

	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 (Room 1)</i> <b>Amorphous Materials on the Meso-scale: Achieving Experimental Length and Timescales</b> Christopher A. Schuh, Department of Materials Science and Engineering, MIT, USA					<i>Plenary (Room 1)</i> <b>Amorphous Materials on the Meso-scale: Achieving Experimental Length and Timescales</b> Christopher A. Schuh, Department of Materials Science and Engineering, MIT, USA					10:10
11:00	<i>Plenary (Room 1)</i> <b>Multiscale Modeling and Realization of Photo-responsive Polymers</b> Maenghyo Cho, School of Mechanical and Aerospace Engineering, Seoul National University, KOREA					<i>Plenary (Room 1)</i> <b>Multiscale Modeling and Realization of Photo-responsive Polymers</b> Maenghyo Cho, School of Mechanical and Aerospace Engineering, Seoul National University, KOREA					11:00
11:50	Lunch					Lunch					11:50

	Symposium C-1	Symposium E-1	Symposium F-1	Symposium I-1	Symposium O-1	Symposium J-1	Symposium M-1	Symposium L-1	Symposium A-1		
	<b>Symposium C-1</b> <i>Chair:</i> Emmanuel Clouet, CEA Saclay, SRMP, France		<b>Symposium F-1</b> <i>Chair:</i> Yunzhi Wang, The Ohio State University, United States of America		<b>Symposium O-1</b> <i>Chairs:</i> Lars Pastewka, University of Freiburg, Germany. Izabela Szlufarska, University of Wisconsin, United States of America	<b>Symposium J-1</b> <i>Chairs:</i> Jinghong Fan, Alfred University, United States of America. Sinan Keten, Northwestern University, United States of America	<b>Symposium M-1</b> <i>Chair:</i> Thomas Voigtmann, German Aerospace Center, Cologne, Germany	<b>Symposium L-1</b> <i>Chairs:</i> Jerome Weiss, CNRS/ University of Grenoble-Alpes, France. Yinan Cui, University of California, Los Angeles, United States of America	<b>Symposium A-1</b> <i>Chair:</i> Anton Van der Ven, University of California Santa Barbara, United States of America		
13:30	<i>Invited</i> <b>Kinetic Monte Carlo model of screw dislocation-solute coevolution in W-Re alloys</b> Jaime Marian, Dept. of Materials Science and Engineering, University of California Los Angeles, United States of America		<i>Invited</i> <b>An Integrated Experimental and Computational Approach to Microstructure-Property Relationships in Structural Materials</b> Yunzhi Wang, The Ohio State University, United States of America		<b>A numerical insight into third body flow regimes within dry contacts</b> Guilhem Mollon, INSA Lyon - LaMCoS, France	<i>Invited</i> <b>A multiscale failure analysis for layered composites with statistical account of manufacturing defects</b> Ramesh Talreja, Texas A&M University, United States of America	<i>Invited</i> <b>Structure-property Relations in Sheared Dense Flocculated Suspensions</b> Jan Vermant, ETH Zurich, Switzerland	<i>Invited</i> <b>Flow and failure of (amorphous) materials - a nonequilibrium phase transition?</b> Peter Schall, University of Amsterdam, Netherlands	<i>Invited</i> <b>Atomistic to continuum: coarse-graining in and out of equilibrium</b> Celia Reina, University of Pennsylvania, United States of America	13:30	
13:45					<b>A novel multiscale framework for modeling of diamond tools wear</b> Adriana Quacquarelli, Université de Lyon, LaMCoS, INSA-Lyon, CNRS UMR5259, F-69621, France					13:45	
14:00	<b>Thermally activated solute-drag strengthening by interstitial impurities in BCC Cr</b> Christian Brandl, Karlsruhe Institute of Technology, Germany		<b>Development of a multiscale simulation system based on microstructure of fine-grained aluminum</b> Atsushi Sagara, Dept. of Finemechanics, Tohoku Univ., Japan		<b>A Micro/Macro multi-physical approach to model braking materials</b> Mathieu Renouf, LMGC, CNRS, Univ. Montpellier, France	<i>Invited</i> <b>Multiscale Modeling of Fiber Reinforced Materials for Future Aerospace Structures</b> Anthony M Waas, U., Washington, Seattle, WA 98195; also Univ. of Michigan, Aerospace Engineering, Ann Arbor, MI 48109, United States of America	<i>Invited</i> <b>Yielding, annealing, and memory in cyclically deformed glasses</b> Srikanth Sastry, JNCASR, India	<i>Invited</i> <b>Reversibility and Criticality in Amorphous and Crystalline Solids</b> Charles Reichhardt, Los Alamos National Laboratory, United States of America	<b>Finite-temperature Localized Stress and Strain for Atomic Models</b> Ranganathan Parthasarathy, Tennessee State University, United States of America	14:00	
14:15	<b>Generalized yield criterion in BCC metals from first principles</b> Antoine Kraych, Institut Lumière Matière, Université Lyon 1, France		<b>Image-based crystal plasticity analysis on the activities of slip systems in polycrystal alpha-Ti</b> Yoshiki Kawano, Kitami Institute of Technology, Japan		<b>Thermodynamics of sliding contact: Joule-Thomson effect</b> Vera Deeva, Tomsk Polytechnic University, Russia				<b>Uncertainty Quantification for Classical Effective Potentials</b> Sarah Longbottom, School of Engineering, University of Warwick, UK	14:15	
14:30	<b>Dislocation Motion in High Entropy Alloys</b> Luchan Zhang, National University of Singapore, Singapore		<b>Micro structure-based Crystal Plasticity Modeling of Duplex Titanium Alloy During Hot Deformation</b> Jun Zhang, Institute of Systems Engineering, China Academy of Engineering Physics, China		<b>Sliding contact mechanics of thin viscoelastic layers with rough profiles</b> Nicola Menga, Department of Mechanics, Mathematics and Management, Polytechnic University of Bari, Italy	<i>Invited</i> <b>A-DISC (Adaptive Discrete-Smeared Crack) Model for Multi-Scale Progressive Damage Analysis of Composite Structures</b> Tong-Earn Tay, National University of Singapore, Singapore	<b>Linear viscoelasticity on matter out of equilibrium</b> Leticia Lopez-Flores, Universidad Autonoma de San Luis Potosi, Mexico	<i>Invited</i> <b>Exploring Crystal-plastic Constitutive Rules with the OOF Tool</b> Andrew Reid, NIST, United States of America	<b>The role of null-lagrangians in the continuum interpolation of the linear chain with hyper-pre-stress</b> Alexandre Danescu, Ecole Centrale de Lyon, France	14:30	
14:45	<b>Modeling the climb-assisted glide of edge dislocations through a random distribution of nanosized vacancy clusters</b> Marie Landeiro Dos Reis, SRMP-CEA Saclay, France		<b>Nonlocal multiscale modeling of deformation behavior of polycrystalline copper by second-order homogenization method</b> Makoto Uchida, Osaka city Univ., Japan		<b>The adhesive behavior of elastic contacts in the presence of interfacial shear stresses</b> Giuseppe Carbone, Department of Mechanics, Mathematics and Management - Polytechnic University of Bari, Italy		<b>Memory effects in functional polymers: The interplay between entropic elasticity and kinetic arrest</b> Fathollah Varnik, Ruhr-University Bochum, Germany		<b>Practical Time Averaging of nonlinear dynamics</b> Amit Acharya, Carnegie Mellon University, United States of America	14:45	
15:00			<b>Residual stress prediction for turning of Ti-6Al-4V considering the microstructure evolution</b> Donald S Shih, Magnesium Research Center, Kumamoto University, Japan		<b>Soft Matter Mechanics: numerical and experimental methodologies for dry and lubricated tribological problems</b> Carmine Putignano Putignano, Polytechnic University of Bari, Italy	<b>Analysis for the Plane Problem of Layered Magnetolectric Composite with Collinear Interfacial Cracks</b> Wenxiang Tian, School of Aerospace Engineering and Applied Mechanics, Tongji Univ, China	<b>Modelling and Experimental Verified Coupled Visco hyper electro-elastic Behaviour of Dielectric Elastomer Circular Actuator</b> Arpit Srivastava, IIT KANPUR, INDIA - 208016, India	<b>Objective fusion of multiscale experiments and multiscale models using Bayesian inference</b> Surya Raju Kalidindi, Georgia Tech, United States of America		15:00	
15:15	Coffee Break					Coffee Break					15:15

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	<b>Symposium C-2</b> <i>Chair:</i> Stefan Sandfeld, Chair of Micromechanical Materials Modelling, TU Bergakademie Freiberg, Germany	<b>Symposium E-2</b>	<b>Symposium F-2</b> <i>Chair:</i> Selim Esedoglu, University of Michigan, United States of America	<b>Symposium I-2</b>	<b>Symposium O-2</b> <i>Chairs:</i> Mark Owen Robbins, Johns Hopkins University, United States of America. Tasuku Onodera, Hitachi, Ltd., Japan	<b>Symposium J-2</b> <i>Chairs:</i> Anthony Waas, University of Washington, United States of America. Junqian Zhang, Shanghai University, China	<b>Symposium M-2</b> <i>Chair:</i> Emanuela Zaccarelli, University of Rome I, Italy	<b>Symposium L-2</b> <i>Chairs:</i> Charles Reichhardt, Los Alamos National Laboratory, United States of America. Peter Schall, University of Amsterdam, Netherlands		<b>Symposium A-2</b> <i>Chair:</i> Celia Reina, University of Pennsylvania, United States of America	
