



September 22–27, 2024
Prague Congress Center, Czech Republic

Session Program

Room: North Hall

09:00 AM	09:30 AM	Coffee break	Forum Hall Foyer 2
Symposium G - Monday Morning / 09:30 AM-11:20 AM			Chair: Lorenz Romaner
09:30 AM	10:00 AM	Keynote Lecture: Finding patterns and outliers in materials data	Claudia Draxl
10:00 AM	10:20 AM	ML prediction of photoluminescence in double perovskites from high-throughput DFT ground state data	Bernd Meyer
10:20 AM	10:40 AM	Hydrogen Diffusion in Magnesium Using Machine Learning Potentials	Dario Massa
10:40 AM	11:00 AM	A Machine Learning Approach for Predicting Stability of Metal-Organic Frameworks	Alauddin Ahmed
11:00 AM	11:20 AM	Simple empirical method from machine learning for classification of materials as metals or insulators	Jean Baptiste Fankam Fankam
11:20 AM	12:20 PM	Lunch	Forum Hall Foyer 2
Symposium G - Monday Afternoon / 12:20 PM-02:10 PM			Chair: Claudia Draxl
12:20 PM	12:40 PM	Computational workflows for experimental materials characterization	Jan Janssen
12:40 PM	01:00 PM	Representation of computational materials and simulation workflows – leveraging ontologies and knowledge graphs	Abril Azocar Guzman
01:00 PM	01:20 PM	Integrating Data-Driven Strategies to Expedite the Discovery of Materials for Sustainable Applications	Jyotirmoy Deb
01:20 PM	01:40 PM	TRANSFERRED to Tuesday, 5:10 PM.	Zhouran Zhang
01:40 PM	02:00 PM	A Comparative Study of Machine Learning Models and Vector Analysis Techniques for Improved Prediction of Quaternary Material Systems Based on Word Embeddings	Lei Zhang
02:10 PM	02:40 PM	Coffee break	Forum Hall Foyer 2
Symposium G - Monday Afternoon / 02:40 PM-04:30 PM			Chair: Yury Lysogorskiy
02:40 PM	03:00 PM	Benchmarking Study of Deep Generative Machine Learning Models for Inverse Polymer Design	Ying Li
03:00 PM	03:20 PM	Prediction of microstructure and properties of metallic materials by integrating molecular dynamics and deep generative models	Yasushi Shibuta
03:20 PM	03:40 PM	Accelerating Materials Design via Computation and Machine Learning Combined Approaches	Yanming Wang
03:40 PM	04:00 PM	Material design by combining AI and computational materials science	Donghwa Lee
04:00 PM	04:20 PM	Enhancing Scientific Collaboration: Towards Standardised and Accessible Workflows within the MaterialDigital and MSE Community	Jörg Schaarschmidt
04:30 PM	05:00 PM	Refreshment break	Forum Hall Foyer 2
Symposium G - Monday Evening / 05:00 PM-06:50 PM			Chair: Oleg Peil
05:00 PM	05:20 PM	Machine learning assisted prediction of solubility limits in binary phase diagrams	Martin Zelený
05:20 PM	05:40 PM	Automated thermodynamic assessments: Residual functions for phase diagram data	Tobias Spitaler
05:40 PM	06:00 PM	Phosphorus segregation into α -Fe grain boundaries: Insights from atomistic modelling and Bayesian inference	Lorenz Romaner
06:00 PM	06:20 PM	Descriptors of Gas Diffusion Layer to Use in Proton Exchange Membrane Fuel Cells Simulations	Víctor Román
06:20 PM	06:40 PM	Understanding fluoride ion conduction mechanism BaSnF ₄ for fluoride ion battery	Xiliang LIAN



