20	Coffee Break					Coffee Break					09:20
	Symposium C-3 Chair: <u>Francis Guillaume</u> , DEN- Département des Matériaux pour le Nucléaire, CEA, Université Paris-Saclay, France	Symposium E-3 Chairs: <u>Benoit Devincere</u> , LEM, CNRS-ONERA, France. <u>Alejandro Strachan</u> , Purdue University, United States of America	Symposium F-3 Chair: <u>Carl Krill</u> , Institute of Micro and Nanomaterials, Ulm University, Germany	Symposium M-3 Chair: <u>Thomas Franasch</u> , University of Innsbruck, Austria	Symposium O-3 Chairs: <u>Motoji Kubo</u> , Tohoku University, Japan. <u>Michael Moseler</u> , Fraunhofer Institute for Mechanics of Materials IWM, Germany	Symposium A-3 Chair: <u>Katsuyo Thornton</u> , University of Michigan, Ann Arbor, United States of America	Symposium I-3 Chair: <u>Peter Voorhees</u> , Northwestern University, United States of America.	Symposium L-3 Chairs: <u>Peter M Derlet</u> , Paul Scherrer Institut, Switzerland. <u>Cynthia Reichhardt</u> , Los Alamos National Laboratory, United States of America	Symposium H-1 Chair: <u>Turab Lookman</u> , Los Alamos National Laboratory, United States of America	Symposium J-3 Chairs: <u>Ramesh Talreja</u> , Texas A&M University, United States of America. <u>Tong-Earn Tay</u> , National University of Singapore, Singapore	
09:45	<i>Invited</i> Quantifying the effect of hydrogen on dislocation dynamics in microcrystals: A three-dimensional discrete dislocation dynamics study <u>Jaafar El-Awady</u> , Johns Hopkins University, United States of America	<i>Invited</i> 3D mesoscopic study of the stability of three-dimensional short cracks in FCC metals using the Discrete-Continuous Model <u>Benoit Devincere</u> , LEM, CNRS-ONERA, France	<i>Invited</i> Biomaterialization in molluscan shells: from ideal to hierarchical grain growth <u>Dana Zoellner</u> , B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany	<i>Invited</i> Heterogeneous thermal properties in a glass from molecular dynamics calculations <u>Jean-Louis Barralet</u> , Univ. Grenoble Alpes, France	<i>Invited</i> Scale dependence of friction: how elasticity destroys superlubricity <u>Mark Owen Robbins</u> , Dept. of Physics and Astronomy, Johns Hopkins University, United States of America	<i>Invited</i> Challenges and gaps in length and time scaling of dislocation models <u>David L McDowell</u> , Woodruff School of Mechanical Engineering, Georgia Institute of Technology, United States of America	<i>Invited</i> Interaction of moving grain boundaries with solutes: bridging time scales between atomistics and continuum <u>Yuri Mishin</u> , George Mason University, United States of America	<i>Invited</i> Intermittent micro-plasticity and its relation to dislocation structure - a line stability analysis. <u>Peter M Derlet</u> , Paul Scherrer Institut, Switzerland	<i>Invited</i> Multiscale modeling of electro-responsive gels <u>Masao Doi</u> , Beihang University, China	<i>Invited</i> Fundamentals of generalized particle (GP) multiscale methods with applications to analyses of alternately-arranged soft and hard layers <u>Jinghong Fan</u> , Kazuo Inamori School of Engineering, Alfred University, United States of America	09:45
10:00										10:00	
10:15	Discrete dislocation plasticity modelling of hydrogen dislocation interactions in micro-cantilevers <u>Haiyang Yu</u> , Dept. of Materials, Univ. of Oxford, UK	<i>Invited</i> Role of cracks, voids and interfaces in hot spot formation and initiation of energetic materials <u>Alejandro Strachan</u> , School of Materials Engineering, Purdue University, United States of America	Mesoscale modeling of cement: texture, mechanics and durability <u>Katerina Ioannidou</u> , Dept. of Civil and Environmental Engineering, Massachusetts Institute of Technology, United States of America	Structural-dynamical phase transition in the phase space of histories of a polydisperse hard sphere liquid <u>Matteo Campo</u> , Johannes Gutenberg University Mainz, Germany	Coarse-grain simulations of polymer solutions with hydrodynamics and long-range interactions <u>Hiroshi Washizu</u> , Univ. Hyogo, Japan	From discrete to continuum dislocations and back: a two dimensional study of microstructure and interaction energies <u>Hengxu Song</u> , TU Bergakademie Freiberg, Germany	Phenomenological model for prediction of interaction parameters in grain boundary segregation <u>Pavel Lejcek</u> , Institute of Physics, AS CR, Praha, Czech Republic	<i>Invited</i> Discrete dislocation dynamics simulations of complexity in crystal plasticity: strain burst statistics and machine learning <u>Lasse Laurson</u> , Aalto University, Finland	Non-monotonic particle size effect on the glass transition in polymer-particle blends and its application to shape memory polymers <u>Elias M. Zirdelj</u> , Ruhr-University Bochum, Germany	The effect of layer thickness ratio on the plastic deformation mechanisms of nonoriented Ti/TiN nanolayered composite: a molecular dynamics study <u>Georges Y Aouf</u> , Dept. of Industrial and manufacturing system Engineering, Univ. of Michigan, United States of America	10:15
10:30	Dislocation climb models from atomistic scheme to dislocation dynamics <u>Yang Xiang</u> , Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong		Actuation in metal-polymer nanocomposites: chemoelectromechanical coupling on interfaces <u>Jana Wilmers</u> , Chair of Solid Mechanics, University of Wuppertal, Germany	Time- and history-dependent structure and morphology of vander-Waals liquids forming physical gels and porous glasses <u>Magdalena Medina-Novola</u> , Instituto de Fisica, Universidad Autonoma de San Luis Potosi, Mexico	A multi-scale approach for the design of novel lubricants <u>Georgios Bletsos</u> , National Technical University of Athens, Greece	Advances in microstructure prediction: a FFT-based dislocation dynamics approach <u>Francesca Boioli</u> , LEM, CNRS-ONERA, Chatillon, France	<i>Invited</i> Influence of solutes at grain boundaries on phase transformations and mechanical response <u>Stephen M Foiles</u> , Sandia National Laboratories, United States of America		Thermomechanical behavior of shape-memory polyurethane copolymer: a coarse-grained molecular dynamics simulation <u>Sungwoo Park</u> , Seoul National University, South Korea, Korea	The attenuation of stress wave propagation in multilayer structure <u>Fengyuan Yang</u> , Tsinghua University, China	10:30
10:45	Investigation of the Hall-Petch Effect with DD Simulation <u>Maoyuan Jiang</u> , EDF - R&D, Les Renardières, France	Precipitation hardening effects on extension twinning in magnesium <u>Haidong Fan</u> , Sichuan University, China	Mechanics of cilia beating - a relationship between metachronal wavelength and fluid flow rate <u>Jon Hall</u> , The University of Sheffield, UK	Impact of ionic liquid ordering on their triboreological properties <u>Konstantinos Gkagkas</u> , Advanced Material Research Division, Toyota Motor Europe NV/SA, Belgium	Plasticity and microstructure evolutions at the mesoscale: towards an integrated framework. <u>Laurent Capolungo</u> , Los Alamos National Laboratory, United States of America			Nanoindentation in the ultra-nano scale: Microstructure-property relationships using statistical approaches <u>Stefanos Papanikolaou</u> , West Virginia University, United States of America	Investigation of photo-mechanical behavior of azobenzene-based polymer: a coarse-grained molecular dynamics study <u>Junghwan Moon</u> , Seoul National University, Korea	Multiscale molecular-dynamics simulations of structure and mechanics of polymer nanocomposites <u>Alexey Lyulin</u> , Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands	10:45
11:00	Break					Break					11:00
	Symposium C-4 Chair: <u>Dan Mordehai</u> , Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel, Israel	Symposium E-4 Chairs: <u>Haifeng Song</u> , Institute of Applied Physics and Computational Mathematics, China. <u>Chenghua Sun</u> , Swinburne University of Technology, Australia	Symposium F-4 Chair: <u>Dana Zoellner</u> , B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany	Symposium M-4 Chair: <u>Leticia Lopez Flores</u> , University of San Luis Potosi, Mexico	Symposium O-4 Chairs: <u>Aiichiro Nakano</u> , Univ. of Southern California, United States of America. <u>Shandan Bai</u> , KYOCERA Corp., Japan	Symposium A-4 Chair: <u>David L McDowell</u> , Woodruff School of Mechanical Engineering, Georgia Institute of Technology, United States of America	Symposium I-4 Chairs: <u>Shen J Dillon</u> , University of Illinois, USA. <u>Daniel Pino Munoz</u> , Mines ParisTech / PSL Research University, France	Symposium L-4 Chair: <u>Lasse Laurson</u> , Aalto University	Symposium H-2 Chair: <u>Hansohl Cho</u> , Los Alamos National Laboratory, United States of America	Symposium J-4 Chairs: <u>Brian Cox</u> , Arachne Consulting Inc., United States of America. <u>Tomonaga Okabe</u> , Tohoku University, Japan	
11:15	<i>Invited</i> Hydrogen consequences on cyclic behavior of $\lt;001>$ nickel single crystals: a multi-scale approach. <u>Xavier Feaugas</u> , Université de la Rochelle, France	High-performance first-principles calculation software development with applications to the zirconium <u>Haifeng Song</u> , Institute of Applied Physics and Computational Mathematics, China	<i>Invited</i> Showdown! Pitting computer simulations against time-resolved experimental measurements of grain growth in 3D <u>Carl Krill</u> , Institute of Micro and Nanomaterials, Ulm University, Germany	<i>Invited</i> Mechanical behavior and emerging morphologies in active matter <u>Ignacio Pagonabarraga</u> , CECAM, EPFL, Switzerland	<i>Invited</i> Molecular simulation to better understand soot-detergent interactions in engine oils <u>Sophie Loehle</u> , Total M&S, France	<i>Invited</i> Effective transport properties of polycrystalline materials <u>Katsuyo Thornton</u> , University of Michigan, Ann Arbor, United States of America	<i>Invited</i> Atomistic modeling of helium segregation to grain boundaries in tungsten and its effect on decohesion <u>Enrique Martinez Saez</u> , Material Science and Technology Division, MST-8, Los Alamos National Laboratory, United States of America	<i>Invited</i> Dynamic phases, pinning, and pattern formation for driven dislocation assemblies <u>Cynthia Reichhardt</u> , Los Alamos National Laboratory, United States of America	<i>Invited</i> Hydrogels with dynamic sacrificial bonds - from toughness to adhesion to composites - <u>Jian Ping Gong</u> , Faculty of Advanced Life Science, Hokkaido University, Japan	<i>Invited</i> Validation of analytical models for ply cracking of general symmetric composite laminates <u>Tomonaga Okabe</u> , Department of Aerospace Engineering, Tohoku University, Japan	11:15
11:30		Catalyst design for ammonia synthesis of ammonia <u>Chenghua Sun</u> , Swinburne University of Technology, Australia								11:30	