15:45	<i>Invited</i> <b>Finite deformation Mesoscale Field Dislocation Mechanics</b> Amit Acharya, Carnegie Mellon University, United States of America		<i>Invited</i> <b>New algorithms for simulating grain boundary motion</b> Selim Esedoglu, University of Michigan, United States of America		<b>Two simple models for pull-off decay of self-affine rough surfaces</b> Antonio Papangelo, Politecnico di Bari, Italy	<i>Invited</i> <b>Simulation-based Design of Bioinspired Impact-resistant Nanocellulose Films with Bouligand Microstructure</b> Sinan Ketten, Northwestern University, United States of America	<b>MMM in aircraft industries: use cases for simulation of additive manufacturing</b> Annett Seide, MTU Aero Engines AG, Germany	<i>Invited</i> <b>The role of system size, internal disorder, and dislocation patterning on the nature of plastic fluctuations</b> Jerome Weiss, CNRS/University of Grenoble-Alpes, France		<i>Invited</i> <b>Bridging the chasm between phenomenological theories and electronic structure</b> Anton Van der Ven, University of California Santa Barbara, United States of America	15:45
16:00					<b>Droplet Spreading on a Surface Exhibiting Solid-liquid Interfacial Premelting</b> Yang Yang, East China Normal University, China		<b>VISCOELASTIC BEHAVIOUR OF HETEROGENEOUS MATERIALS STUDIED THANKS TO AN EXTENSION OF CRAFT SOFTWARE IN HARMONIC REGIME</b> Julien Boisse Boisse, University of Lorraine, France, France				16:00
16:15	<b>Anisotropic and non-symmetric continuum dislocation dynamics</b> Thomas Hochrainer, TU Graz, Austria		<b>The Role of Grain Shape in Discrete Element Modeling of Snow Mechanics</b> Carolin Willibald, Institute for Snow and Avalanche Research (SLF, ETH), Switzerland		<b>Comparative Study on the Adsorption of Volatile Organic Compounds on the Surfaces of Two-Dimensional Materials: Toward the Early Lung Cancer Detection</b> Van An Dinh, Nanotechnology Program, Vietnam Japan University, Viet Nam	<i>Invited</i> <b>Amelogenesis: Nature's 3D printing system for multi-scale laminates</b> Brian Cox, Arachne Consulting, United States of America	<b>Multi-scale modelling of Zener Pinning during the solid solution treatment of a Nickel-based Superalloy</b> Magnus Jack Anderson, The University of Birmingham, UK	<i>Invited</i> <b>Temporal and spatial plastic instability of micrometer-scaled materials</b> Yinan Cui, Mechanical and Aerospace Engineering Department, University of California, Los Angeles, United States of America		<b>Two-component Dirac-Kohn-Sham calculation for multiscale modeling of materials</b> Koichi Nakamura, Kyoto Univ. Japan	16:15
16:30	<b>Numerical simulation of model problems in Plasticity based on Field Dislocation Mechanics</b> Leo Morin, PIMM, Arts et Métiers-ParisTech, CNAM, CNRS, UMR 8006, 151 bd de l'Hopital, 75013 Paris, France		<b>Experimental-Computational Analysis of Primary Static Recrystallization in DC04 Steel</b> Martin Diehl, Max-Planck-Institut fuer Eisenforschung GmbH, Germany		<b>Adsorption of the Volatile Organic Compounds on Graphene including Van de Waals Interaction</b> Thi Viet Bac Phung, Nanotechnology Program, Vietnam Japan University - Vietnam National University, Viet Nam		<b>Assessment of residual stresses in welds made of multiphase alloys</b> Victor De rancourt, Commissariat a l'energie atomique, France			<b>Combination of Kinetic Monte Carlo Method and First Principles Calculation to Explore Stable Structure of Solute Cluster in Al-Si Based Alloys</b> Kenjiro Sugio, Hiroshima Univ., Japan	16:30
16:45	<b>Direct computation of the stress field due to geometrically necessary dislocation densities</b> Yichao Zhu, Dalian University of Technology, China		<b>Large scale phase-field simulations of solid state sintering</b> Johannes Hoetzer, Karlsruhe University of Applied Sciences, Germany		<b>Diffusion of a Cu nanodroplet on an amorphous carbon surface</b> Yu-Chen Chiu, National Chiao Tung University, Taiwan	<b>Role of geometrical features on mechanical properties in bio-inspired staggered composites</b> Siladitya Pal, Indian Institute of Technology Roorkee, India	<b>Atomic analysis of crystalline nucleation and growth in the supercooled liquid of glass-forming binary alloy</b> Masato Wakeda, Research Center for Structural Materials, National Institute for Materials Science, Japan	<b>Dislocations associated with stick-slip friction of lubricants in boundary lubrication</b> Yongsheng Leng, George Washington Univ, United States of America		<b>Electronic structure analysis of Fermi level instability in Fe-rich Si alloy</b> Chen Ying, School of Engineering, Tohoku University, Japan	16:45
17:00	<b>Meshfree Analysis for Kink Band Formation in Mg-based LPSO Phase Based on Crystal Plasticity Cosserat Model Considering Disclination Density</b> Yuichi Kimura, Grad. School of Science and Technology, Keio Univ., Japan		<b>Phase-field simulations of coupled dendritic-eutectic growth</b> Marco Seiz, Institute of Applied Materials - Computational Materials Science, Karlsruhe Institute of Technology, Germany		<b>First principal modeling of oxygen and carbon adsorption on Fe (110) surface with symmetrical tilt Sigma3(111) grain boundary</b> Ivan Lobzenko, Toyota Technological Institute, Japan	<b>Dynamic homogenization for acoustic metamaterials</b> Celia Reina, University of Pennsylvania, United States of America	<b>Crystal growth in fluid flow: Nonlinear response effects</b> Hailong Peng, German Aerospace Center, Germany	<b>Comparison of surface-indentation and pillar-compression at the nanoscale of FCC metals: Unification of size effects using 3D Discrete Dislocation Dynamics</b> Hengxu Song, west virginia university, United States of America		<b>From first-principles defect chemistry to device damage models of radiation effects in III-V semiconductors</b> Peter A Schultz, Sandia National Laboratories, United States of America	17:00
17:15	<b>Dynamic recrystallization model for Mg/LPSO alloys coupling phase-field model and dislocation-based crystal plasticity model</b> Sho Kujirai, Grad. School of Science and Technology, Keio Univ., Japan		<b>The use of thermodynamic tensor models for phase-field simulations of spinodal decomposition in quaternary alloys coupled with CALPHAD data</b> Yuri Amorim Coutinho, Dept. of Materials Engineering, KU Leuven, Belgium		<b>Theoretical study of the effects of boron doping on the electronic structure of g-C3N4/TiO2(001) heterojunction</b> Jianhong Dai, Harbin Institute of Technology at weihai, China	<b>Cracking behavior of ferrite-pearlite pipeline steel with hierarchical and concurrent multiscale modeling schemes</b> Taolong Xu, Southwest Petroleum University of China, China	<i>Invited</i> <b>Time-dependent active microrheology in dilute colloidal suspensions</b> Thomas Franosch, Innsbruck Univ., Austria	<b>Statistical models for cross slip and reaction rate processes in continuum dislocation dynamics</b> Vignesh Vivekanandan, Purdue University, United States of America		<b>How to model ordering processes in metallic hydrides? A Tight-Binding Ising modeling proposal and its application to Zr-H</b> Paul Eyméoud, Institut de Radioprotection et de Sécurité Nucléaire/PSN-RES/SEMIA/LPTM, France	17:15
17:30								<b>Designing Interfaces: a combinatorial approach to geometrical manipulation of interfaces</b> Hakan Yavas, Czech Technical University, Czech Republic			17:30
17:45 - 20:00	<b>Poster session 1 - Wine &amp; cheese party</b>					<b>Poster session 1 - Wine &amp; cheese party</b>					17:45 - 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) Plasticity in crystals and glasses: from the atoms up David Rodney, Institut Lumière Matière, University of Lyon, France					Plenary (Room 1) Plasticity in crystals and glasses: from the atoms up David Rodney, Institut Lumière Matière, University of Lyon, France					08:30
09:20	Coffee Break					Coffee Break					09:20
	<b>Symposium C-3</b> Chair: Francois Willaime, DEN-Departement des Materiaux pour le Nucleaire, CEA, Universite Paris-Saclay, France	<b>Symposium E-3</b>	<b>Symposium F-3</b> Chair: Carl Krill, Institute of Micro and Nanomaterials, Ulm University, Germany	<b>Symposium I-3</b>	<b>Symposium O-3</b> Chairs: Momiji Kubo, Tohoku University, Japan. Michael Moseler, Fraunhofer Institute for Mechanics of Materials IWM, Germany	<b>Symposium J-3</b> Chairs: Ramesh Talreja, Texas A&M University, United States of America. Tong-Earn Tay, National University of Singapore, Singapore	<b>Symposium M-3</b> Chair: Thomas Franosch, University of Innsbruck, Austria	<b>Symposium L-3</b> Chairs: Peter M Derlet, Paul Scherrer Institut, Switzerland. Cynthia Reichhardt, Los Alamos National Laboratory, United States of America	<b>Symposium H-1</b> Chair: Turab Lookman, Los Alamos National Laboratory, United States of America	<b>Symposium A-3</b> Chair: Katsuyo Thornton, University of Michigan, Ann Arbor, United States of America	