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Session Program

Room: Terrace 2A

09:00 AM	09:30 AM	Coffee break	Forum Hall Foyer 2
Symposium I - Monday Morning / 09:30 AM-11:20 AM			Chair: Marco Salvalaglio
09:30 AM	10:00 AM	Keynote Lecture: Towards Predicting Interface Structure in Crystalline Materials: from Frank-Bilby to Peierls-Nabarro	Jian Han
10:00 AM	10:20 AM	Grain boundaries in fcc metals with energetically stable nanofacets	Tobias Brink
10:20 AM	10:40 AM	Coherent and Semicoherent α/β Interfaces in Titanium: structure, thermodynamics, migration	Siqi Wang
10:40 AM	11:00 AM	Grain boundary amorphization as a transformation induced plasticity	Jean Furstoss
11:20 AM	12:20 PM	Lunch	Forum Hall Foyer 2
Symposium I - Monday Afternoon / 12:20 PM-02:10 PM			Chair: Mikko Alava
12:20 PM	12:50 PM	Keynote Lecture: Grain Boundary Segregation and Dynamic Solute Drag in Multicomponent Alloys	Fadi Abdeljawad
12:50 PM	01:10 PM	Solute segregation to extended defects in Fe-Cr alloys : an ab-initio based spin-atomic Monte Carlo simulation	Hilal Bozkurt
01:10 PM	01:30 PM	Coupled mechanics-diffusion-reaction models: Volumetric reactions, reaction localisation and computational homogenisation	Mikhail Poluektov
01:30 PM	01:50 PM	Atomistic Modeling of Interphase Boundary Diffusion	Yuri Mishin
01:50 PM	02:10 PM	Proton diffusion in two model grain boundaries of monoclinic zirconia	Jean-Paul Crocombette
02:10 PM	02:40 PM	Coffee break	Forum Hall Foyer 2
Symposium I - Monday Afternoon / 02:40 PM-04:30 PM			Chair: Fadi Abdeljawad
02:40 PM	03:10 PM	CANCELLED	-
03:10 PM	03:30 PM	Multiscale modeling of the solute atom segregation towards grain boundaries	Joé Petrazoller
03:30 PM	03:50 PM	The Interplay of Triple Junction and Long-Range Solute Attraction Effects on Grain-boundary Solute Clustering in Polycrystals	Frederic Sansoz
03:50 PM	04:10 PM	Thermodynamically Consistent Coupling of Fluctuating Hydrodynamics and Kinetic Monte Carlo for Gas-Solid Interfaces	Changho Kim
04:10 PM	04:30 PM	CANCELLED	
04:30 PM	05:00 PM	Refreshment break	Forum Hall Foyer 2



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Session Program

Room: Terrace 2B

09:00 AM	09:30 AM	Coffee break	Forum Hall Foyer 2
Symposium M - Monday Morning / 09:30 AM-11:20 AM			Chair: Sebastian Pfaller
09:30 AM	10:00 AM	Keynote Lecture: Playing with Entanglements to Structure Polymer Materials	Kurt Kremer
10:00 AM	10:20 AM	Conformation-Induced Stiffening Effect of Crosslinked Polymer Thin Films	Zhengyang Zhang
10:20 AM	10:40 AM	Molecular Structure Generation for Multicomponent Block Copolymers: From Self-Consistent Field Theory to Molecular Dynamics Simulations	Peter Brommer
10:40 AM	11:00 AM	Realization of random fields to describe the linear elasticity of short fiber composites. A comparison of Gaussian and non-Gaussian random fields	Ilona Małgorzata Widera
11:00 AM	11:20 AM	Coarse-grained molecular dynamics study of polycarbonate: Effect of molecular structure on mechanical properties	Yoshitaka Umeno
11:20 AM	12:20 PM	Lunch	Forum Hall Foyer 2
Symposium M - Monday Afternoon / 12:20 PM-02:10 PM			Chair: Andrea Giuntoli
12:20 PM	12:50 PM	Keynote Lecture: Tailoring Molecular Topology to Control the Mechanical Properties of Polymeric and Nanoparticle Networks	Sinan Keten
12:50 PM	01:10 PM	Mapping microstructure to shock-induced temperature fields using molecular dynamics and machine learning	Alejandro Strachan
01:10 PM	01:30 PM	Identification of elastic properties of interphase and interface in graphene-polymer nanocomposites by atomistic simulations	Fabrice Detrez
01:30 PM	01:50 PM	Transition of polymer chains from elastic to plastic regions under deformation: the role of conformation heterogeneity	Panayiota Katsamba
01:50 PM	02:10 PM	Coarse-graining aggregate polymer nanocomposites : towards a microscopic Interpretation of the Payne Effect	Samy Merabia
02:10 PM	02:40 PM	Coffee break	Forum Hall Foyer 2
Symposium M - Monday Afternoon / 02:40 PM-04:30 PM			Chair: Fabrice Detrez
02:40 PM	03:10 PM	Keynote Lecture: Computational Modeling of Polymers and Polymer Nanocomposites Across Scales: From Atoms to Macroscopic Behavior	Vagelis Harmandaris
03:10 PM	03:30 PM	Chemically-specific multiscale mechanical simulation of polymer nanocomposites: improving tractability with machine learning	Maxime Vassaux
03:30 PM	03:50 PM	Structural and Mechanical Properties of Vulcanized SBR	Spyridon Kallivokas
03:50 PM	04:10 PM	Scale-bridging Modelling and Simulation of Polymers	Sebastian Pfaller
04:10 PM	04:30 PM	Fracture Simulations of Amorphous Materials Across Scales	Felix Weber
04:30 PM	05:00 PM	Refreshment break	Forum Hall Foyer 2
Symposium M - Monday Evening / 05:00 PM-06:50 PM			Chair: Matej Praprotnik
05:00 PM	05:30 PM	Keynote Lecture: Deep Coarse-grained Molecular Modeling	Julija Zavadlav
05:30 PM	05:50 PM	A novel coarse-grained modeling scheme for thermal transport properties of thermoplastic polymers	Seunghwa Yang
05:50 PM	06:10 PM	Propagator-Biased Chain Generation: accurately reverse mapping phase segregated block copolymers	Mateus Garcia Rodolfo
06:10 PM	06:30 PM	Efficient coarse-grained modeling of many-atom van der Waals interactions for Polymer Melt simulations	Ian Sosa