11:45	Atomistic and continuum approaches to analyse precipitation hardening in metallic alloys <u>Javier Llorca</u> , IMDEA Materials Institute, Spain	A solid-solution structure model for multi-component alloys <u>Xinqyu Gao</u> , Institute of Applied Physics and Computational Mathematics, China	Coarsening and grain-growth in an SOFC-anode under surface and grain boundary self-diffusion: a multiphase-field approach <u>Paul Hoffrogge</u> , Karlsruhe University of Applied Sciences, Germany	Time dependent interaction between intruders in granular media <u>Hisao Hatakawa</u> , Yukawa Institute for Theoretical Physics, Kyoto University, Japan	A molecular dynamics study on the wear mechanisms of hydrogenated diamond-like carbon <u>Yang Wang</u> , Institute for Materials Research, Tohoku University, Japan	A new E-VPSC polycrystal formulation: fundamentals <u>Carlos Tome</u> , Los Alamos National Laboratory, United States of America	Thermodynamic properties of bcc Fe grain boundaries with segregation of 3d-transition-metal solutes <u>Zhuo Xu</u> , AIST, Japan	Effect of solute atoms and Peierls stress on the critical behaviour of discrete dislocations <u>Peter Dusan Ispanovity</u> , Eotvos University, Hungary	Elastic properties and effective interactions of <i>in silico</i> realistic microgels <u>Lorenzo Rovigatti</u> , Institute for Complex Systems, Uos Sapienza - CNR, Italy	<i>Invited</i> Two-way coupled modeling of lithium diffusion and diffusion induced finite elastoplastic bending of bilayer electrodes in lithium-ion batteries <u>Junqian Zhang</u> , Shanghai University, China	11:45
12:00	Dislocation-precipitate interaction in Al-Mg-Si alloys <u>Inga Gudem Ringdalen</u> , Dept. of Materials and Nanotechnology, SINTEF, Norway	First-principles prediction of plastic deformation modes in alloys <u>Song Lu</u> , KTH Royal Institute of Technology, Sweden	Solidification simulation in additive manufacturing process of Ti-alloy by ICME approach <u>Yusuke Shimono</u> , Itochu Techno-Solutions Corp., Japan	History-dependent shear jamming of granular materials under oscillatory shear <u>Michio Otsuki</u> , Graduate School of Engineering Science, Osaka Univ., Japan	Effect of tribochemical reactions on diamond-like carbon and wear under water lubrication: a molecular dynamics simulation investigation <u>Jing Zhang</u> , Inst. for Materials Research, Tohoku Univ., Japan	A new E-VPSC polycrystal formulation: applications <u>Youngeung Jeong</u> , Changwon National Univ., Korea	A new thermodynamic model for the austenite-ferrite massive transformation in Fe-C-X alloys <u>Alexandre Maheven</u> , INSA Lyon, France	<i>Invited</i> Temporal and spatial plastic instability of micrometer-scaled materials <u>Yinan Cui</u> , Mechanical and Aerospace Engineering Department, University of California, Los Angeles, United States of America	Controlling the mechanics of a synthetic hydrogel with motor-like internal contractility <u>Cornelis Storm</u> , Theory of Polymers and Soft Matter, Technische Universiteit Eindhoven, The Netherlands		12:00
12:15		The local-orbital construction of strongly correlated electrons based on the PAW method <u>Yu Liu</u> , Institute of Applied Physics and Computational Mathematics, China	Phase field model of microstructural evolution in metal alloy for designing mechanical property <u>Dongchoul Kim</u> , Dept. of Mechanical Engineering, Sogang Univ., Korea	Structural predictor for nonlinear sheared dynamics in simple glass-forming liquids <u>Trond S. Ingebrigtsen</u> , University of Tokyo, Japan	Formation mechanism of tribofilm of silicon carbide under water lubrication: molecular dynamics simulations <u>Fumiya Nakamura</u> , Tohoku Univ., Japan	Modeling microstructural material variability with uncertainty quantification and machine learning techniques <u>Reese Jones</u> , Sandia National Laboratories, United States of America	Multiscale simulation of solid phase sintering of nano copper powder <u>Xinyu Zhu</u> , School of Materials Science and Engineering, Jiamusi Univ, China		Study on viscoelastic behavior of natural rubber with multiscale approach <u>Byungjo Kim</u> , Seoul National University, Korea	Micro-scale model of thermomechanics in solidifying saturated porous media <u>Michal Benes</u> , Czech Technical University in Prague, Czech Republic	12:15
12:30	Lunch					Lunch					12:30
14:00	Excursion					Excursion					14:00

	Room 1	Room 2	Room 3	Room 4	Room 5	Room 6	Room 7	Room 8	Room 9	Room 10	
08:00	Registration					Registration					08:00
08:30	Plenary (Room 1, Chair: Erik Bitzek, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany) Grain boundary sliding, fracture and dislocation motion in ceramics Yuichi Ikuhara, The University of Tokyo/Japan Fine Ceramics Center, Japan					Plenary (Room 1, Chair: Erik Bitzek, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany) Grain boundary sliding, fracture and dislocation motion in ceramics Yuichi Ikuhara, The University of Tokyo/Japan Fine Ceramics Center, Japan					08:30
09:20	Coffee Break					Coffee Break					09:20
	Symposium C-5 Chair: Christopher Woodward, Air Force Research Laboratory, United States of America	Symposium E-5 Chairs: Anthony D Rollett, Carnegie Mellon University, United States of America. Evgeniya Kabilman, Austrian Institute of Technology, Austria	Symposium F-5 Chair: Ingo Steinbach, Ruhr-University Bochum, Germany	Symposium N-1 Chair: Danny Perez, Los Alamos National Laboratory, United States of America	Symposium O-5 Chairs: Hitoshi Washizu, University of Hyogo, Japan. Sophie Loehle, TOTAL Marketing & Services, Solaize, France	Symposium A-5 Chair: Sinisa Di Mesarovic, Washington State University, United States of America	Symposium I-5 Chairs: Stephen M Foiles, Sandia National Laboratories, United States of America. Mitra L Taheri, Drexel University, United States of America	Symposium G-1 Chairs: Byoungchan Lee, KyungHee Univ., Korea. Keonwook Kang, Yonsei University, Korea	Symposium H-3 Chair: Hansohi Cho, Los Alamos National Laboratory, United States of America	Symposium B-1 Chair: Lorenzo Malerba, CIEMAT, Energy, Environment and Technology Research Centre, Spain	
09:45	Invited Plasticity and fracture in transition metal carbides Giacomo Po, University of California Los Angeles, Mechanical Engineering Department, United States of America	Invited Use of FFT-based micromechanical modeling for analysis of synchrotron-based diffraction experiments Anthony D Rollett, Carnegie Mellon University, United States of America	Invited Solidification microstructure formation by phase-field simulation with multi-GPU acceleration Tomohiro Takaki, Kyoto Institute of Technology, Japan	Invited Increasing the power of accelerated molecular dynamics methods and plans to exploit the coming exascale Arthur F Voter, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, United States of America	Invited On the formation of superlubricious layers during boundary lubrication of diamond and diamond-like carbon Michael Moseler, Fraunhofer Institute for Mechanics of Materials IWM, Germany	Invited Parameters to consider in the modelling of dislocation boundary evolution Grethe Winther Winther, Technical University of Denmark, Denmark	Invited Heterogeneous disconnections nucleation mechanisms during grain boundary migration Nicolas Combe, CEMES Toulouse, France	Invited A systematic method to develop a potential model for harsh environments Takui Oda, Dept. of Nuclear Engineering, Seoul National Univ., Korea	Invited Polydomain liquid crystal elastomers I Kaushik Bhattacharya, California Institute of Technology, United States of America	Thermal stability of carbon-vacancy complexes in iron alloys and steels Milan J Konstantinovic, Belgian nuclear institute, SCK.CEN, Belgium	09:45
10:00										Computational study of phosphorous migration to grain-boundary in alpha-iron Ken-ichi Ebihara, Center for Computational Science & e-Systems, Japan Atomic Energy Agency, Japan	10:00
10:15	Atomic scale investigation of plasticity in Laves phases Julien Gienoe, Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Germany	Computational design of hysteresis-free and linear super-elastic, and ultralow modulus ferroelastic materials Jiaming Zhu, City University of Hong Kong, Hong Kong	Phase-field study of eutectic colony formation in NiAl-34Cr Michael Kellner, Institute of Applied Materials – Computational Materials Science (IAM-CMS), Karlsruhe Institute of Technology, Germany	Invited Atomistic processes at interfaces on extended timescales Jutta Rogal, Ruhr University Bochum, United States of America, Germany	Unveiling the chemical reactions involved in moisture-induced weakening of adhesion between aluminum and epoxy resin: a hybrid quantum-classical simulation study Shuji Oqata, Nagoya Institute of Technology, Japan	Data mining of indentation induced dislocation microstructures Dominik Steinberger, Chair of Micromechanical Materials Modelling, TU Bergakademie Freiberg, Germany	Motion of grain boundaries based on disconnections Chaozhen Wei, Hong Kong University of Science and Technology, Hong Kong	Molecular dynamics study of the bulk cascades in W-Re alloy Hunngyu Lee, Yonsei University, Korea	Mechanical behavior of hydrated polymers at nanoscale: from elasticity to rupture William Goncalves, Institute of Fluid Science, Tohoku University, Sendai, Miyagi 980-8577, Japan	Properties of interstitials in concentrated Fe-Cr alloys from first principles Marcin Roland Zemla, Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland	10:15
10:30	Nucleation of dislocation in ultra-hard ceramic nanoparticles modelled by molecular dynamics and nudged elastic band simulations Jonathan Amodéo, MATEIS, Univ. Lyon 1, France	A biphasic continuum model for large deformation visco-elastic mechanics of uncured carbon fibre prepreps Amir Hosein, Sakhaei, Mathematics and Physical Sciences, University of Exeter, UK	Solidification analysis by non-equilibrium phase field model using thermodynamics data estimated by machine learning Sukeharu Nomoto, ITOCHU Techno-Solutions Corporation, Japan		Efficient evaluation of adhesion free energy between a liquid and polymer-grafted substrate Masayuki Uraganase, Nagoya Institute of Technology, Japan	Lattice continua for polycrystal grains: climb and glide of dislocations, diffusion and grain boundary kinematics. Sinisa Di Mesarovic, Washington State University, United States of America	Invited Dislocation-mediated boundary motion, dislocation-boundary interaction, and their effect on the mechanical behavior in fcc materials Bob Svendsen, Material Mechanics, RWTH Aachen University, Germany	Defect energetics in W-based transition-metal ternary systems Younghak Shin, KyungHee Univ., Korea	Structural properties of mixtures of stars polymers and long chains Emanuele Locatelli, Faculty of Physics, University of Vienna, Austria	Defect production in cascade overlap with defect clusters in iron and tungsten Jesper Byggmatar, Department of Physics, University of Helsinki, Finland	10:30