09:45	Invited Quantifying the effect of hydrogen on dislocation dynamics in microcrystals: A three-dimensional discrete dislocation dynamics study Jaafar El-Awady, Johns Hopkins University, United States of America		Invited Biomineralization in molluscan shells: From ideal to hierarchical grain growth Dana Zoellner, B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany		Invited Scale Dependence of Friction: How Elasticity Destroys Superlubricity Mark Owen Robbins, Dept. of Physics and Astronomy, Johns Hopkins University, United States of America	Invited Fundamentals of Generalized Particle (GP) Multiscale Methods with Applications to Analyses of Alternatively-Arranged Soft and Hard Layers Jinghong Fan, Kazuo Inamori School of Engineering, Alfred University, United States of America	Invited Heterogeneous thermal properties in a glass from molecular dynamics calculations Jean-Louis Barrat, Univ. Grenoble Alpes, France	Invited Mechanics of Dislocation-density Fields on Different Length Scales Alfonso H.W. Ngan, University of Hong Kong, Hong Kong	Invited Multiscale modeling of electro-responsive gels Masao Doi, Beihang University, China	Invited Challenges and gaps in length and time scaling of dislocation models David L McDowell, Woodruff School of Mechanical Engineering, Georgia Institute of Technology, United States of America	09:45
10:00											10:00
10:15	Discrete dislocation plasticity modelling of hydrogen dislocation interactions in micro-cantilevers Haiyang Yu, Dept. of Materials, Univ. of Oxford, UK		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		Coarse-Grain Simulations of Polymer Solutions with Hydrodynamics and Long-range Interactions Hitoshi Washizu, Univ. Hyogo, Japan	The effect of layer thickness ratio on the plastic deformation mechanisms of nonoriented Ti/TiN nanolayered composite: A molecular dynamics study Georges Y Ayoub, Dept. of Industrial and manufacturing system Engineering, Univ. of Michigan, United States of America	Structural-dynamical phase transition in the phase space of histories of a polydisperse hard sphere liquid Matteo Campo, Johannes Gutenberg University Mainz, Germany, Germany	Invited Discrete dislocation dynamics simulations of complexity in crystal plasticity: strain burst statistics and machine learning Lasse Laurson, Aalto University, Finland	Non-monotonic particle size effect on the glass transition in polymer-particle blends and its application to shape memory polymers Elias M. Zirdehi, Ruhr-University Bochum, Germany	From discrete to continuum dislocations and back: a two dimensional study of microstructure and interaction energies. Hengxu Song, TU Bergakademie Freiberg, Germany	10:15
10:30	Dislocation climb models from atomistic scheme to dislocation dynamics Yang Xiang, Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong		Actuation in Metal-Polymer Nanocomposites: Chemoelectromechanical Coupling on Interfaces Jana Wilmers, Chair of Solid Mechanics, University of Wuppertal, Germany		A Multi-Scale Approach for the Design of Novel Lubricants Georgios Bletsos, National Technical University of Athens, Greece	The attenuation of stress wave propagation in multilayer structure Fengyuan Yang, Tsinghua University, China	Soft deformable colloids make strong liquids with stress-driven relaxation Emanuela Zaccarelli, CNR Institute for Complex Systems, Rome, Italy		Thermomechanical behavior of shape-memory polyurethane copolymer: A coarse-grained molecular dynamics simulation Sungwoo Park, Seoul National University, South Korea, Korea	Advances in microstructure prediction: a FFT-based Dislocation Dynamics approach Francesca Bolioli, LEM, CNRS-ONERA, Chatillon, France	10:30
10:45	Investigation of the Hall-Petch Effect with DD Simulation Maoyuan Jiang, EDF - R&D, Les Renardières, France		Design of spontaneous formation-based 3D plasmonic optical structure, using multiphysics modeling Jihwan Song, Dept. of Mechanical Engineering, Hanbat National University, Korea		Impact of ionic liquid ordering on their triborheological properties Konstantinos Gkagkas, Advanced Material Research Division, Toyota Motor Europe NV/SA, Belgium	Multiscale molecular-dynamics simulations of structure and mechanics of polymer nanocomposites Alexey Lyulin, Group Theory of Polymers and Soft Matter, Eindhoven University of Technology, Netherlands	Time- and History-dependent Structure and Morphology of van-der-Waals Liquids forming Physical Gels and Porous Glasses Magdaleno Medina-Noyola, Instituto de Fisica, Universidad Autonoma de San Luis Potosi, Mexico	Nanoindentation in the ultra-nano scale: Microstructure-property relationships using statistical approaches Stefanos Papanikolaou, west virginia university, United States of America	Investigation of photo-mechanical behavior of azobenzene-based polymer: A coarse-grained molecular dynamics study Junghwan Moon, School of Mechanical and Aerospace Engineering, Seoul National University, Korea	Plasticity and microstructure evolutions at the mesoscale: towards and integrated framework. Laurent Capolungo, Los Alamos National Laboratory, United States of America	10:45
11:00	Break					Break					11:00
	<b>Symposium C-4</b> Chair: Dan Mordehai, Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel, Israel	<b>Symposium E-4</b>	<b>Symposium F-4</b> Chair: Dana Zoellner, B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany	<b>Symposium I-4</b>	<b>Symposium O-4</b> Chairs: Aichiro Nakano, Univ. of Southern California, United States of America. Shandan Bai, KYOCERA Cop., Japan	<b>Symposium J-4</b> Chairs: Brian Cox, Arachne Consulting Inc., United States of America. Tomonaga Okabe, Tohoku University, Japan	<b>Symposium M-4</b> Chair: Leticia Lopez Flores, University of San Luis Potosi, Mexico	<b>Symposium L-4</b> Chairs: Lasse Laurson Aalto University, Finland. Alfonso H.W. Ngan, University of Hong Kong, Hong Kong	<b>Symposium H-2</b> Chair: Hansohl Cho, Los Alamos National Laboratory, United States of America	<b>Symposium A-4</b> Chair: David L McDowell, Woodruff School of Mechanical Engineering, Georgia Institute of Technology, United States of America	
11:15	Invited Hydrogen consequences on cyclic behaviour of <001> nickel single crystals: a multi-scale approach. Xavier Feaugas, Universite de la rochelle, France		Invited Showdown! Pitting computer simulations against time-resolved experimental measurements of grain growth in 3D Carl Krill, Institute of Micro and Nanomaterials, Ulm University, Germany		Invited Molecular simulation to better understand soot-detergent interactions in engine oils Sophie Loehle, Total M&S, France	Invited Validation of analytical models for ply cracking of general symmetric composite laminates Tomonaga Okabe, Department of Aerospace Engineering, Tohoku University, Japan	Invited Mechanical behavior and emerging morphologies in active matter Ignacio Pagonabarraga, CECAM, EPFL, Switzerland	Invited Dynamic phases, pinning, and pattern formation for driven dislocation assemblies Cynthia Reichhardt, Los Alamos National Laboratory, United States of America	Invited Hydrogels with Dynamic Sacrificial Bonds- From Toughness to Adhesion to Composites - Jian Ping Gong, Faculty of Advanced Life Science, Hokkaido University, Japan	Invited Effective Transport Properties of Polycrystalline Materials Katsuyo Thornton, University of Michigan, Ann Arbor, United States of America	11:15
11:30											11:30
11:45	Atomistic and continuum approaches to analyse precipitation hardening in metallic alloys Javier Llorca, IMDEA Materials Institute, Spain		Coarsening and grain-growth in an SOFC-anode under surface and grain boundary self-diffusion: A Multiphase-field approach Paul Hoffrogge, Karlsruhe University of Applied Sciences, Germany		A Molecular Dynamics Study on the Wear Mechanisms of Hydrogenated Diamond-like Carbon Yang Wang, Institute for Materials Research, Tohoku University, Japan	Invited Two-way coupled modeling of lithium diffusion and diffusion induced finite elastoplastic bending of bilayer electrodes in lithium-ion batteries Junqian Zhang, Shanghai University, China	Time dependent interaction between intruders in granular media Hisao Hayakawa, Yukawa Institute for Theoretical Physics, Kyoto University, Japan	Invited Intermittent micro-plasticity and its relation to dislocation structure - a linear stability analysis. Peter M Derlet, Paul Scherrer Institut, Switzerland	Elastic properties and effective interactions of <i>in silico</i> realistic microgels Lorenzo Rovigatti, Institute for Complex Systems, Uos Sapienza - CNR, Italy	A new E-VPSC polycrystal formulation: fundamentals Carlos Tome, Los Alamos National Laboratory, United States of America	11:45