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Room: South Hall 2A

09:00 AM	09:30 AM	Coffee break	Forum Hall Foyer 2
Symposium K - Monday Morning / 09:30 AM-11:20 AM			Chair: Amin Esfandiarpour
09:30 AM	10:00 AM	Keynote Lecture: Navigating and exploiting the high-dimensional configuration spaces of high entropy alloys	Jörg Neugebauer
10:00 AM	10:20 AM	Multiscale modelling of phase stability and properties of Cr-Ta-Ti-V-W high-entropy alloys	Jan Wróbel
10:20 AM	10:40 AM	Machine-learning interatomic potentials for FCC high-entropy alloys	Aslak Fellman
10:40 AM	11:00 AM	Atomic simulation of grain boundary migration in high-entropy alloys	Tomotsugu Shimokawa
11:00 AM	11:20 AM	Inertia effect of deformation in amorphous solids: a mesoscale model	Minqiang Jiang
11:20 AM	12:20 PM	Lunch	Forum Hall Foyer 2
Symposium K - Monday Afternoon / 12:20 PM-02:10 PM			Chair: Duc Nguyen-Manh
12:20 PM	12:50 PM	Keynote Lecture: Analysis of different noise sources on dislocation mobility	Enrique Martinez
12:50 PM	01:10 PM	Composition Search for Designing Ultra-Strong FCC Multicomponent Alloys via Atomistic Simulations	Amin Esfandiarpour
01:10 PM	01:30 PM	Predicting the strength of multi-principal element alloys: a mechanistic data-driven approach	Markus Sudmanns
01:30 PM	01:50 PM	Atomistic simulations of the shock and spall behavior of the refractory high-entropy alloy HfNbTaTiZr	Daniel Thürmer
02:10 PM	02:40 PM	Coffee break	Forum Hall Foyer 2
Symposium K - Monday Afternoon / 02:40 PM-04:30 PM			Chair: Jesper Byggmästar
02:40 PM	03:10 PM	Keynote Lecture: Strong impact of thermal vibrations and chemical complexity on diffusion in high-entropy alloys revealed from accurate ab initio machine learning	Xi Zhang
03:10 PM	03:30 PM	Finite temperature phase stability of Fe-Cr-Mn-Ni: from DFT to CALPHAD	Jan Wróbel
03:30 PM	03:50 PM	Thermal stability of High Entropy Alloy Nanoparticles: an atomic scale study	Anissa Acheche
03:50 PM	04:10 PM	Towards a Machine Learning Interatomic Potential for Ti-6Al-4V	Connor Allen
04:10 PM	04:30 PM	Modeling diffusion phenomena in Cantor-type High Entropy Alloys validated by interdiffusion experiments	Ahmadreza Riyahi Khorasgani
04:30 PM	05:00 PM	Refreshment break	Forum Hall Foyer 2
Symposium K - Monday Evening / 05:00 PM-06:50 PM			Chair: Xi Zhang
05:00 PM	05:30 PM	Keynote Lecture: Complex concentrated alloys and the TRIP effect: Exploring new benefits	Cem Tasan
05:30 PM	05:50 PM	Multi-scale characterization of 3D printable CrCoNi-based ODS-MPEAs by methods of advanced stereo-STEM cross-correlated with EDS – resourcing experimental data to act as potential input into the quantitative models	Milan Heczko