10:45	Multiscale discrete dislocation dynamics modeling of nano-indentation near the grain boundary Xu Zhang, School of Mechanics and Engineering, Southwest Jiaotong University, China	Strong coupling of deformation and microstructure/microchemistry evolution in hot compression tests Evgeniya Kabilman, Light Metals Technologies Ranshofen, Center for Low-Emission Transport, Austrian Institute of Technology, Austria	Phase field modeling of deformation twinning in β-metastable titanium alloys Juba Hamma, LEM, UMR 104 CNRS-ONERA, Université Paris Saclay F-92322 Châtillon, France		Ultimate response of confined fluids under extreme conditions: a molecular dynamics analysis Alejandro Porras-Vazquez, NSA Lyon, France			A numerical study of channel deformation and fracture in irradiated stainless steel single crystals Jean-Michel Scherer, DEN-Service d'Etudes des Matériaux Irradiés, CEA, Université Paris-Saclay, France	Harnessing instabilities in magnetorheological elastomers Kostas Danas, CNRS, Ecole Polytechnique, France	Multiscale modelling of radiation damage evolution in Fe and Fe-based alloys Fredric Granberg, Department of Physics, University of Helsinki, Finland	10:45
11:00	Break					Break					11:00
	Symposium C-6 Chair: Jaime Marian, Dept. of Materials Science and Engineering, University of California Los Angeles, United States of America	Symposium E-6 Chairs: Ying-Jun Gao, Guangxi University, China. Masaki Tanaka, Kyushu Univ., Japan	Symposium F-6 Chair: Benoit Appolaire, Institut Jean Lamour, Univ. de Lorraine, France	Symposium N-2 Chair: Erik Bitzek, FAU Erlangen-Nuernberg, Germany	Symposium O-6 Chairs: Yoshitaka Umemo, The University of Tokyo, Japan. Yoshinori Shihara, Toyota Technological Institute, Japan	Symposium A-6 Chair: Emma Griffiths, University of Cape Town, South Africa	Symposium I-6 Chairs: Garritt Tucker, Colorado School of Mines, United States of America. Chuang Deng, University of Manitoba, Canada	Symposium G-2 Chairs: Seunghwa Ryu, Korea Advanced Institute of Science and Technology, Korea. Keonwook Kang, Yonsei University, Korea	Symposium H-4 Chair: Meredith Silberstein, Cornell University, United States of America	Symposium B-2 Chair: Davide Pizzocri, Politecnico di Milano, Italy	
11:15	Invited Effect of interstitial solutes on the structure and mobility of screw dislocations in bcc metals Francois Guillaume, DEN-Département des Matériaux pour le Nucléaire, CEA, Université Paris-Saclay, France	Phase field crystal simulation of crack extension and brittle-ductile transition behavior on nano-scale Ying-Jun Gao, Guangxi University, China	Invited Atomistically informed full-field simulation of tempered martensite: quenching, tempering and mechanical characterization Ingo Steinbach, Ruhr-University Bochum, Germany	Invited Modeling microstructure evolution in rapid solidification phenomena using structural phase field crystal models Nikolas Provatas, McGill University, Canada	Invited Modeling the plastic deformation of a metal crystal induced by contact with a rough rigid surface Lucia Nicola, Delft University of Technology, Netherlands	Invited Design of patchy nanoparticles via the self-assembly of triblock terpolymers in selective solvents Eliot Fried, Okinawa Institute of Science and Technology, Japan	Invited Migration mechanisms of faceted vicinal grain boundaries Shari Hadian, Max-Planck-Institut fuer Eisenforschung, Germany	Multiscale modeling of strength enhancement of aluminium honeycombs under combined shear-compression at high strain rate Han Heng Zhao, Ecole Normale Paris-Saclay, France	Invited Enhanced dissipation behavior of main-chain LCE networks Thao D Nguyen, Johns Hopkins University, United States of America	Invited Atomic scale calculations of nuclear fuel properties to sustain multiscale modeling of fuel behavior Emeric Bourasseau, CEA/DEN/DEC, Centre CEA de Cadarache, France	11:15
11:30		Continuum elasticity and correlations of plastic strain fluctuations in sheared glasses: the effect of hard boundaries Muhammad Hassani, Ruhr-University Bochum, Germany						Multiscale mechanical analysis of silicon and silicon dioxide as high capacity anode materials for lithium ion batteries. Janghyuk Moon, School of Energy System Engineering, Chung-Ang Univ., Korea			11:30
11:45	Effect of solutes on dislocation motion in dilute hcp and bcc alloys Tomohito Tsuru, Japan Atomic Energy Agency, Japan	Modeling approaches to tetragonal-to-monoclinic transformations in MgO partially stabilized zirconia Michael Budnizki, TU Bergakademie Freiberg, Germany	Characterisation and modelling of drawn martensite Marius Gintalas, The University of Cambridge, Department of Materials Science & Metallurgy, 27 Charles Babbage Road, Cambridge CB3 0FS, UK	The phase field method: crystal structures and facets Peter Voorhees, Northwestern University, United States of America	On the potential use of liquid crystals as 'smart' lubricants – an MD simulation study Kerstin Falk, Dept. of Tribology, Fraunhofer IWM, Freiburg, Germany	Nanoporous composites: giving polymers strength and helping metals move Emma Griffiths, University of Cape Town, South Africa	Multiscale model for the structure and energy of low-angle general grain boundaries in Al, Cu and Ni Shuyang Dai, Wuhan University, China	Finite element analysis of the effect of interfacial bubbles on performance of epoxy coatings under the alternating hydrostatic pressure Liliu, Institute of Metal Research, Chinese Academy of Sciences, China	Thermo-mechanically coupled model for large strain of ultra-high molecular weight semi-crystalline polymers Christelle A. Bernard, Frontier Research Institute for Interdisciplinary Sciences (FRIS), Tohoku Univ., Japan	Influence of vibrational entropy on the concentrations of uranium vacancies in UO Jean-Paul Crocombette, CEA Saclay, France	11:45
12:00	Investigation of the energy pathway for generation of dislocations in silicon at $\Sigma 3$ grain boundaries with the kinetic activation-relaxation technique Simen Nut Hansen Ellissen, Norwegian Univ. of Science and Technology, Norway	Delamination cracks in wire-drawn fully pearlitic steels Masaki Tanaka, Kyushu Univ., Japan	3D modeling of microstructure evolution in Ni-based superalloys under creep loading Maeva Cottura, Institut Jean Lamour, France	Invited Using free energy calculations and statistical mechanics to probe the brittle to ductile transition of bcc metals Thomas Swinburne, CInAM, CNRS/Aix-Marseille University, France	Sliding on physisorbed cetyltrimethylammonium bromide (CTAB) Johannes Laurin Hoermann, University of Freiburg, Germany	Multiscale modeling of advanced materials for hybrid organic-inorganic solar cells Alexander E. Kobryn, Nanotechnology Research Center, National Research Council Canada, Canada	Invited The influence of normal stress on the structural transformation and migration of grain boundaries Chuang Deng, University of Manitoba, Canada	Multiscale modeling and design of high-strength and low-density 3D-architected metamaterial systems Hussein M Zbib, Washington State University, United States of America	Design principles for high modulus and toughness of assembled hairy nanoparticles Sinan Ketan, Northwestern University, United States of America	Modelling of defect and rare gas transport properties in UO atomic to the grain Marjorie Bertolus, CEA, DEN, France	12:00
12:15	Prediction of mechanical twinning in post-perovskite structure Philippe Carrez, Lille University, Lab. UMET UMR-CNRS 8207, France	FTMP-based modeling and simulations of inhomogeneous recovery-triggered accelerated creep rupture in lath martensite structures Yasulaka Matsubara, Kobe Univ., Japan	Phase field study of the effect of coherency strains and applied load in material couples Sourav Chatterjee, Department of Materials Engineering, KU Leuven, Belgium		Atomistic simulations of amines as organic friction modifiers Manuel Cobian, LTDS ECL, Université de Lyon, France	From cellulose and lignin to kerogen: molecular simulations of a geological process Roland Pellenz, <MSE>2, MIT- CNRS -AMU, United States of America		Multiscale-multiphysics simulations of metal nanotips under high electric field Mihkel Veske, Helsinki Institute of Physics, University of Helsinki, Finland	Effect of chain alignment on entanglements, diffusion and polymer weld strength Marco Galvani, Dept. Physics and Radioprotection et de Sûreté Nucléaire/PSN-RES/SEM/LPTM, France, France	Intragranular bubble impact on nuclear fuel thermomechanical properties Jack Aravro, Institut de Radioprotection et de Sûreté Nucléaire/PSN-RES/SEM/LPTM, France, France	12:15
12:30	Lunch					Lunch					12:30

	Room 1	Room 2	Room 3	Room 4	Room 5	Room 6	Room 7	Room 8	Room 9	Room 10	
	Symposium C-7 Chair: David Rodney , Institut Lumiere Matiere, Universite Lyon 1, France	Symposium E-7 Chairs: Daisuke Matsunaka , Shinshu Univ., Japan, Shiyu Du , Chinese Academy of Sciences, China	Symposium F-7 Chair: Tomohiro Takaki , Kyoto Institute of Technology, Japan	Symposium N-3 Chair: Arthur F. Voter , Los Alamos National Lab, United States of America	Symposium O-7 Chairs: Lucia Nicola , Delft University of Technology, Netherlands, Shuji Ogata , Nagoya Institute of Technology, Japan	Symposium A-7 Chair: Michael Zaiser , FAU University of Erlangen-Nuremberg, Germany	Symposium I-7 Chairs: Nicolas Combe , CEMES Toulouse, France, Brandon Runnels , University of Colorado Colorado Springs, United States of America	Symposium G-3 Chairs: Seunghwa Ryu , Korea Advanced Institute of Science and Technology, Korea, Keonwook Kang , Yonsei University, Korea	Symposium H-5 Chair: Alexey Lyulin , Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands	Symposium B-3 Chair: Kazuto Arakawa , Shimane University, Japan	
14:00	<i>Invited</i> Predictive simulations of crystal plasticity: multiscale or cross-scale Vasily V Bulatov , Lawrence Livermore National Laboratory, Germany	<i>Invited</i> The activation parameters for dislocation nucleation in molybdenum nanoparticles under compression Dan Mordehai , Mechanical Engineering, Technion, 32000 Haifa, Israel	<i>Invited</i> A Cosserat crystal plasticity and phase field theory for grain boundary migration Benoit Appolaire , Institut Jean Lamour, Univ. de Lorraine, France	<i>Invited</i> Kinetics of fivefold-twinned nanowire growth Kristen Fichthorn , Penn State University, United States of America	<i>Invited</i> Toward exascale atomistic simulations of interfaces Akihiro Nakano , Univ. of Southern California, United States of America	<i>Invited</i> Mathematical challenges for a mesoscale theory of dislocations Thomas Hochrainer , TU Graz, Austria	<i>Invited</i> Insights into recrystallisation: atomistic simulations of the properties of grain boundaries in heavily deformed material Chris P Race , University of Manchester, UK	<i>Invited</i> Simulations on severely transient FSI problems associated with shock compression of matters in extreme conditions Jai-ick Yoh , Seoul National University, Korea	<i>Invited</i> Simulation and experiment study of the structure-property relation of polymer nanocomposites Jun Liu , Beijing University of Chemical Technology, China	<i>Invited</i> Formation of radiation-induced Re and Os precipitation in W and its effects on mechanical properties Guang-Hong Lu , Beihang University, China	14:00