12:00	Dislocation-precipitate interaction in Al-Mg-Si alloys Inga Gudem Ringdalen, Dept. of Materials and Nanotechnology, SINTEF, Norway		Solidification Simulation in Additive Manufacturing Process of Ti-Alloy by ICME approach Yusuke Shimono, Itochu Techno-Solutions Corp., Japan		Effect of Tribochemical Reactions on Diamond-like Carbon and Wear under Water Lubrication: A Molecular Dynamics Simulation Investigation Jing Zhang, Inst. for Materials Research, Tohoku Univ., Japan		History-dependent shear jamming of granular materials under oscillatory shear Michio Otsuki, Graduate School of Engineering Science, Osaka Univ., Japan		Integrated modeling and experiments of viscoelastic gels Shawn Chester, New Jersey Institute of Technology, United States of America	A new E-VPSC polycrystal formulation: applications Youngung Jeong, Changwon National Univ., Korea	12:00
12:15			Phase Field Model of Microstructural Evolution in Metal Alloy for Designing Mechanical Property Dongchoul Kim, Dept. of Mechanical Engineering, Sogang Univ., Korea		Formation Mechanism of Tribofilm of Silicon Carbide under Water Lubrication: Molecular Dynamics Simulations Fumiya Nakamura, Tohoku Univ., Japan	Micro-Scale Model of Thermomechanics in Solidifying Saturated Porous Media Michal Benes, Czech Technical University in Prague, Czech Republic	Structural predictor for nonlinear sheared dynamics in simple glass-forming liquids Trond S. Ingebrigtsen, University of Tokyo, Japan	Effect of solute atoms and Peierls stress on the critical behaviour of discrete dislocations Peter Dusan Ispanovity, Eotvos University, Hungary	Study on viscoelastic behavior of natural rubber with multiscale approach Byungjo Kim, Seoul National University, Korea	Modeling microstructural material variability with uncertainty quantification and machine learning techniques Reese Jones, Sandia National Laboratories, United States of America	12:15
12:30	Lunch					Lunch					12:30
14:00	Excursion					Excursion					14:00

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08:00	Registration					Registration					08:00
08:30	Plenary (Room 1) Grain Boundary Sliding, Fracture and Dislocation Motion in Ceramics Yuichi Ikuhara, The University of Tokyo/Japan Fine Ceramics Center, Japan					Plenary (Room 1) 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	Symposium F-5 Chair: Ingo Steinbach, Ruhr-University Bochum, Germany	Symposium I-5	Symposium O-5 Chairs: Hitoshi Washizu, University of Hyogo, Japan. Sophie Loehle, TOTAL Marketing & Services, Solaize, France	Symposium B-1 Chair: Lorenzo Malerba, SCK-CEN, the Belgian Nuclear Energy Research Centre, Belgium	Symposium N-1 Chair: Danny Perez, Los Alamos National Laboratory, United States of America	Symposium G-1 Chairs: Byeongchan Lee, KyungHee Univ., Korea. Keonwook Kang, yonsei university, Korea	Symposium H-3 Chair: Hansohl Cho, Los Alamos National Laboratory, United States of America	Symposium A-5 Chair: Sinisa Dj Mesarovic, Washington State University, United States of America	
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 Solidification microstructure formation by phase-field simulation with multi-GPU acceleration Tomohiro Takaki, Kyoto Institute of Technology, Kyoto Institute of Technology, Japan		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	Thermal stability of carbon-vacancy complexes in iron alloys and steels Milan J Konstantinovic, Belgian nuclear institute, SCK.CEN, Belgium	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 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 1 Kaushik Bhattacharya, California Institute of Technology, United States of America	Invited Parameters to consider in the modelling of dislocation boundary evolution Grethe Winther Winther, Technical University of Denmark, Denmark	09:45
10:00						Computational study of phosphorus 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 Guenole, Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Germany		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		Unveiling the chemical reactions involved in moisture-induced weakening of adhesion between aluminum and epoxy resin: a hybrid quantum-classical simulation study Shuji Ogata, Nagoya Institute of Technology, 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	Invited From transition states to dynamics over long time scales Graeme Henkelman, University of Texas at Austin, United States of America	Molecular dynamics study of the bulk cascades in W-Re alloy Hyunggyu 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	Data Mining of Indentation Induced Dislocation Microstructures Dominik Steinberger, Chair of Micromechanical Materials Modelling, TU Bergakademie Freiberg, Germany	10:15
10:30	Nucleation of dislocation in ultra-hard ceramic nanoparticles modelled by molecular dynamics and nudged elastic band simulations Jonathan Amodeo, MATEIS, Univ. Lyon 1, France		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 Uranagase, Nagoya Institute of Technology, Japan	Computational Design of Radiation Damage Tolerant Single-Phase Alloys Penghui Cao, MIT, United States of America		Defect Energetics in W-Based Transition-Metal Ternary Systems Youngguk Shin, KyungHee Univ., Korea	Structural properties of mixtures of stars polymers and long chains Emanuele Locatelli, Faculty of Physics, University of Vienna, Austria	local-energy and local-stress analysis of tensile behaviours of tilt and twist grain boundaries in Al and Cu Hao Wang, Shanghai Univ., China	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		Phase field modeling of deformation twinning in beta-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	Multiscale modelling of radiation damage evolution in Fe and Fe-based alloys Fredric Granberg, Department of Physics, University of Helsinki, Finland		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	Lattice continua for polycrystal grains: Climb and glide of dislocations, diffusion and grain boundary kinematics. Sinisa Dj Mesarovic, Washington State University, United States of America	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	Symposium F-6 Chair: Benoit Appolaire, Institut Jean Lamour, Univ. de Lorraine, France	Symposium I-6	Symposium O-6 Chairs: Yoshitaka Umeno, The University of Tokyo, Japan. Yoshinori Shihara, Toyota Technological Institute, Japan	Symposium B-2 Chair: Davide Pizzocri, Politecnico di Milano, Italy	Symposium N-2 Chair: Graeme Henkelman, University of Texas at Austin, United States of America	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 Silberstein, Cornell University, United States of America	Symposium A-6 Chair: Markus Lazar, Darmstadt University of Technology, Germany	
11:15	Invited Effect of interstitial solutes on the structure and mobility of screw dislocations in bcc metals Francois Willaime, DEN-Département des Matériaux pour le Nucléaire, CEA, Université Paris-Saclay, France		Invited Atomistically informed full-field simulation of tempered martensite: Quenching, tempering and mechanical characterization Ingo Steinbach, Ruhr-University Bochum, Germany		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 Atomic scale calculations of nuclear fuel properties to sustain multiscale modeling of fuel behavior Emeric Bourasseau, CEA/DEN/DEC, Centre CEA de Cadarache, France	Invited Modeling Microstructure Evolution in Rapid Solidification Phenomena Using Structural Phase Field Crystal Models Nikolas Provatas, McGill University, Canada	Multiscale modeling of strength enhancement of aluminium honeycombs under combined shear-compression at high strain rate Han Henri 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 Design of patchy nanoparticles via the self-assembly of triblock terpolymers in selective solvents Eliot Fried, Okinawa Institute of Science and Technology, Japan	11:15
11:30								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		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		On the potential use of liquid crystals as 'smart' lubricants – an MD simulation study Kerstin Falk, Dept. of Tribology, Fraunhofer IWM, Freiburg, Germany	Influence of vibrational entropy on the concentrations of uranium vacancies in UO Jean-Paul Crocombette, CEA Saclay, France	Invited Accelerated Sampling with Local Entropy Gideon Simpson, Drexel University, United States of America	Finite element analysis of the effect of interfacial bubbles on performance of epoxy coatings under the alternating hydrostatic pressure Li Liu, Institute of Metal Research, Chinese Academy of Sciences, China	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	Nanoporous Composites: Giving Polymers Strength and Helping Metals Move Emma Griffiths, University of Cape Town, South Africa	11:45
12:00	Investigation of the energy pathway for generation of dislocations in silicon at E3 grain boundaries with the kinetic Activation-Relaxation Technique Simen Nut Hansen Eliassen, Norwegian Univ. of Science and Technology, Norway		3D modeling of microstructure evolution in Ni-based superalloys under creep loading Maeva Cottura, Institut Jean Lamour, France		Sliding on physisorbed cetyltrimethylammonium bromide (CTAB) Johannes Laurin Hoermann, University of Freiburg, Germany	Modelling of defect and rare gas transport properties in UO atomic to the grain Marjorie Bertolus, CEA, DEN, France		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 Nitin Krishnamurthy Hansoge, Northwestern University, United States of America	Multiscale modeling of advanced materials for hybrid organic-inorganic solar cells Alexander E. Kobryn, Nanotechnology Research Center, National Research Council Canada, Canada	12:00
12:15	Prediction of mechanical twinning in post-perovskite structure Philippe Carrez, Lille University, Lab. UMET UMR-CNRS 8207, France		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	Intragranular bubble impact on nuclear fuel thermomechanical properties Fabienne Ribeiro, Institut de Radioprotection et de Sécurité Nucléaire/PSN-RES/SEMIA/LPTM, France, France		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 Astronomy, Johns Hopkins Univ., United States of America	From cellulose and lignin to kerogen: molecular simulations of a geological process Roland Pellenq, <MSE>2, MIT- CNRS - AMU, United States of America	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		
<b>08:00</b>	<b>Registration</b>				<b>Registration</b>				<b>08:00</b>		
<b>08:30</b>	<i>Plenary</i> (Room 1) <b>Property optimisation of titanium alloys based on phase stability evaluation and microstructure design</b> Rui Yang, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China				<i>Plenary</i> (Room 1) <b>Property optimisation of titanium alloys based on phase stability evaluation and microstructure design</b> Rui Yang, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China				<b>08:30</b>		
<b>09:20</b>	<b>Coffee Break</b>				<b>Coffee Break</b>				<b>09:20</b>		
	<b>Symposium C-9</b> <i>Chair:</i> Vasily Bulatov, Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, United States of America	<b>Symposium E-9</b>	<b>Symposium F-9</b> <i>Chair:</i> Ernst Kozeschnik, Institute of Materials Science and Technology, TU Wien, Austria	<b>Symposium I-9</b>	<b>Symposium O-9</b> <i>Chair:</i> Yusuke Ootani, Tohoku University, Japan. Shuichi Uehara, Tohoku University, Japan	<b>Symposium B-5</b> <i>Chair:</i> Jean-Paul Crocombette, CEA, Univ. Paris-Saclay, France	<b>Symposium G-5</b> <i>Chair:</i> Keonwook Kang, yonsei university, Korea. Akiyuki Takahashi, Tokyo University of Science, Japan	<b>Symposium D-1</b>	<b>Symposium H-7</b> <i>Chair:</i> Patrick R. Onck, Univ. of Groningen, Netherlands	<b>Symposium A-9</b> <i>Chair:</i> Eliot Fried, Okinawa Institute of Science and Technology, Japan	
<b>09:45</b>	<i>Invited</i> <b>Interstitial Shuffling Mechanism for Solute-Induced Embrittlement of Titanium</b> Daryl C. Chrzan, Department of Materials Science and Engineering, University of California, Berkeley, United States of America		<i>Invited</i> <b>Programmable Materials - tuning effective materials response</b> Peter Gumbsch, Fraunhofer IWM, Germany		<i>Invited</i> <b>Combined experimental and computational study on the superlubricity mechanism of 2D Materials at the microscale</b> Tianbao Ma, Tsinghua University, China	<b>He impurities in boron carbide : structure, kinetics, and Raman signatures</b> Guido Roma, CEA, Univ. Paris-Saclay, France	<i>Invited</i> <b>Metallic materials under extreme pressure: Interplay of plasticity and phase transitions</b> Nina Gunkelmann, Clausthal University of Technology, Germany	<i>Invited</i> <b>Data-Driven Discovery of new materials</b> Isao Tanaka, Dept. Materials Science and Engineering, Kyoto Univ. , Japan	<i>Invited</i> <b>Computational modeling approach for the rational design of DNA nanostructures</b> Do-Nyun Kim, Department of Mechanical and Aerospace Engineering, Seoul National University, Korea	<b>From gradient elasticity to Angström-mechanics of dislocations</b> Markus Lazar, Darmstadt University of Technology, Germany	<b>09:45</b>
<b>10:00</b>					<b>Irradiation damage in nuclear graphite at the atomic scale</b> Alain Chartier, DEN, Service de la Corrosion et du Comportement des Matériaux dans leur Environnement, CEA Saclay, France					<b>Group-theoretical construction for constitutive equation of the first strain gradient elasticity</b> Ryuichi Tarumi, Graduate School of Engineering Science, Osaka Univ., Japan	<b>10:00</b>
<b>10:15</b>	<b>Screw dislocation mediated solution strengthening of substitutional <math>\alpha</math>-Ti alloys - First principles investigation</b> Piotr Kwasniak, Warsaw University of Technology, Poland		<b>Towards the understanding and prediction of weight-specific saturation magnetization of cemented carbides by means of first-principles magnetic moment calculations – Effect of solutes in the binder phase</b> Martina Lattemann, Sandvik Coromant R&D, Sweden		<b>Quantum chemistry vs. rheology of some EMIM-based ionic liquids</b> Andras Veres, AC2T research GmbH, Viktor-Kaplan-Str. 2/C, 2700 Wiener Neustadt, Austria	<b>Using computational modeling to understand radiation damage tolerance in complex oxides both from the bottom-up and the top-down</b> Blas Pedro Uberuaga, Los Alamos National Laboratory, United States of America	<b>Dislocation dynamics modeling of fracture behavior with considering dislocation shielding effect</b> Akiyuki Takahashi, Tokyo University of Science, Japan	<i>Invited</i> <b>Machine Learning and Materials Discovery*</b> Gus Hart, Brigham Young University, United States of America	<b>Quantitative Multiscale Modelling of Bionano Interface</b> Vladimir Lobaskin, School of Physics, University College Dublin, Ireland	<b>Physically based strain gradient plasticity model for length scale dependent yield strength</b> Peter Gudmundson, Department of Solid Mechanics, KTH Royal Institute of Technology, Sweden	<b>10:15</b>
<b>10:30</b>	<b>Microstructural effects on strain rate sensitivity in dual-phase titanium alloys</b> Sana Waheed, Dept. of Mechanical Engineering, Imperial College London, UK		<b>Equilibrium crystal shape of GaAs by ab-initio thermodynamics</b> In Won Yeu, Center for Electronic Materials, Korea Institute of Science and Technology, Korea		<b>Lubrication with a refrigerant : a challenge made possible thanks to fluid/surface chemistry</b> Nicolas Fillot, Univ Lyon, INSA-Lyon, , CNRS UMR5259, LaMCoS, F-69621 Villeurbanne, France	<b>Development of defect mechanics-based multi-scale simulation techniques for reliability study of high performance electronic devices in radiation environments</b> Yukeun Eugene Pak, Advanced Institutes Convergence Technology, Korea	<b>Dynamic behaviors of dislocations and grain boundaries induced by phonon scattering in nanoscale</b> Soon Kim, Dept. of Mechanical Engineering, UNIST, Korea		<b>Multiscale modelling of intrinsically-disordered proteins</b> Patrick R. Onck, University of Groningen, Netherlands	<b>FTMP-based Seamless Description of Deformation-Fracture Transitions</b> Tadashi Hasebe, Kobe Univ., Japan	<b>10:30</b>
<b>10:45</b>	<b>Understanding thermal alleviation in cold dwell fatigue in titanium alloys using crystal plasticity model</b> Zebang Zheng, Dept. of Materials, Imperial College London, UK		<b>Elastic field of lattice defects in low-dimensional nano-carbon materials</b> Xiao-Wen Lei, Dept. of Mechanical Engineering, Univ. of Fukui, Japan		<b>Meso-scale SPH simulation for friction and wear between elastic-plastic solids with various asperities</b> Natsuko Nakagawa Sugimura, Dept. of Mechanical Engineering, Tokyo City Univ., Japan	<b>Using IM3D to simulate nano-beam and nano-target effects in ion radiation</b> Ju Li, Massachusetts Institute of Technology, United States of America	<b>Investigation on 1/2&lt;11-1&gt;{112} and 1/2&lt;11-1&gt;{123} mixed dislocations in BCC iron by classical molecular dynamics</b> Tomohisa Kumagai, Central Research Institute of Electric Power Industry, Japan	<b>Data-Driven Materials Design in an Industrial Environment</b> Thomas Eckl, Robert Bosch GmbH, Germany	<b>Inter-chain cross-correlations of entangled polymers for multi-chain models</b> Yuichi Masubuchi , Nagoya Univ., Japan	<b>On the crucial role played by instantaneous and hidden multifield features of lattice dynamics in their nonlocal pseudocontinuum modeling</b> Miguel Charlotte, University of Toulouse, Institute Clement Ader, CNRS – UMR 5312 INSA/UPS/SAE-SupAero/Mines Albi, France	<b>10:45</b>
<b>11:00</b>	<b>Break</b>				<b>Break</b>					<b>11:00</b>	