14:15											14:15
14:30	Molecular dynamics simulations of dislocation avalanche emissions in FCC and BCC crystals Javier Varillas , New Technologies Research Centre, University of West Bohemia in Pilsen, Czech Republic	Dislocation density-based crystal plasticity analysis for the evolution of atomic vacancies during plastic slip deformation Tetsuya Ohashi , Kitami institute of technology, Japan	Phase-field modeling of precipitation growth and ripening during heat-treatment conditions in Ni-base superalloys Michael Fleck , Metals and Alloys, University Bayreuth, Germany	Accelerated quantum molecular dynamics simulations of chemistry under extreme conditions Romain Perrot , Los Alamos National Laboratory, United States of America	Molecular dynamics simulation study on the structure, role, and formation mechanism of tribofilms of silicon-based materials in water Yusuke Ootani , Institute for Materials Research, Tohoku University, Japan	Dislocation multiplication in the discrete-continuum transition regime Karin Schulz , Karlsruhe Institute of Technology, Germany	Continuum dislocation dynamic based grain fragmentation Modeling for severe plastic deformation in FCC metals Ali Al-Hadi I. Kobaisy , Department of Mechanical Engineering, American University of Beirut, Lebanon	Modeling and simulation of shock waves in solids using branched Hugoniot Won-Suk Ohm , Yonsei University, Korea	Microstructural effects in the dynamic response of random 3D structural polymeric foams Axinte Ionita , Los Alamos National Laboratory, United States of America	Elastic fields and interaction between self-interstitial atom defects in bcc metals. Sergei L Dudarev , UK Atomic Energy Authority, UK	14:30
14:45	Scrutinizing screw dislocation glide initiation at finite temperatures in BCC metals Tomonaki Suzudo , Japan Atomic Energy Agency, Japan	Structural stability of long-period stacking ordered magnesium alloys Daisuke Matsunaka , Dept. of Mechanical Systems Engineering, Shinshu Univ., Japan	Two-dimensional simulation of cyclic phase transformation in Fe-C-Mn-Si alloy using non-equilibrium multi-phase-field model Masahito Segawa , ITOCHU Techno-Solutions Corporation, Japan	Hydrogen diffusion in TiHx: insights from PRD accelerated QMD Ivan Novoselov , Dukhov Research Institute of Automatics, Russia	Influence of tribo-film structure generated from MoDTC on friction behavior: a molecular dynamics simulation Masahiro Saito , Institute for Materials Research, Tohoku Univ., Japan	The fundamental instability of dislocation transport equations Michael Zaiser , FAU University of Erlangen-Nuremberg, Germany	Atomistic investigation on interaction of stress-assisted grain boundary motion with crack Mohammad Aramfar , Univ. Manitoba, Canada	Branched Hugoniot curve of aluminum in strong shock using molecular dynamics Jimin Choi , Yonsei Univ., Korea	Monte Carlo simulation predicting generation and growth of spherulites in thermoplastic polymer Ryota Osawa , Dept. of Mechanical Engineering, Tohoku Univ., Japan	Molecular dynamics simulation study of the interaction of Re with interstitial defects in tungsten bulk Huihui Deng , School of Physics and Electronics, Hunan University, China	14:45
15:00	Uranium plastic deformation: a multiscale approach Pavel A Pokaashkin , Dukhov Research Institute of Automatics (VNIIA), Russia	First-principles-based prediction of yield strength in the Rh/NiPdPtCu high entropy alloy Bingjun Yin , LAMMM, EPFL, Switzerland	Prediction of the microstructure evolution in electron beam melting alloy 718 through phase field modelling Chamara Kumara , Department of Engineering Science, University West, Sweden	<i>Invited</i> Shape fluctuation of metallic nanoclusters: observations from long-timescale simulations Bao Huang , Xiamen University, China	Shear-induced amorphization of silicon and diamond yields liquid-like amorphous solids Gianni Moras , Fraunhofer Institute for Mechanics of Materials IWM, Germany	2D continuum theory of dislocations Istvan Groma , Eotvos Lorand University, Hungary	<i>Invited</i> Effect of grain boundary structure on its dynamic response using molecular dynamics Sanyu Fensin , Los Alamos National Lab, United States of America	Shear relaxation behind the shock front in <110> molybdenum Roman Koslowski , Department of Mechanical Engineering, Technion – Israel Institute of Technology, 32000 Haifa, Israel	Determination of mechanical properties of polymers from coarse grained molecular dynamics simulations: a few case studies Sumit Basu , Indian Institute of Technology Kanpur, India	Hydrogen super-saturated layers in plasma loaded tungsten: a global model combining density functional theory data, thermodynamic and Kinetic models Yves Farné , Aix-Marseille University, France	15:00
15:15	Understanding the grain refinement mechanism in surface mechanical attrition treatment of Fe14Ni18Cr by molecular dynamics simulations Ali Rida , University of Technology of Troyes, France	Metal-coated carbon nanotube reinforced aluminum composites Samaneh Nasiri , Institute for Materials Simulation WW8, Department of Materials Science, Friedrich-Alexander University Erlangen-Nuemberg, Germany	Phase-field simulation of solidification morphology in laser powder deposition of Fe-B alloys Xiaoxia Li , School of Materials Science and Engineering, Jiamusi Univ., China	<i>Invited</i> A new damage implementation for smooth particle hydrodynamics and its application to simulating the wear response of metals. Alban de Vaucorbeil , Monash University, Australia	Continuum dislocation dynamics for finite deformation mesoscale plasticity Anter El-Azab , Purdue University, United States of America	Hypervelocity shock behavior of graphene-metal nanocomposites via molecular dynamics simulations Stefano Signetti , Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea	Modulating elastomer strength and toughness with metal ligand cross-linking Meredith Silberstein , Cornell University, United States of America	Mobility of small vacancy and interstitial prismatic dislocation loops in BCC tungsten Jan Fikar , Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Switzerland			15:15
15:30	Coffee Break										15:30
	Symposium C-8 Chair: Yinan Cui , Mechanical and Aerospace Engineering Department, University of California, Los Angeles, United States of America	Symposium E-8 Chairs: Hao Wang , Institute of Metal Research, CAS, China, Jun-Ping Du , Kyoto University, Japan	Symposium F-8 Chair: Martin Diehl , Max-Planck-Institut fuer Eisenforschung GmbH, Germany	Symposium N-4 Chair: Laurent Karim Beland , Queen's University, Canada	Symposium O-8 Chairs: Tianbao Ma , Tsinghua University, China, Yang Wang , Institute for Materials Research, Tohoku University, Japan	Symposium A-8 Chair: Thomas Hochrainer , TU Graz, Austria	Symposium I-8 Chair: Srikanth Patala , North Carolina State University, United States of America	Symposium G-4 Chairs: Keonwook Kang , Yonsei University, Korea, Byeongchan Lee , KyungHee Univ., Korea	Symposium H-6 Chair: Alexey Lyulin , Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands	Symposium B-4 Chair: Gary S Was , University of Michigan, United States of America	
16:00	<i>Invited</i> Thermal fluctuations of dislocations reveal the interplay between their core energy and long-range elasticity. Pierre-Antoine Geslin , Mateis lab, INSA Lyon/CNRS, France	Effect of hydrogen on the vacancy diffusion in metals Jun-Ping Du , Elements Strategy Initiative for Structural Materials, Kyoto University, Japan	<i>Invited</i> From state parameter-based microstructure modeling to temperature and strain rate-dependent yield stress Ernst Kozeschnik , Institute of Materials Science and Technology, TU Wien, Austria	<i>Invited</i> Multiscale diffusion method for simulations of long-time defect evolution with application to dislocation climb Kristopher Baker , Knolls Atomic Power Laboratory, United States of America	Friction mechanism of nanostructured steel in lubricant: a coarse-grained molecular dynamics study Yoshitaka Umeno , The University of Tokyo, Japan	<i>Invited</i> Pattern formation in doubly curved thin shells Eleni Katifori , University of Pennsylvania, United States of America	<i>Invited</i> New approaches for understanding nanocrystalline mechanics: physical microstructures, grain boundary descriptors and deformation mechanisms Garritt Tucker , Colorado School of Mines, United States of America	Effect of surface and internal defects on the mechanical properties of metallic glasses Seunghwa Ryu , Dept. of Mechanical Engineering, Korea Advanced Institute of Science and Technology, Korea	Coarse-grained molecular dynamics simulation of fluid rubber under cyclic tensile deformation Takashi Kojima , The Yokohama Rubber Co., Ltd., Japan	<i>Invited</i> Kinetics of precipitation in Fe-Cr and Fe-Cr-C alloys under Irradiation Frederic Soisson , CEA Saclay, France	16:00
16:15		Promotional effects of anisotropic strain on vacancy mobility in tungsten: the independence on the sign of strain Zhong Zhu Li , Department of Physics, Beihang University, China			Coarse-grained molecular dynamic simulation on the wear mechanism of polymer brush with different chain topologies Zhongmin Liu , Institute for Material Research, Tohoku Univ., Japan			Weighted Voronoi tessellation for metallic glasses by molecular dynamics and powder packing by discrete element method Junyoung Park , Dept. of Mechanical Design Engineering, Kumoh National Institute of Technology, Korea	Modelling of influence of fatigue damage on oxygen diffusion in rubbers Jan Heczko , NTIS - New Technologies for the Information Society, Faculty of Applied Sciences, University of West Bohemia, Czech Republic	16:15	
16:30	Tension of fluctuating dislocation lines Max Boivininger , Culham Centre for Fusion Energy, UK	Ab initio investigation on the stacking fault energy and the c/a ratio in hexagonal metals and alloys Gang Zhou , Institute of Metal Research, Chinese Academy of Sciences, China	Modelling of grain boundary segregation and precipitation in multi-component Al alloys subjected to heat treatment Dongdong Zhao , Norwegian University of Science and Technology (NTNU), 7491, Trondheim, Norway	Accelerated quantum molecular dynamics Enrique Martinez Saez , Material Science and Technology Division, MST-8, Los Alamos National Laboratory, Los Alamos, 87545 NM, USA, United States of America	Molecular dynamics simulation study on friction of bottlebrush polymer with a cationic anchor block adsorbed on substrate Shuichi Uehara , Institute for Materials Research, Tohoku Univ., Japan	Phase-field model for microstructure change in L1₂ type ordering with lattice distortion Ryuichiro Oguma , Fukuoka Univ., Japan	Grain boundary sliding: the best supporting role in ductile localization Alexandre Dimanov , LMS, CNRS-UMR7649, Ecole Polytechnique, France	Potential of lineal-path function as a characterization parameter related to material properties Tong-Seok Han , Yonsei University, Korea	On the modeling and calculation of tensile properties of real rubber using molecular dynamics simulation Osamu Hino , TOYO TIRE&RUBBER CO., LTD., Japan	The complex problem of the experimental validation of atomistic and microstructural evolution models Lorenzo Malerba , CIEMAT, Energy, Environment and Technology Research Centre, Spain	16:30
16:45	Stress-dependent activation parameters for cross-slip in FCC metals Alon Malka-Markovitz , Technion—Israel Institute of Technology, Israel	Role of vacancies and grain boundaries for 2D materials for the catalytic ammonia synthesis Qinve Li , Monash University, Australia	Modeling the microstructure and electrical conductivity evolution during aging of Al-Mg-Si alloys Yiliang Xu , Norwegian University of Science and Technology, Norway	On the effect of hydrogen on vacancy diffusion Sebastian Echeverri Restrepo , Department of Metallic Materials & Ceramics, SKF, Netherlands	Temperature dependent dynamics simulation of traction fluid by molecular dynamics method Eiji Tomiyama , Research Organization for Information Science and Technology, Japan	Coupling multi-component phase field models for oxide systems to thermodynamic databases – breaking the curse of dimensionality Inge Bellemans , Department of Materials, Textiles and Chemical Engineering, Ghent University, Belgium			A molecular dynamics study of dissolution of covalent adaptable networks in organic solvent Yaquang Sun , Dept. of Mechanics, Beijing Jiaotong Univ., China	Physically based prediction of radiation hardening: application to steels and model alloys Ghiath Monnet , EDF - R&D, MMC, France	16:45
17:00	The influence of precipitate size and shape on the strengthening and hardening rate as observed within metallic alloys Benjamin Szalewski , Army Research Laboratory, United States of America	First-principles investigation on the stability and oxygen adsorption behavior of a Ti₂AlNb/TiAl interface Yue Li , School of Materials Science and Engineering, Harbin Institute of Technology at Weihai, China	Thermo-kinetic modeling of long-term precipitate evolution in heat-resistant alloys Jae-Hyeok Shim , Korea Institute of Science and Technology, Korea			<i>Invited</i> A sharp phase field method Alphonse Finel , Laboratoire d'Etude des Microstructures, CNRS, ONERA, France			A minimal micromechanical model for the viscoelasticity in biophysical filamentous networks Erik Van der Giessen , Univ. of Groningen, Netherlands	Oxygen diffusion in bcc Fe under the influence of foreign atoms and vacancies Xiaoshuang Wang , Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany	17:00
17:15	Molecular dynamics simulations of dislocation dynamics Guy Makov , Ben-Gurion University of the Negev, Israel	DFT predictions of hydrogen storage properties of Mg₂TiX₂ (X= F, O, S, P and Cl) Yuying Chan , School of Materials Science and Engineering, Harbin Institute of Technology at Weihai, China	Simultaneous transformation kinetics model for additive manufacturing Narendran Raghavan , Oak Ridge National Laboratory, United States of America								17:15
17:30	Break										17:30
17:45	Poster session 2 - Wine & cheese party										17:45
20:00											20:00

	Room 1	Room 2	Room 3	Room 4	Room 5	Room 6	Room 7	Room 8	Room 9	Room 10	
08:00	Registration					Registration					08:00
08:30	Plenary (Room 1, Chair: Dongsheng Xu, IMR-CAS, China) Property optimisation of titanium alloys based on phase stability evaluation and microstructure design Rui Yang, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China					Plenary (Room 1, Chair: Dongsheng Xu, IMR-CAS, China) Property optimisation of titanium alloys based on phase stability evaluation and microstructure design Rui Yang, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China					08:30
09:20	Coffee Break					Coffee Break					09:20
	Symposium C-9 Chair: Vasily Bulatov , Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, United States of America	Symposium E-9 Chairs: Andrej Ostapovc , Institute of Physics of Materials ASCR, Czech Republic. Yujie Wei , Chinese Academy of Sciences, China	Symposium F-9 Chair: Ernst Kozeschnik , Institute of Materials Science and Technology, TU Wien, Austria	Symposium G-5 Chairs: Keonwook Kang , Yonsei University, Korea. Akiyuki Takahashi , Tokyo University of Science, Japan	Symposium O-9 Chairs: Yusuke Ootani , Tohoku University, Japan. Shuichi Uehara , Tohoku University, Japan	Symposium A-9 Chair: Eliot Fried , Okinawa Institute of Science and Technology, Japan	Symposium I-9 Chairs: Yuri Mishin , George Mason University, United States of America. Yang Xiang , Hong Kong University of Science and Technology, Hong Kong	Symposium D-1 Chairs: Daniel Urban , Fraunhofer IWM, Germany	Symposium H-7 Chair: Patrick R. Onck , Univ. of Groningen, Netherlands	Symposium B-5 Chair: Jean-Paul Crocombette , CEA, Univ. Paris-Saclay, France	
09:45	<i>Invited</i> Interstitial shuffling mechanism for solute-induced embrittlement of titanium Daryl C. Chrzan, Department of Materials Science and Engineering, University of California, Berkeley, United States of America	<i>Invited</i> The motion of a single dislocation from molecular dynamics simulations and its physical interpretation Yujie Wei, Chinese Academy of Sciences, China	<i>Invited</i> Programmable materials - tuning effective materials response Peter Gumbsch, Fraunhofer IWM, Germany	<i>Invited</i> Metallic materials under extreme pressure: interplay of plasticity and phase transitions Nina Gunkelmann, Clausthal University of Technology, Germany	<i>Invited</i> Combined experimental and computational study on the superlubricity mechanism of 2D materials at the microscale Tianbao Ma, Tsinghua University, China	Group-theoretical construction for constitutive equation of the first strain gradient elasticity Ryuichi Tarumi, Graduate School of Engineering Science, Osaka Univ., Japan	<i>Invited</i> Grain Boundary Microstates Under Irradiation: A Moment in Time? Mitra I. Taheri, Drexel University, Department of Materials Science & Engineering, United States of America	<i>Invited</i> Data-driven discovery of new materials Isao Tanaka, Dept. Materials Science and Engineering, Kyoto Univ., Japan	<i>Invited</i> Computational modeling approach for the rational design of DNA nanostructures Do-Nyun Kim, Department of Mechanical and Aerospace Engineering, Seoul National University, Korea	He impurities in boron carbide: structure, kinetics, and Raman signatures Guido Roma, CEA, Univ. Paris-Saclay, France	09:45
10:00						Physically based strain gradient plasticity model for length scale dependent yield strength Peter Gudmundson, Department of Solid Mechanics, KTH Royal Institute of Technology, Sweden					10:00
10:15	Screw dislocation mediated solution strengthening of substitutional α-Ti alloys - first principles investigation Piotr Kwasniak, Warsaw University of Technology, Poland	Atomistic study on the super-elasticity of single crystal bulk NiTi shape memory alloy under adiabatic condition Bing Wang, School of Mechanics and Engineering, Southwest Jiaotong University, China	Equilibrium crystal shape of GaAs by ab-initio thermodynamics In Won Yeu, Center for Electronic Materials, Korea Institute of Science and Technology, Korea	Dislocation dynamics modeling of fracture behavior with considering dislocation shielding effect Akiyuki Takahashi, Tokyo University of Science, Japan	Quantum chemistry vs. rheology of some EMIM-based ionic liquids Andras Vemes, AC2T research GmbH, Viktor-Kaplan-Str. 2/C, 2700 Wiener Neustadt, Austria	FTMP-based seamless description of deformation-fracture transitions Tadashi Hasebe, Kobe Univ., Japan	The role of grain boundaries under long-time radiation Jing Luo, Dalian University of Technology, China	<i>Invited</i> Machine learning and materials discovery Gus Hart, Brigham Young University, United States of America	Quantitative multiscale modelling of bionano interface Vladimir Lobaskin, School of Physics, University College Dublin, Ireland	Irradiation damage in nuclear graphite at the atomic scale Aïain Chartier, DEN, Service de la Corrosion et du Comportement des Matériaux dans leur Environnement, CEA Saclay, France	10:15
10:30	Microstructural effects on strain rate sensitivity in dual-phase titanium alloys Sana Waheed, Dept. of Mechanical Engineering, Imperial College London, UK	Atomistic modelling of fracture with non-linear elastic boundary conditions Punit Patel, University of Warwick, UK	Elastic field of lattice defects in low-dimensional nano-carbon materials Xiao-Wen Lei, Dept. of Mechanical Engineering, Univ. of Fukui, Japan	Dynamic behaviors of dislocations and grain boundaries induced by phonon scattering in nanoscale Soon Kim, Dept. of Mechanical Engineering, UNIST, Korea	Lubrication with a refrigerant: a challenge made possible thanks to fluid/surface chemistry Nicolas Fillard, Univ Lyon, INSA-Lyon, CNRS UMR5259, LaMCoS, F-69621 Villeurbanne, France	On the crucial role played by instantaneous and hidden multifield features of lattice dynamics in their nonlocal pseudocontinuum modeling Miguel Charlotte, University of Toulouse, Institute Clement Ader, CNRS - UMR 5312 INSAUPS/ISAE-SupAero/Mines Albi, France	<i>Invited</i> Quantifying point defect fluxes to interfaces and the role of interface structure Shen J Dillon, University of Illinois, United States of America		Multiscale modelling of intrinsically-disordered proteins Patrick R. Onck, University of Groningen, Netherlands	Using computational modeling to understand radiation damage tolerance in complex oxides both from the bottom-up and the top-down Blas Pedro Uberuaga, Los Alamos National Laboratory, United States of America	10:30
10:45	Understanding thermal alleviation in cold dwell fatigue in titanium alloys using crystal plasticity model Zehang Zheng, Dept. of Materials, Imperial College London, UK	Atomistic simulation of the deformation and crack nucleation mechanisms in titanium alloys Dongsheng Xu, Institute of Metal Research, Chinese Academy of Sciences, China		Investigation on $1/2\langle 111 \rangle$ and $1/2\langle 11\bar{1} \rangle$ mixed dislocations in BCC iron by classical molecular dynamics Tomohisa Kumagai, Central Research Institute of Electric Power Industry, Japan	Meso-scale SPH simulation for friction and wear between elastic-plastic solids with various asperities Natsuko Nakagawa Sugimura, Dept. of Mechanical Engineering, Tokyo City Univ., Japan		Data-driven materials design in an industrial environment Thomas Eckl, Robert Bosch GmbH, Germany	Tracing the interplay of polymer topology and hydrodynamics Lisa B. Weiss, University of Vienna, Austria	Development of defect mechanics-based multi-scale simulation techniques for reliability study of high performance electronic devices in radiation environments Yukeun Eugene Pak, Advanced Institutes Convergence Technology, Korea	10:45	