	<b>Symposium C-10</b> <i>Chair:</i> Tomohito Tsuru, Japan Atomic Energy Agency, Japan	<b>Symposium E-10</b>	<b>Symposium F-10</b> <i>Chair:</i> Ricardo Lebensohn, Los Alamos National Laboratory, United States of America	<b>Symposium I-10</b>	<b>Symposium K-1</b> <i>Chair:</i> Momoji Kubo, Institute for Materials Research, Tohoku University, Japan. Tomoaki Niiyama, Kanazawa Univ., Japan	<b>Symposium B-6</b> <i>Chair:</i> Jaime Marian, University of California Los Angeles, United States of America	<b>Symposium G-6</b> <i>Chair:</i> Akiyuki Takahashi, Tokyo University of Science, Japan. Keonwook Kang, yonsei university, Korea	<b>Symposium D-2</b>	<b>Symposium H-8</b> <i>Chair:</i> Patrick R. Onck, Univ. of Groningen, Netherlands	<b>Symposium A-10</b> <i>Chair:</i> Mikhail Tashkinov, Perm National Research Polytechnic University, Russia	
<b>11:15</b>	<i>Invited</i> <b>First Principles Calculations of Dislocations in Model Engineering Alloys (Ni, Ni3Al, hcp-Ti, and a Refractory Metal BCC-HEA)</b> Christopher Woodward, Air Force Research Laboratory, United States of America		<i>Invited</i> <b>Data Analytics for Mining Process-Structure-Property Linkages for Hierarchical Materials</b> Surya Raju Kalidindi, Georgia Tech, United States of America		<b>Supercomputer Post-K Project “Challenge of Basic Science – Exploring Extremes through Multi-Physics and Multi-Scale Simulations”</b> Momoji Kubo, Tohoku Univ., Japan	<i>Invited</i> <b>Ion Irradiation as a Surrogate for Reactor Irradiation: The Expected and the Surprises</b> Gary S Was, University of Michigan, United States of America	<b>Repulsive Correction in Tersoff Potential for Irradiated Si</b> Youhwan Jo, Kyung Hee University, Korea	<i>Invited</i> <b>Using Machine-Learning to Create Predictive Material Property Models</b> Chris Wolverton, Northwestern University, United States of America	<i>Invited</i> <b>Modeling and Simulation of DNA Foldback Intercoll Structure</b> Moon Ki Kim, School of Mechanical Engineering, Sungkyunkwan University, Korea	<b>Interdiffusion and atomic mobilities in fcc Ag-Mg, Ag-Mn and Ag-Mg-Mn alloy</b> Qianhui Min, Powder Metallurgy Research Institute, Central South University, China	<b>11:15</b>
<b>11:30</b>					<b>Predicting avalanches and failure: wood and paper</b> Mikko Alava, Aalto University, Finland		<b>Phase-field modeling of microstructural evolution of Fe-Cr-Al system</b> Kunok Chang, Kyung Hee Univ., Kyung Hee Univ., Korea			<b>Stacking and Multilayered Nature of Martensite in Copper Based Shape Memory Alloys</b> Osman Adiguzel, Firat University , Turkey	<b>11:30</b>
<b>11:45</b>	<b>Hybrid QM/MM study of dislocation glide in tungsten in the presence of plasma components</b> Petr Grigorev, Warwick Centre for Predictive Modelling, UK		<b>Maximization of strengthening effect of microscopic morphology in duplex elastoplastic solids</b> Ikumu Watanabe, National Institute for Materials Science, Japan		<i>Invited</i> <b>Universal avalanche statistics across 16 decades in length: From nanocrystals (and neurons) to earthquakes and stars?</b> Karin Dahmen, University of Illinois at Urbana Champaign, United States of America	<b>Dose Effect on the Irradiation Induced Loop Density and Burgers Vector in Ion-Irradiated Ferritic/Martensitic Steel HT9 Through In-Situ TEM</b> Djamel Kaoumi, North Carolina State University, United States of America	<b>Dissolution kinetics of ejecta in hydrogen at megabar pressure</b> Arslan B. Mazitov, Dukhov Research Institute of Automatics (VNIIA), Moscow, Russian Federation, Russia	<b>Designing mesoscale structures of Li-ion battery electrode using FIB-SEM image via machine learning</b> Yoichi Takagishi, Kobelco Research Institute Inc., Japan	<b>DNA-particle vitrimer systems</b> Francesco Sciortino, Sapienza Universita' di Roma, Italy	<b>Mesoscale understanding of ionic conduction in yttria stabilized zirconia</b> Abhijit Chatterjee, Dept. of Chemical Engineering, Indian Institute of Technology Bombay, India	<b>11:45</b>
<b>12:00</b>	<b>Real-space electronic structure studies on the energetics of dislocations in Al-Mg materials system and its connection to mesoscale models</b> Vikram Gavini, University of Michigan, United States of America		<b>Assessment of formability limit diagram prediction by crystal plasticity finite element method</b> Duancheng Ma, Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria			<b>Novel Deformation Mechanism of Helium Irradiated Copper</b> Weizhong Han, Xi'an Jiaotong University, China	<b>MD simulation study of displacement damage in bulk wurtzite GaN by proton irradiation.</b> Sang Hyuk Yoo, Dept. of Mechanical Engineering, Yonsei Univ., Korea	<b>Stability Engineering of Halide Perovskite via Machine Learning</b> Wan-Jian YIN, Soochow University, China	<b>Tunable seat belt behavior in nanocomposite interfaces inspired from bacterial adhesion pilli</b> Kerim Can Dansuk, Northwestern University, United States of America	<b>Analysis of statistical properties of porous media with complex microstructure using multipoint morphology descriptors</b> Mikhail Tashkinov, Perm National Research Polytechnic University, Russia	<b>12:00</b>
<b>12:15</b>			<b>Analysis of gradient microstructures using crystal plasticity</b> Balaji Selvarajou, IHPC, Singapore, Singapore		<b>System-spanning shear avalanches induced by thermal structural relaxation in metallic glasses</b> Tomoaki Niiyama, College of Science and Engineering, Kanazawa Univ., Japan	<b>Isotope effect on quantum diffusion of interstitial hydrogen in face-centered cubic metals</b> Hajime Kimizuka, Osaka University, Japan		<b>Systematic evaluation of ionization potentials of divalent cation binary oxides</b> Yoyo Hinuma, Center for Frontier Science, Chiba Univ., Japan	<b>Origin of large scale spatial organization of DNA-polymer in bacterial chromosomes</b> Aparajit Chatterji, IISER-Pune, India 411008,India	<b>Accelerating stochastic simulations with path integrals</b> Steve Fitzgerald, University of Leeds, UK	<b>12:15</b>
<b>12:30</b>	<b>Lunch</b>				<b>Lunch</b>					<b>12:30</b>	

	Room 1	Room 2	Room 3	Room 4	Room 5	Room 6	Room 7	Room 8	Room 9	Room 10
	<b>Symposium C-11</b> <i>Chair:</i> Nikhil Chandra Admal, University of California Los Angeles, United States of America	<b>Symposium E-11</b>	<b>Symposium F-11</b> <i>Chair:</i> Peter Gumbsch, Fraunhofer IWM, Germany	<b>Symposium I-11</b>	<b>Symposium K-2</b> <i>Chairs:</i> Ferenc Kun, University of Debrecen, Hungary. Ian Main, University of Edinburgh, UK	<b>Symposium B-7</b> <i>Chair:</i> Marjorie Bertolus, CEA/DEN/DEC, Centre CEA de Cadarache, France	<b>Symposium N-5</b> <i>Chair:</i> Jutta Rogal, ICAMS Ruhr University Bochum, Germany	<b>Symposium D-3</b>	<b>Symposium H-9</b> <i>Chair:</i> Kees Storm, Eindhoven University of Technology, Netherlands	
14:00	<i>Invited</i> <b>A Multi-Scale Dislocation Language - Data Mining, Statistical Analysis, and Steps Towards a Community-Driven Data Base</b> Stefan Sandfeld, TU Bergakademie Freiberg, Germany		<i>Invited</i> <b>Mesoscale plasticity models of polycrystalline materials for efficient computation of microstructure/property relationships</b> Ricardo Lebensohn, Los Alamos National Laboratory, United States of America		<i>Invited</i> <b>Predictability of catastrophic failure in porous media</b> Ian Main, University of Edinburgh, UK	<i>Invited</i> <b>Thermal properties of fluorite-type metal dioxides: CeO<sub>2</sub>, ThO<sub>2</sub>, UO<sub>2</sub>, NpO<sub>2</sub>, PuO<sub>2</sub> and AmO<sub>2</sub></b> Masato Kato, Japan Atomic Energy Agency, Japan	<i>Invited</i> <b>Dynamics of C atoms nearby extended defects: a multi technique approach</b> Charlotte S Becquart, Univ.Lille, CNRS, INRA, ENSCL, UMR 8207, UMET, Unité Matériaux et Transformations, France	<i>Invited</i> <b>Finding the needle in the haystack: Materials discovery through high-throughput ab initio computing and data mining</b> Geoffroy Hautier, Université catholique de Louvain, Belgium	<i>Invited</i> <b>Micromechanics and instabilities in soft composite materials</b> Stephan Rudykh, University of Wisconsin - Madison, United States of America	14:00
14:15										14:15
14:30	<b>Deformation Behaviour of Pristine and Helium-Implanted Tungsten: Spherical Nano-indentation, X-ray Micro-diffraction &amp; Crystal-plasticity</b> Suchandrima Das, Dept. of Engineering, Univ. of Oxford, UK		<b>Development of a new consistent discrete Green operator for FFT-based methods to solve heterogeneous problems with eigenstrains</b> Konlavi Senyo Eloh, University of Lorraine, France		<b>Deciphering the dynamics of precursors to failure in quasi-brittle solids: an inspiration for understanding the statistics of earthquakes ?</b> Laurent Ponson, Institut Jean le Rond d'Alembert, CNRS - Sorbonne University, Paris, France	<b>SCIANTIX: A new inert gas behaviour module ready for use</b> Davide Pizzocri, Politecnico di Milano, Italy	<b>Localised on-the-fly Kinetic Monte Carlo</b> Johannes Bulin, Fraunhofer-Institut SCAI, Germany	<b>High-entropy alloys investigation using machine-learned potentials</b> Tatiana Kostiuchenko, Dept. of Material Science and Engineering, Skolkovo Institute of Science and Technology, Moscow, Russia	<b>Deformation analysis of UV curing 3d printed materials by combined molecular dynamics-finite element method</b> Gunjin Yun, Seoul National University, Korea	14:30
14:45	<b>The Nye tensor formalism for the DDD-FFT approach</b> Lionel GELEBART, CEA Université Paris-Saclay, DEN/DMN/SRMA, France		<b>Efficient FFT-based Homogenisation without Linear Reference Medium</b> Till Junge, EPFL, Mech. Engineering, Multiscale Mechanics Modeling, Switzerland		<b>Avalanche precursors and fracture strength in the limit of high disorder</b> Ferenc Kun, Department of Theoretical Physics, University of Debrecen, Hungary	<b>Modeling swelling in U3Si2 nuclear fuel using a multi-scale computational approach</b> Larry Agesen, Idaho National Laboratory, United States of America	<b>A Preconditioning scheme for Minimum Energy Path finding methods</b> Stela Makri, University of Warwick, UK	<b>Stability evaluation of high-entropy alloys via accurate on-lattice model</b> Evgenii Meshkov, All-Russian Research Institute of Automatics (VNIA), Russia	<b>Modelling and 3D Printing Kelvin Cell Acoustic Metamaterial</b> Huina Mao, Dept. of Aeronautical and Vehicle Engineering, KTH Royal Institute of Technology, Sweden	14:45
15:00	<b>FTMP-based Simulations and Evaluation of Geometrically-Necessary Boundaries (GNBs) of Dislocation</b> Shiro Ihara, Dept. of Mechanical Engineering, Kobe Univ., Japan		<b>Multiscale modelling of the effective viscoplastic behavior of constituents of the mantle transition zone (Mg<sub>2</sub>SiO<sub>4</sub> wadsleyite and ringwoodite): bridging atomic and polycrystal scales</b> Olivier Castelnuovo, Process and Engineering in Mechanics and Materials, CNRS/ENSAM/CNAM, Paris, France		<b>Jump statistics of epicenters in thermally induced cracking of fiber bundles</b> Naoki Yoshioka, RIKEN Center for Computational Science, Japan	<i>Invited</i> <b>Why Multiscale Modeling of Nuclear Fuel is Absolutely Essential and Why it is so Challenging</b> Michael R Tonks, University of Florida, United States of America	<i>Invited</i> <b>Temperature Programmed Molecular Dynamics - Accessing rare events using a combination of finite time sampling and bias potentials</b> Abhijit Chatterjee, Dept. of Chemical Engineering, Indian Institute of Technology Bombay, India	<b>Atomistically informed atomic mobility databases for continuum diffusion simulations</b> Katrin Abrahams, Scalebridging Thermodynamic and Kinetic Simulation (ICAMS), Ruhr-University Bochum, Germany	<b>Theoretical approach for EUV resist fabrication: DFT-MD-FDM study</b> Muyoung Kim, Division of Multiscale Mechanical Design, School of Mechanical and Aerospace Engineering, Seoul National University, Korea	15:00
15:15	<b>Improved phase field model of dislocation intersections</b> Songlin Zheng, China Academy of Engineering Physics, China		<b>Scalable and Directionally-Sensitive Three-Dimensional Quantifying of Orientation and Dislocation Density Gradients in Crystal Plasticity Computer Simulations</b> Markus Kuehbach, Max-Planck-Institut für Eisenforschung GmbH, Germany		<b>Time dependent fracture under unloading in a fiber bundle model</b> Reka Korei, Department of Theoretical Physics, University of Debrecen, Hungary			<b>The European Materials Modelling Council: standardization, interoperability and data management tools for materials modelling</b> Luca Bergamasco, Politecnico di Torino, Italy		15:15
15:30	<b>Coffee Break</b>					<b>Coffee Break</b>				15:30
	<b>Symposium C-12</b> <i>Chair:</i> Irene Beyerlein, University of California at Santa Barbara, United States of America	<b>Symposium E-12</b>	<b>Symposium F-12</b> <i>Chair:</i> Yasushi Shibuta, The University of Tokyo, Japan	<b>Symposium I-12</b>	<b>Symposium K-3</b> <i>Chairs:</i> Takahiro Hatano, University of Tokyo, Japan. Akio Nakahara, Nihon Univ., Japan	<b>Symposium B-8</b> <i>Chair:</i> Guang-Hong Lu, Beihang University, China	<b>Symposium N-6</b> <i>Chair:</i> Erik Bitzek, FAU Erlangen-Nuernberg, Germany	<b>Symposium D-4</b>	<b>Symposium H-10</b> <i>Chair:</i> Kees Storm, Eindhoven University of Technology, Netherlands	
16:00	<b>Modeling the interaction between martensitic phase transformations and dislocation dynamics</b> Rachel Derby, TU Bergakademie Freiberg, Germany		<i>Invited</i> <b>Microstructure formation in large-scale molecular dynamics simulation</b> Yasushi Shibuta, The University of Tokyo, Japan		<i>Invited</i> <b>Creep of strongly disordered materials: Plasticity, damage and approach to failure</b> Michael Zaiser, Inst. of Materials Simulation, Dept of Materials Science, FAU University of Erlangen-Nuremberg, Germany	<b>Kinetic Monte Carlo study of tungsten fuzz formation under low energy helium irradiation</b> Zhangcan Yang, School of Energy and Power Engineering, Huazhong University of Science and Technology, China	<i>Invited</i> <b>Modelling metals, alloys and cement paste across length and time scales</b> Laurent Karim Beldand, Queen's University, Canada	<i>Invited</i> <b>Exploration of large ab initio data spaces to design structural materials with superior mechanical properties</b> Joerg Neugebauer, Max-Planck-Institut fuer Eisenforschung, Germany	<b>Tracing the interplay of polymer topology and hydrodynamics</b> Lisa B. Weiss, University of Vienna, Austria	16:00
16:15	<b>The effect of microscopic slip deformation on the yield stress in dispersion hardened alloys analyzed by using crystal plasticity FEM</b> Yelm Okuyama, Dept. of Materials Science and Engineering, Kyushu University, Japan					<b>Constrained thermodynamic model for multi-component alloys under irradiation: A matrix formulation from first-principles Hamiltonian</b> Duc Nguyen-Manh, Materials Science and Scientific Computing Department, Culham Centre for Fusion Energy, UKAEA, UK			<b>Relation between Macroscopic Flows in a Contraction-Expansion Channel and Dynamics of Well-Entangled Polymer Chains</b> Takeshi Sato, Dept. of Chemical Engineering, Kyoto Univ., Japan	16:15
16:30	<b>Deformation Behaviour for Two-Phase Composites under Large Deformations using Micromechanical Analysis</b> Srihari Dodla, Madanapalle Institute of Technology (MITS) Madanapalle, India		<b>Directed assembly of structured nanoparticles through rapid micromixing</b> Arash Nikoubashman, Johannes Gutenberg University of Mainz, Germany		<b>Creep rupture and Omori-Utsu law: Fiber bundle model approach</b> Takahiro Hatano, University of Tokyo, Japan	<b>Kinetic Monte-Carlo Simulations of Radiation Damage in W(Re,Os) Alloys</b> Matthew James Lloyd, Department of Materials, University of Oxford, UK	<b>BCA-MD-KMC hybrid simulation for long time helium plasma irradiation inducing fuzzy nanostructure on tungsten</b> Atsushi M Ito, National Institute for Fusion Science, National Institutes of Natural Sciences, Japan	<b>Toward a machine learning aided interatomic potential for multi-element alloys: Application to binary compounds</b> Doyle Dickel, Mississippi State University, United States of America	<b>Dynamical properties of suspensions of star block-copolymers in shear flow.</b> Diego Felipe Jaramillo - Cano, Faculty of Physics, University of Vienna, Austria	16:30
16:45	<b>Dislocation dynamics simulation of FCC single crystals in high strain rate deformation</b> Ronan Madec, CEA, DAM, DIF, France		<b>Various interfaces related to twinning in hexagonal metals</b> Vaclav Paidar, Institute of Physics AS CR Prague, Czech Republic		<b>Temperature dependent shear friction in metallic glass</b> Akio Ishii, Osaka Univ., Japan	<b>Modeling Re-precipitate hardening in neutron irradiated W and W-Re alloys: from point defects to macroscopic hardening</b> Jaime Marian, University of California Los Angeles, United States of America	<b>Atomistic Modelling of Pipe Diffusion: a Direct Comparison of MD, KMC, aKMC and DMD</b> Erik Bitzek, FAU Erlangen-Nuernberg, Germany	<b>Machine Learning potentials for modeling irradiation defects in iron and tungsten</b> Alexandra Goryaeva, DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France	<b>Heterogeneous flow and internal friction in amorphous carbon</b> Richard Jana, Albert Ludwigs Universitaet Freiburg, Germany	16:45
17:00	<b>Comparison of two methods to cross-slip modeling by means of mathematical theory of moving curves</b> Miroslav Kolar, Czech Technical University in Prague, Czech Republic		<b>Mesoscale modeling of cement: texture, mechanics and durability</b> Katerina Ioannidou, Dept. of Civil and Environmental Engineering, Massachusetts Institute of Technology, United States of America		<b>Mechanism of controlled crack formation induced by memory effect of clay paste</b> Akio Nakahara, Nihon Univ., Japan	<i>Invited</i> <b>In-situ TEM of Formation Processes of Defects in Tungsten under Irradiation: Comparison between Electron and Self-ion Irradiations</b> Kazuto Arakawa, Shimane University, Japan	<b>Strategies for optimal construction of Markov chain representations of atomistic dynamics</b> Danny Perez, Los Alamos National Laboratory, United States of America	<b>Effect of friction and ductility on relaxation dynamics and mechanical memory of crumpled materials</b> Mehdi Habibi, Wageningen University, Netherlands	<b>Increasing the thermal conductivity of polymer nanocomposites filled with carbon nanotubes via molecular dynamics simulation</b> Yangyang Gao, Beijing University of Chemical Technology, China	17:00