11:00	Break					Break					11:00
	Symposium C-10 Chair: Tomohito Tsuru , Japan Atomic Energy Agency, Japan	Symposium E-10 Chairs: Irene Beverlein , University of California at Santa Barbara, USA. Dongsheng Xu , Institute of Metal Research, CAS, China	Symposium F-10 Chair: Ricardo Lebensohn , Los Alamos National Laboratory, United States of America	Symposium G-6 Chairs: Akiyuki Takahashi , Tokyo University of Science, Japan. Keonwook Kang , Yonsei University, Korea	Symposium K-1 Chairs: Momoki Kubo , Institute for Materials Research, Tohoku University, Japan. Tomoki Niiyama , Kanazawa Univ., Japan	Symposium A-10 Chair: Steve Fitzgerald , University of Leeds, UK	Symposium I-10 Chair: Sanyu Fensin , Los Alamos National Lab, United States of America	Symposium D-2 Chair: Tilmann Hicke , MPIE, Germany	Symposium H-8 Chair: Patrick R. Onck , Univ. of Groningen, Netherlands	Symposium B-6 Chair: Jaime Marian , University of California Los Angeles, United States of America	
11:15	<i>Invited</i> First principles calculations of dislocations in model engineering alloys (Ni, Ni₃Al, hcp-Ti, and a refractory metal BCC-HEA) Christopher Woodward, Air Force Research Laboratory, United States of America	Study of atomic trajectories during twinning transformation in magnesium Andrej Ostapovc, Institute of Physics of Materials ASCR, Czech Republic	<i>Invited</i> Data analytics for mining process-structure-property linkages for hierarchical materials Surya Raju Kalidindi, Georgia Tech, United States of America	Repulsive correction in Tersoff potential for irradiated Si Younwan Jo, Kyung Hee University, Korea	Supercomputer post-K project "Challenge of basic science - exploring extremes through multi-physics and multi-scale simulations" Momoki Kubo, Tohoku Univ., Japan	Interdiffusion and atomic mobilities in fcc Ag-Mg, Ag-Mn and Ag-Mg-Mn alloy Qianhui Min, Powder Metallurgy Research Institute, Central South University, China	<i>Invited</i> Structure and mobility of dissociated vacancies at twist grain boundaries and screw dislocations in ionic compounds Blas Pedro Uberuaga, Los Alamos National Laboratory, United States of America	<i>Invited</i> Using machine-learning to create predictive material property models Chris Wolverton, Northwestern University, United States of America	<i>Invited</i> Modeling and simulation of DNA foldback intercoil structure Moon Ki Kim, School of Mechanical Engineering, Sungkyunkwan University, Korea	<i>Invited</i> Ion irradiation as a surrogate for reactor irradiation: the expected and the surprises Gary S Was, University of Michigan, United States of America	11:15
11:30		Understanding nanocontact plasticity through massive MD simulations Jorge Alcalá, Universidad Politécnica de Catalunya, Spain		Phase-field modeling of microstructural evolution of Fe-Cr-Al system Kunok Chang, Kyung Hee Univ., Kyung Hee Univ., Korea	<i>Invited</i> Universal avalanche statistics across 16 decades in length: from nanocrystals (and neurons) to earthquakes and stars? Karin Dahmen, University of Illinois at Urbana Champaign, United States of America	Stacking and multilayered nature of martensite in copper based shape memory alloys Osman Adiguzel, Firat University, Turkey					11:30
11:45	Hybrid QM/MM study of dislocation glide in tungsten in the presence of plasma components Petr Grgorev, Warwick Centre for Predictive Modelling, UK	Atomistically informed mesoscale modeling of fracture Hamad ul Hassan, ICAMS, Ruhr-Universität Bochum, Germany	Maximization of strengthening effect of microscopic morphology in duplex elastoplastic solids Ikumu Watanabe, National Institute for Materials Science, Japan	Dissolution kinetics of ejecta in hydrogen at megabar pressure Arsian B. Mazilov, Dukhov Research Institute of Automatics (VNIIA), Moscow, Russian Federation, Russia		Mesoscale understanding of ionic conduction in yttria stabilized zirconia Abhijit Chatterjee, Dept. of Chemical Engineering, Indian Institute of Technology Bombay, India	<i>Invited</i> Reverse engineering the kinetics of grain growth Carl Krill, Institute of Micro and Nanomaterials, Ulm University, Germany	Designing mesoscale structures of Li-ion battery electrode using FIB-SEM image via machine learning Yoichi Takagishi, Kobelco Research Institute Inc., Japan	DNA-particle vitrimer systems Francesco Sciortino, Sapienza Università di Roma, Italy	Dose effect on the irradiation induced loop density and Burgers vector in ion-irradiated ferritic/martensitic steel HT9 through in-situ TEM Djamel Kaoumi, North Carolina State University, United States of America	11:45
12:00	First-principles calculations of deformation twins in hexagonal titanium alloys Daisuke Matsunaka, Dept. of Mechanical Engineering, Shinshu Univ., Japan	Lattice distortion effect on cross-slip in high entropy alloys and Lennard-Jones systems for face-centered cubic Chao-Chun Yen, National Tsing Hua University, Taiwan	Assessment of formability limit diagram prediction by crystal plasticity finite element method Duancheng Ma, Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria	MD simulation study of displacement damage in bulk wurtzite GaN by proton irradiation Sang Hyuk Yoo, Dept. of Mechanical Engineering, Yonsei Univ., Korea	Predicting avalanches and failure: wood and paper Mikko Alava, Aalto University, Finland	Accelerating stochastic simulations with path integrals Steve Fitzgerald, University of Leeds, UK		Stability engineering of halide perovskite via machine learning Wan-Jian Yin, Soochow University, China	Relation between macroscopic flows in a contraction-expansion channel and dynamics of well-entangled polymer chains Takeshi Sato, Dept. of Chemical Engineering, Kyoto Univ., Japan	Novel deformation mechanism of helium irradiated copper Weizhong Han, Xi'an Jiaotong University, China	12:00
12:15		Atomic structure of gamma/alpha2 interface and its influence on plastic deformation of lamellar TiAl alloys Hao Wang, Institute of Metal Research, CAS, China	Analysis of gradient microstructures using crystal plasticity Balaji Selvarajou, IHPC, Singapore, Singapore		System-spanning shear avalanches induced by thermal structural relaxation in metallic glasses Tomoki Niiyama, College of Science and Engineering, Kanazawa Univ., Japan		Systematic evaluation of ionization potentials of divalent cation binary oxides Yoyo Hinuma, Center for Frontier Science, Chiba Univ., Japan	Origin of large scale spatial organization of DNA-polymer in bacterial chromosomes Aparajit Chatterji, IISER-Pune, India 411008, India	Isotope effect on quantum diffusion of interstitial hydrogen in face-centered cubic metals Haiime Kimizuka, Osaka University, Japan	12:15	
12:30	Lunch					Lunch					12:30

	Room 1	Room 2	Room 3	Room 4	Room 5	Room 6	Room 7	Room 8	Room 9	Room 10	
	Symposium C-11 Chair: Nikhil Chandra Admal , University of California Los Angeles, United States of America	Symposium E-11 Chairs: Xiaoyu Yang , Computer network information center, CAS, China, Denise Reimann , ICAMS, Ruhr-Universität Bochum, Germany	Symposium F-11 Chair: Peter Gumbsch , Fraunhofer IWM, Germany	Symposium N-5 Chair: Julia Rogal , ICAMS Ruhr University Bochum, Germany	Symposium K-2 Chairs: Ferenc Kun , University of Debrecen, Hungary, Jan Main , University of Edinburgh, UK		Symposium I-11 Chairs: Bob Svendsen , RWTH Aachen University, Germany, Jeremy K Mason , University of California, Davis, United States of America	Symposium D-3 Chairs: Danil Chrzan , UC Berkeley, USA	Symposium H-9 Chair: Kees Storm , Eindhoven University of Technology, Netherlands	Symposium B-7 Chair: Mariorie Bertolus , CEAD/ENDEC, Centre CEA de Cadarache, France	
14:00	<i>Invited</i> A multi-scale dislocation language - data mining, statistical analysis, and steps towards a community-driven data base Stefan Sandfeld , TU Bergakademie Freiberg, Germany	<i>Invited</i> Thermodynamically consistent directional distortional hardening of wrought Mg alloys: experimental investigation and constitutive modeling Baodong Shi , NECSR, School of Mechanical Engineering, Yanshan Univ., China	<i>Invited</i> Mesoscale plasticity models of polycrystalline materials for efficient computation of microstructure/property relationships Ricardo Lebensohn , Los Alamos National Laboratory, United States of America	<i>Invited</i> Understanding the impact of extended defects on the behaviour of C atoms: a multi technique approach Christophe Domain , EDF, France	<i>Invited</i> Predictability of catastrophic failure in porous media Jan Main , University of Edinburgh, UK		<i>Invited</i> Recent advances in the full-field modeling of microstructural evolutions using a finite-element level set integrated framework Daniel Pino Munoz , Mines ParisTech / PSL Research University, France	<i>Invited</i> Finding the needle in the haystack: materials discovery through high-throughput ab initio computing and data mining Geoffroy Hautier , Université catholique de Louvain, Belgium	<i>Invited</i> Micromechanics and instabilities in soft composite materials Stephan Rudykh , University of Wisconsin - Madison, United States of America	<i>Invited</i> Thermal properties of fluorite-type metal dioxides: CeO₂, ThO₂, UO₂, NpO₂, PuO₂ and AmO₂ Masato Kato , Japan Atomic Energy Agency, Japan	14:00
14:15											14:15
14:30	The effect of dislocation character on dislocation line tension in bcc tungsten and its impact on kink-pair enthalpy David Cereceda , Dept. of Mechanical Engineering, Villanova University, United States of America	A computational infrastructure for multiscale materials simulation Xiaoyu Yang , Computer network information center of the Chinese Academy of Sciences, China	Development of a new consistent discrete Green operator for FFT-based methods to solve heterogeneous problems with eigenstrains Kornlavi Senyo Fioh , University of Lorraine, France	Localised on-the-fly kinetic Monte Carlo Johannes Bulin , Fraunhofer-Institut SCAI, Germany	Deciphering the dynamics of precursors to failure in quasi-brittle solids: an inspiration for understanding the statistics of earthquakes ? Laurent Ponson , Institut Jean le Rond d'Alembert, CNRS - Sorbonne University, Paris, France		<i>Invited</i> The effect of strong anisotropic grain boundary energy and mobility on microstructure formation and evolution: mesoscale modeling and simulation Brandon Runnels , University of Colorado Colorado Springs, United States of America	High-entropy alloys investigation using machine-learned potentials Tatiana Kostuchenko , Dept. of Material Science and Engineering, Skolkovo Institute of Science and Technology, Moscow, Russia	Deformation analysis of UV curing 3d printed materials by combined molecular dynamics-finite element method Gunjin Yun , Seoul National University, Korea	SCIANTIX: a new inert gas behaviour module ready for use Davide Pizzocci , Politecnico di Milano, Italy	14:30
14:45	Atomistic modeling of thermally activated plasticity in UO₂ Jean-Paul Crocombette , CEA Saclay, SRMP, France	Using machine learning methods to homogenize damage from micro- to macroscale Alexander Hartmaier , ICAMS, Ruhr-Universität Bochum, Germany	Efficient FFT-based homogenisation without linear reference medium Till Jung , EPFL, Mech. Engineering, Multiscale Mechanics Modeling, Switzerland	A preconditioning scheme for minimum energy path finding methods Sela Makri , University of Warwick, UK	Avalanche precursors and fracture strength in the limit of high disorder Ferenc Kun , Department of Theoretical Physics, University of Debrecen, Hungary			Stability evaluation of high-entropy alloys via accurate on-lattice model Evgenii Meshkov , All-Russian Research Institute of Automatics (VNIIA), Russia	Modelling and 3D printing Kelvin cell acoustic metamaterial Huina Mao , Dept. of Aeronautical and Vehicle Engineering, KTH Royal Institute of Technology, Sweden	Modeling swelling in U₃Si₂ nuclear fuel using a multi-scale computational approach Larry Aagesen , Idaho National Laboratory, United States of America	14:45
15:00	FTMP-based simulations and evaluation of geometrically-necessary boundaries (GNBs) of dislocation Shiro Ihara , Dept. of Mechanical Engineering, Kobe Univ., Japan	Graph theory analysis of rich fiber-scale data yields very fast simulations of damage evolution in composites Brian N Cox , Arachne consulting, United States of America	Multiscale modelling of the effective viscoplastic behavior of constituents of the mantle transition zone (Mg₂SiO₄ wadsleyite and ringwoodite): bridging atomic and polycrystal scales Patrick Cordier , Unité Matériaux et Transformations, CNRS / Univ. Lille, Lille, France	<i>Invited</i> Temperature programmed molecular dynamics - accessing rare events using a combination of finite time sampling and bias potentials Abhijit Chatterjee , Dept. of Chemical Engineering, Indian Institute of Technology Bombay, India	Jump statistics of epicenters in thermally induced cracking of fiber bundles Naoki Yoshioka , RIKEN Center for Computational Science, Japan		<i>Invited</i> A machine learning exploration of grain boundary mobility mechanisms Srikanth Patela , North Carolina State University, United States of America	Atomistically informed atomic mobility databases for continuum diffusion simulations Karin Abrahams , Scalebridging Thermodynamic and Kinetic Simulation (ICAMS), Ruhr-University Bochum, Germany	Theoretical approach for EUV resist fabrication: DFT-MD-FDM study Muyoung Kim , Division of Multiscale Mechanical Design, School of Mechanical and Aerospace Engineering, Seoul National University, Korea	<i>Invited</i> Why multiscale modeling of nuclear fuel is absolutely essential and why it is so challenging Michael R Tonks , University of Florida, United States of America	15:00
15:15	Improved phase field model of dislocation intersections Songlin Zhang , China Academy of Engineering Physics, China	A deep learning-based constitutive model for finite element analysis Angelo Simone , University of Padova, Italy	Scalable and directionally-sensitive three-dimensional quantifying of orientation and dislocation density gradients in crystal plasticity computer simulations Markus Kuehbach , Max-Planck-Institut für Eisenforschung GmbH, Germany		Time dependent fracture under unloading in a fiber bundle model Reka Korei , Department of Theoretical Physics, University of Debrecen, Hungary			The european materials modelling council: standardization, interoperability and data management tools for materials modelling Luca Bergamasco , Politecnico di Torino, Italy			15:15
15:30	Coffee Break					Coffee Break					15:30
	Symposium C-12 Chair: Irene Beverlein , University of California at Santa Barbara, United States of America	Symposium E-12 Chairs: Baodong Shi , NECSR, School of Mechanical Engineering, Yanshan Univ., China, Liqang Zhang , Central South University, China	Symposium F-12 Chair: Yasushi Shibuta , The University of Tokyo, Japan	Symposium N-6 Chair: Chad W Sinclair , Dept. of Materials Engineering, University of British Columbia, Canada	Symposium K-3 Chairs: Takashi Hatano , University of Tokyo, Japan, Akio Nakahara , Nihon Univ., Japan		Symposium I-12 Chairs: Blas Pedro Uberuaga , Los Alamos National Laboratory, United States of America, Chris P Race , University of Manchester, UK	Symposium D-4 Chairs: Minoru Ojani , AIST, Japan	Symposium H-10 Chair: Kees Storm , Eindhoven University of Technology, Netherlands	Symposium B-8 Chair: Guang-Hong Lu , Beihang University, China	
16:00	Modeling the interaction between martensitic phase transformations and dislocation dynamics Rachel Derby , TU Bergakademie Freiberg, Germany	Diffusivities and atomic mobilities in bcc Ti-Mo-Nb-Ta-Zr alloys Weimin Bai , School of Materials Science and Engineering, Central South Univ., China	<i>Invited</i> Microstructure formation in large-scale molecular dynamics simulation Yasushi Shibuta , The University of Tokyo, Japan	<i>Invited</i> Modelling metals, alloys and cement paste across length and time scales Laurent Karim Beland , Queen's University, Canada	<i>Invited</i> Creep of strongly disordered materials: plasticity, damage and approach to failure Michael Zaiser , Inst., of Materials Simulation, Dept. of Materials Science, FAU University of Erlangen-Nuremberg, Germany		<i>Invited</i> Formation and shrinkage of grain boundary loops in two-dimensional colloidal crystals Roel Dullens , University of Oxford, UK	<i>Invited</i> Exploration of large ab initio data spaces to design structural materials with superior mechanical properties Joerg Neugebauer , Max-Planck-Institut fuer Eisenforschung, Germany	<i>Invited</i> In silico design of self-assembly nanostructured polymer systems by multiscale molecular modelling Maurizio Fermeglia , University of Trieste, Italy	Kinetic Monte Carlo study of tungsten fuzz formation under low energy helium irradiation Zhangcan Yang , School of Energy and Power Engineering, Huazhong University of Science and Technology, China	16:00
16:15	The effect of microscopic slip deformation on the yield stress in dispersion hardened alloys analyzed by using crystal plasticity FEM Yelm Okuyama , Dept. of Materials Science and Engineering, Kyushu University, Japan	Design of Ti-alloy by integrating high throughput experiments and calculations Liqang Zhang , Central South University, China							Constrained thermodynamic model for multi-component alloys under irradiation: a matrix formulation from first-principles Hamiltonian Duc Nguyen-Manh , Materials Science and Scientific Computing Department, Culham Centre for Fusion Energy, UKAEA, UK	16:15	
16:30	Deformation behaviour for two-phase composites under large deformations using micromechanical analysis Srihari Dodla , Madanapalle Institute of Technology (MITS) Madanapalle, India	Simulation of plasticity in amorphous solids Shingo Urata , Innovative Technology Research Center, Asahi Glass Co., Ltd (AGC), Japan	Directed assembly of structured nanoparticles through rapid micromixing Arash Nikoubashman , Johannes Gutenberg University of Mainz, Germany	BCA-MD-KMC hybrid simulation for long time helium plasma irradiation inducing fuzzy nanostructure on tungsten Atsushi M Ito , National Institute for Fusion Science, National Institutes of Natural Sciences, Japan	Creep rupture and Omori-Utsu law: fiber bundle model approach Takashi Hatano , University of Tokyo, Japan		Growth and characterization of two-dimensional poly(quasi)crystals Petri Hirvonen , Dept. of Applied Physics, Aalto Univ., Finland	Toward a machine learning aided interatomic potential for multi-element alloys: application to binary compounds Doyl Dickey , Mississippi State University, United States of America	Dynamical properties of suspensions of star block-copolymers in shear flow. Diego Felipe Jaramillo-Cano , Faculty of Physics, University of Vienna, Austria	Kinetic Monte-Carlo simulations of radiation damage in W(Re,Os) alloys Matthew James Lloyd , Department of Materials, University of Oxford, UK	16:30
16:45	Dislocation dynamics simulation of FCC single crystals in high strain rate deformation Ronan Madec , CEA, DAM, DIF, France	Computational generation of the yield surfaces using stress based loading Mayank Chouksey , Indian Institute of Technology, Kanpur, India	Various interfaces related to twinning in hexagonal metals Vaclav Paidar , Institute of Physics AS CR Prague, Czech Republic	Atomistic modelling of pipe diffusion: a direct comparison of MD, KMC, aKMC and DMD Erik Bitzek , FAU Erlangen-Nuernberg, Germany	Temperature dependent shear friction in metallic glass Akio Ishii , Osaka Univ., Japan		A parallel algorithm for high resolution 3D phase field simulations of polycrystalline solidification Pavel Strachota , Czech Technical University in Prague, Czech Republic	Machine learning potentials for modeling irradiation defects in iron and tungsten Alexandra Gonjaveva , DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France	Heterogeneous flow and internal friction in amorphous carbon Richard Jana , Albert Ludwigs Universitaet Freiburg, Germany	Modeling Re-precipitate hardening in neutron irradiated W and W-Re alloys: from point defects to macroscopic hardening Jaime Marian , University of California Los Angeles, United States of America	16:45
17:00	Comparison of two methods to cross-slip modeling by means of mathematical theory of moving curves Miroslav Kolar , Czech Technical University in Prague, Czech Republic		Multiscale mean-field modelling of mechanochemical processes in heterogeneous materials for energy storage Mikhail Poluektov , International Institute for Nanocomposites Manufacturing, WMG, University of Warwick, UK	Strategies for optimal construction of Markov chain representations of atomistic dynamics Danny Perez , Los Alamos National Laboratory, United States of America	Mechanism of controlled crack formation induced by memory effect of clay paste Akio Nakahara , Nihon Univ., Japan		Properties of β/w phase interfaces in Ti and their implications on mechanical properties and ω morphology Shuo Cao , Institute of Metal Research, Chinese Academy of Science, China	Effect of friction and ductility on relaxation dynamics and mechanical memory of crumpled materials Mahdi Habibi , Wageningen University, Netherlands	Increasing the thermal conductivity of polymer nanocomposites filled with carbon nanotubes via molecular dynamics simulation Yangyang Gao , Beijing University of Chemical Technology, China	<i>Invited</i> In-situ TEM of formation processes of defects in tungsten under irradiation: comparison between electron and self-ion irradiations Kazuto Arakawa , Shimane University, Japan	17:00
17:15			Impact of local symmetry breaking on the physical properties of tetrahedral liquids Rui Shi , University of Tokyo, Japan	Simulating the collective diffusion mechanism of amorphous solids at experimentally relevant time scales Yunjiang Wang , Institute of Mechanics, Chinese Academy of Sciences, China	Effects of shockwave-induced nanobubble collapse on precision polishing: molecular dynamics study Yoshimasa Aoyama , Dept. of Materials Science, Tohoku Univ., Japan			Big-data insights into solute-GB segregation Liam Huber , MPIE, Germany	Thermal transport in polymer-based nanocomposite materials across multiple scales Matteo Fasano , Energy Department, Politecnico di Torino, Italy		17:15