17:15			<b>Effect of composition domain boundary on spinodal decomposition in binary system by phase-field method</b> Guen-Sik Min, Hanyang Univ., Korea		<b>Effects of Shockwave-Induced Nanobubble Collapse on Precision Polishing : Molecular Dynamics Study</b> Yoshimasa Aoyama, Dept. of Materials Science, Tohoku Univ., Japan		<b>Simulating the collective diffusion mechanism of amorphous solids at experimentally relevant time scales</b> Xunjiang Wang, Institute of Mechanics, Chinese Academy of Sciences, China	<b>Big-data insights into solute-GB segregation</b> Liam Huber, MPIE, Germany	<b>Thermal transport in polymer-based nanocomposite materials across multiple scales</b> Matteo Fasano, Energy Department, Politecnico di Torino, Italy	17:15
19:00 - 21:00	<b>Banquet Taiko-En</b>					<b>Banquet Taiko-En</b>				19:00 - 21:00

	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) Integrated Earthquake Simulation Enhanced with High Performance Computing Muneo Hori, Earthquake Research Institute, The University of Tokyo, Japan					Plenary (Room 1) 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	Symposium F-13 Chair: Takayuki Aoki, Tokyo Institute of Technology, Japan	Symposium I-13	Symposium K-4 Chairs: Tetsuo Mohri, IMR, Tohoku University, Japan. Akihiro Nakatani, Dept. of Adaptive Machine Systems, Osaka Univ., Japan	Symposium B-9 Chair: Michael Tonks, University of Florida, United States of America	Symposium N-7 Chair: Shotaro Hara, Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan	Symposium D-5	Symposium H-11 Chair: Erik Van der Giessen, University of Groningen, Netherlands		
09:45	Invited Mesoscopic studies of slip and twinning processes in hcp polycrystalline materials Irene Beyerlein, University of California at Santa Barbara, United States of America		Invited Advanced analysis tools for atomistic microstructure modeling Alexander Stukowski, Dept. of Materials Science, Darmstadt University of Technology, Germany		Invited Disclination dipole model of kink deformation in layered solid Akihiro Nakatani, Dept. of Adaptive Machine Systems, Osaka Univ., Japan	Ab Initio Modeling of Self-Interstitial and Vacancy Migration in Zirconium Emmanuel Clouet, CEA Saclay, France	Invited Atomistic Simulations that Reach Anthropological Timescale and Beyond Ju Li, Massachusetts Institute of Technology, United States of America	Invited Computational exploration of strong permanent magnet compounds Takashi Miyake, CD-FMat, AIST, Japan	Invited In silico design of self-assembly nanostructured polymer systems by multiscale molecular modelling Maurizio Fermeglia, University of Trieste, Italy		09:45
10:00						Atomistic modelling of point defect clusters in zirconium and impact on the microstructure evolution and crystal growth under irradiation Ludovic Thuinet, 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		Studying thermo-oxidative degradation of polyimide in oxygen environment using MD simulations Ashwani Kumar Sengar, IIT Kanpur, India		Large-scale coarse-grained molecular dynamics simulations on fracture processes of lamellar structure in crystalline polymers Yuji Higuchi, The University of Tokyo, Japan	Modeling of dislocation climb assisted glide in crystal plasticity models Alankar Alankar, IIT Bombay, India	The Phase Field Method: Crystal Structures and Facets Peter Voorhees, Northwestern University, United States of America	A machine-learning approach for finding new hard-magnetic phases Daniel F. Urban, Fraunhofer IWM, Freiburg, Germany	A Hierarchical Multiscale Simulations Approach for Modeling Failure in Polymer Matrix Composites Jaafar A. El-Awady, Johns Hopkins University, United States of America		10:15
10:30	An Elastic-Viscoplastic Crystal Plasticity Modeling for Plane Strain Deformation of Pure Magnesium Weidong Song, Beijing Institute of Technology, China		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		Grain boundary sliding within the entropy production rate theory Tetsuo Mohri, IMR, Tohoku University, Japan	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	Adaptive resolution simulations coupling molecular dynamics to dissipative particle dynamic Matej Praprotnik, National Institute of Chemistry, Slovenia	High-throughput optimization of finite temperature phase stabilities of Ce-based hard magnetic materials Tilmann Hickel, Max Planck Institut für Eisenforschung, Germany	Multiscale modeling of fuzzy fiber reinforced woven fabric composites Seunghwa Yang, Chung-Ang University, Korea		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.		Design of neural network for thermodynamics data of non-equilibrium multiphase field model Hiroshi Wakameda, ITOCHU Techno-Solutions Corporation, Japan		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	Advances in X-ray Diffraction Line Profile Analysis of Dislocation Loops in Zr - Insights from Atomistic Modelling. Chris P Race, University of Manchester, UK	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	Understanding pairwise magnetic interactions in Fe-based materials with machine learning techniques Osamu Waseda, MPIE, Germany	Linear and non-linear viscoelastic properties of model fractal-like aggregates polymer nanocomposites Samy Merabia, CNRS and Université Lyon 1, France		10:45
11:00	Break					Break					11:00
		Symposium E-14	Symposium F-14 Chair: Markus Kuehbach, Max-Planck-Institut für Eisenforschung GmbH, Germany	Symposium I-14	Symposium K-5 Chair: Masanori Kohyama, AIST, Japan. Masatake Yamaguchi, Center for Computational Science and e-Systems, Japan Atomic Energy Agency, Japan	Symposium B-10 Chair: Frederic Soisson, CEA Saclay, France	Symposium N-8 Chair: Laurent Karim Baland, Queen's University, Canada	Symposium D-6	Symposium H-12 Chair: Erik Van der Giessen, University of Groningen, Netherlands		
11:15			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	Sink strengths of point defects near tilt grain boundaries: A phase field model Pengchuang Liu, Institute of Materials, China academy of engineering physics, China	Invited Bridging Time Scales with Variationally Enhanced Sampling Omar Valsson, Max Planck Institute for Polymer Research, Germany	Invited Novel two-dimensional materials: Materials discovery, data provenance, and workflow reproducibility. Nicola Marzari, EPFL, Switzerland	Topological defect structure in the self-assembly of semiflexible polymers under spherical confinement Mihir Khadilkar, Johannes Gutenberg University Mainz, Germany, Germany		11:15
11:30					Combined analysis of first-principles calculations and fracture mechanics experiments on intergranular embrittlement of an alloy steel Masatake Yamaguchi, Center for Computational Science and e-Systems, 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				Molecular dynamics simulation of the detachment force between graphene and epoxy resin Kazuki Mori, ITOCHU Techno-Solutions Corporation, Japan	11:30
11:45			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	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	Simulations of Branched Polyelectrolytes Filip Uhlik, Charles University, Czech Republic	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	Relation between deformation and electrical conductivity for electroconductive polymer nanocomposites with highly segregated structure Oleg V. Lebedev, Skolkovo Institute of Science and Technology, Russia		11:45
12:00			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	Theoretical derivation of the ABVI model from cluster expansion Hamiltonian Antonio Fernandez Caballero, School of Mechanical, Aerospace and Civil Engineering, University of Manchester, UK	Accelerated mesodynamics Mauricio Ponga, University of British Columbia, Canada	Unraveling the structure-property relationships in fiber-composite materials using Machine Learning and Global Sensitivity Analysis David Cereceda, Villanova University, United States of America			12:00
12:15			Hydrogen Transport and Thermal Desorption in Multiphase Steels Andrej Turk, University of Cambridge, UK					Machine learning assisted by first-principles calculations for designing intermetallic-typed metallic glasses Tokuteru Uesugi, Dep. of Materials Science, Osaka Prefecture Univ., Japan			12:15
12:30	Poster award / Closing remark (Room 1)					Poster award / Closing remark (Room 1)					12:30