19:00 - 21:00	Banquet Taiko-En					Banquet Taiko-En					19:00 - 21:00

	Room 1	Room 2	Room 3	Room 4	Room 11	Room 6	Room 7	Room 8	Room 9	Room 10	
08:00	Registration					Registration					08:00
08:30	Plenary (Room 1, Chair: Karin Dahmen, University of Illinois at Urbana Champaign, USA) Integrated earthquake simulation enhanced with high performance computing Muneo Hori, Earthquake Research Institute, The University of Tokyo, Japan					Plenary (Room 1, Chair: Karin Dahmen, University of Illinois at Urbana Champaign, USA) Integrated earthquake simulation enhanced with high performance computing Muneo Hori, Earthquake Research Institute, The University of Tokyo, Japan					08:30
09:20	Coffee Break					Coffee Break					09:20
	Symposium C-13 Chair: Jaafar A. El-Awady, Johns Hopkins University, United States of America	Symposium E-13 Chairs: Erik Bitzek, FAU Erlangen-Nuernberg, Germany, Kisaragi Yashiro, Gifu University, Japan	Symposium F-13 Chair: Takayuki Aoki, Tokyo Institute of Technology, Japan	Symposium N-7 Chair: Shotaro Hara, Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan	Symposium K-4 Chairs: Tetsuo Mohri, IMR, Tohoku University, Japan, Akihiro Nakatani, Dept. of Adaptive Machine Systems, Osaka Univ., Japan			Symposium D-5 Chairs: Jora Neugebauer, MPIE, Germany	Symposium H-11 Chair: Erik Van der Giessen, University of Groningen, Netherlands	Symposium B-9 Chair: Michael Tonks, University of Florida, United States of America	
09:45	Invited Mesoscopic studies of slip and twinning processes in hcp polycrystalline materials Irene Reyberlein, University of California at Santa Barbara, United States of America	Invited 3D aspects of fracture in crack – obstacle interactions and effects of crack front curvature Erik Bitzek, FAU Erlangen-Nuernberg, Germany	Invited Advanced analysis tools for atomistic microstructure modeling Alexander Stukowski, Dept. of Materials Science, Darmstadt University of Technology, Germany	Invited Bridging time scales with variationally enhanced sampling Omar Valsson, Max Planck Institute for Polymer Research, Germany	Invited Disclination dipole model of kink deformation in layered solid Akihiro Nakatani, Dept. of Adaptive Machine Systems, Osaka Univ., Japan			Invited Computational exploration of strong permanent magnet compounds Takashi Miyake, CD-FMat, AIST, Japan	A hierarchical multiscale simulations approach for modeling failure in polymer matrix composites Jaafar A. El-Awady, Johns Hopkins University, United States of America	Ab initio modeling of self-interstitial and vacancy migration in zirconium Emmanuel Clouet, CEA Saclay, France	09:45
10:00									Some Positive Aspect of Structural Defects in Graphene/Polymer Nanocomposites Studied by Ab-initio, Molecular Dynamics, and Continuum Approaches Seunghwa Yang, Chung-Ang University, Korea	Atomistic modelling of point defect clusters in zirconium and impact on the microstructure evolution and crystal growth under irradiation Ludovic Thuinat, UMET, UMR CNRS 8207, Lille university, F-59655 Villeneuve d'Ascq, France	10:00
10:15	Crystal plasticity formulation involving volume fraction-based deformation twinning model Yuichi Tadano, Department of Mechanical Engineering, Saga University, Japan	Vortex instabilities in the deformation of Cu/Au nanolaminates Lars Pastewka, University of Freiburg, Germany	Studying thermo-oxidative degradation of polyimide in oxygen environment using MD simulations Ashwani Kumar Sengar, IIT Kanpur, India	Simulations of branched polyelectrolytes Filip Uhlík, Charles University, Czech Republic	Large-scale coarse-grained molecular dynamics simulations on fracture processes of lamellar structure in crystalline polymers Yuji Higuchi, The University of Tokyo, Japan			A machine-learning approach for finding new hard-magnetic phases Daniel F. Urban, Fraunhofer IWM, Freiburg, Germany	Linear and non-linear viscoelastic properties of model fractal-like aggregates polymer nanocomposites Samy Merabia, CNRS and Université Lyon 1, France	Modeling of dislocation climb assisted glide in crystal plasticity models Ankan Alankar, IIT Bombay, India	10:15
10:30	An elastic-viscoplastic crystal plasticity modeling for plane strain deformation of pure magnesium Weidong Song, Beijing Institute of Technology, China	Molecular dynamics simulation of the interaction between grain boundary and point defects Liang Zhang, The University of Tokyo, Japan	In-plane characterization of structural and thermodynamic properties for steps at faceted chemically heterogeneous solid/liquid interfaces Hongtao Liang, School of Physical and Material Science, East China Normal University, China	Adaptive resolution simulations coupling molecular dynamics to dissipative particle dynamic Matej Praprotnik, National Institute of Chemistry, Slovenia	Grain boundary sliding within the entropy production rate theory Tetsuo Mohri, IMR, Tohoku University, Japan			High-throughput optimization of finite temperature phase stabilities of Ce-based hard magnetic materials Tilmann Hickel, Max Planck Institut für Eisenforschung, Germany	Topological defect structure in the self-assembly of semiflexible polymers under spherical confinement Mihir Khadilkar, Johannes Gutenberg University Mainz, Germany, Germany	The role of oxide grain boundaries in the oxidation of zirconium alloy fuel cladding Maria S Yankova, Materials Performance Centre, School of Materials, University of Manchester, UK	10:30
10:45	The minimum energy pathways identifications of twinning dislocation loop nucleation of extension twinning in magnesium Xiao-Zhi Tang, Inst. of Mechanics, Beijing Jiaotong Univ.	Deformation mode analysis by the eigenvectors of the atomic elastic stiffness Kisaragi Yashiro, Gifu University, Japan	Design of neural network for thermodynamics data of non-equilibrium multiphase field model Hiroshi Wakameda, ITOCHU Techno-Solutions Corporation, Japan	Using diffusive molecular dynamics simulations to investigate grain boundary segregation and grain boundary structural transformations Chad W Sinclair, Dept. of Materials Engineering, University of British Columbia, Canada	Molecular dynamics simulation on intergranular cracking mechanism of iron material in high temperature pressurized water environment Qian Chen, Institute for Materials Research, Tohoku University, Japan			Understanding pairwise magnetic interactions in Fe-based materials with machine learning techniques Osamu Waseda, MPIE, Germany	Molecular dynamics simulation of the detachment force between graphene and epoxy resin Kazuki Mori, ITOCHU Techno-Solutions Corporation, Japan	Advances in X-ray diffraction line profile analysis of dislocation Loops in Zr - insights from atomistic modelling Chris P. Race, University of Manchester, UK	10:45
11:00	Break					Break					11:00
		Symposium E-14 Chairs: Thierry Auger, CNRS, France, Jamila Rahmoun, LAMIH-ENSIAME, Valenciennes University, France	Symposium F-14 Chair: Markus Kuehbach, Max-Planck-Institut für Eisenforschung GmbH, Germany		Symposium K-5 Chairs: Masanori Kohyama, AIST, Japan, Masatake Yamauchi, Japan Atomic Energy Agency, Japan			Symposium D-6 Chairs: Daniel Urban, Fraunhofer IWM, Germany	Relation between deformation and electrical conductivity for electroconductive polymer nanocomposites with highly segregated structure Oleg V. Lebedev, Skolkovo Institute of Science and Technology, Russia	Symposium B-10 Chair: Frederic Soisson, CEA Saclay, France	
11:15		Stability controlled crack evolution in staggered laminate bio-material Yi Yan, Dept. of Adaptive Machine Systems, Osaka University, Japan	Invited Large-scale multiphase flow simulations on a GPU supercomputer Takayuki Aoki, Tokyo Institute of Technology, Japan		Effects of a bulk-region size in the first-principles tensile test of a grain boundary Masanori Kohyama, AIST, Japan			Invited Novel two-dimensional materials: materials discovery, data provenance, and workflow reproducibility. Nicola Marzari, EPFL, Switzerland		Sink strengths of point defects near tilt grain boundaries: a phase field model Pengchuan Liu, Institute of Materials, China academy of engineering physics, China	11:15
11:30		A brittle to ductile transition modeling for liquid metal embrittlement Thierry Auger, CNRS, France			Combined analysis of first-principles calculations and fracture mechanics experiments on intergranular embrittlement of an alloy steel Masatake Yamauchi, Japan Atomic Energy Agency, Japan					Modelling swelling and growth under irradiation using the phase field method Daniel Schwen, Dept. of Fuels Modeling and Simulation, Idaho National Laboratory, United States of America	11:30
11:45		Buckling delamination of ductile thin films on rigid substrates Nadia Ben Dahmane, Univ. Grenoble Alpes, SIMAP, F-38000 Grenoble, France	Transport properties of fluid mixtures in micro- and mesoporous kerogen membrane Patrick Alain Bonnaud, University of Pau and Adour Countries, France		First-principles local energy analysis of grain boundary segregation of sp-elements on bcc Fe Kazuma Ito, Osaka University, Japan			In silico screening of metal-organic frameworks for adsorption driven heat pumps and chillers Mate Erdos, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Netherlands		Phase-field modelling of dislocation loop evolution under irradiation : application to radiation induced segregation prediction near the dislocation cores Gabriel Franck Bouobda Moladje, CNRS, université de Lille, France	11:45
12:00		An analytical model of the peeling forces at edges of multilayers subjected to temperature variations Chengyin Zhang, Shanghai Institute of Applied Mathematics and Mechanics, Shanghai University, China	Numerical simulation of ionic transport through deformable porous media: application to cortical bone tissue modeling Jana Turjanicova, Dept. of Mechanis, Univ. of West Bohemia in Pilsen, Czech Republic		Fast and scalable prediction of local energy at grain boundaries: machine-learning based modeling of first-principles calculations Tomoyuki Tamura, Nagoya Institute of Technology, Japan			Machine learning assisted by first-principles calculations for designing intermetallic-typed metallic glasses Tokuteru Uesugi, Dep. of Materials Science, Osaka Prefecture Univ., Japan		Theoretical derivation of the ABVI model from cluster expansion Hamiltonian Antonio Fernandez Caballero, School of Mechanical, Aerospace and Civil Engineering, University of Manchester, UK	12:00
12:15		Characterization and multi-scale modeling of the mechanical response of the human humerus under dynamic loading Jamila Rahmoun, LAMIH-ENSIAME, Valenciennes University, France									12:15
12:30	Poster award / Closing remark (Room 1)					Poster award / Closing remark (Room 1)					12:30