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Session Program

Room: South Hall 2B

09:00 AM	09:30 AM	Coffee break	Forum Hall Foyer 2
Symposium A - Monday Morning / 09:30 AM-11:20 AM			Chair: Igor Abrikosov
09:30 AM	10:00 AM	Keynote Lecture: Quantum-Accurate Multiscale and Data-driven Methods for the Simulation of Materials Failure	James Kermode
10:00 AM	10:20 AM	From electronic structure to phase diagrams with automated workflows	Sarath Menon
10:20 AM	10:40 AM	Thermodynamic properties at high temperature with DFT	Johann Bouchet
10:40 AM	11:00 AM	Machine learning accelerated thermodynamic search of ductile Cr-based alloys complemented by first-principles simulations	Lassi Linnala
11:00 AM	11:20 AM	Exploration of magnetite surface phase diagrams using a newly developed machine-learning interatomic potential	Baptiste Bienvenu
11:20 AM	12:20 PM	Lunch	Forum Hall Foyer 2
Symposium A - Monday Afternoon / 12:20 PM-02:10 PM			Chair: James Kermode
12:20 PM	12:50 PM	Keynote Lecture: Accelerated free energy computations for first-principles structural study of gold in extreme conditions	Pauline Richard
12:50 PM	01:10 PM	Solid solution strengthening in aluminium alloys from first-principles and machine learning interatomic potentials	Lukas Volkmer
01:10 PM	01:30 PM	A neural network interatomic potential study of α -iron--Carbon binary system	Fan-Shun Meng
01:30 PM	01:50 PM	Quantum mechanics and machine learning simulations of bcc Ti-Nb-Zr alloys in the vicinity of dynamical instability	Igor Abrikosov
01:50 PM	02:10 PM	Accelerating the discovery of low-energy structure configurations: a computational approach that integrates first-principles calculations, Monte Carlo sampling, and Machine Learning	David Cereceda
02:10 PM	02:40 PM	Coffee break	Forum Hall Foyer 2
Symposium A - Monday Afternoon / 02:40 PM-04:30 PM			Chair: Martin Friak
02:40 PM	03:10 PM	Keynote Lecture: Sampling-free thermodynamics in bulk crystalline metals from the mean-field anharmonic bond model	Raynol Dsouza
03:10 PM	03:30 PM	Machine-learning potential for accurate predictions of elastic properties in amorphous W-B-C	Pavel Ondračka
03:30 PM	03:50 PM	Atomic scale calculation of thermophysical properties of molten salt reactor fuel via DFT and PIM MD simulations: inclusion of Americium	Maria Chiara Notarangelo
03:50 PM	04:20 PM	Keynote Lecture: Principles of quantum computing	Mario Ziman
04:30 PM	05:00 PM	Refreshment break	Forum Hall Foyer 2
Symposium A - Monday Evening / 05:00 PM-06:50 PM			Chair: Martin Friak
05:00 PM	05:30 PM	Keynote Lecture: Rethinking Quantum Learning Algorithms	Eric Anschuetz
05:30 PM	05:50 PM	Meta-optimization of Resources on Quantum Computers	Martin Plesch
05:50 PM	06:10 PM	Quantum-computing study of the electronic structure of diamond-structure crystals	Michal Ďuriška
06:10 PM	06:30 PM	Variational Quantum Algorithms for Electronic Structure Calculations	Ivana Mihalikova
06:30 PM	06:50 PM	Hubbard physics with Rydberg atoms: using a quantum spin simulator to simulate strong fermionic correlations, towards strongly correlated materials modelling	Antoine Michel



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Room: 221 + 222

09:00 AM	09:30 AM	Coffee break	Forum Hall Foyer 2
Symposium L - Monday Morning / 09:30 AM-11:20 AM			Chair: Coleman Alleman
09:30 AM	10:00 AM	Keynote Lecture: An Interleaved Physics-based Deep-learning Framework as a New Cycle Jumping Approach for Microstructurally Small Fatigue Crack Growth Simulations	Ashley Spear
10:00 AM	10:20 AM	Inverse calibration of material model parameters using digital image correlation measurement and finite element simulation coupled with non-sequential data assimilation	Sae Sueki
10:20 AM	10:40 AM	Bifurcation Theory of Plasticity, Damage and Failure	Alexander Umantsev
10:40 AM	11:00 AM	The Schwarz Alternating Method for Multiscale Coupling in Solid Mechanics	Alejandro Mota
11:20 AM	12:20 PM	Lunch	Forum Hall Foyer 2
Symposium L - Monday Afternoon / 12:20 PM-02:10 PM			Chair: Ashley Spear
12:20 PM	12:50 PM	Keynote Lecture: The role of chemical potential and residual stress on H trapping and embrittlement at grain boundaries: A first principles cohesive zone model	Rebecca Janisch
12:50 PM	01:10 PM	A Thermodynamic Entropy based Criterion for Defect Formation in Friction Stir Welding	Abdessamad Brahami
01:10 PM	01:30 PM	Modeling of Hydrogen-induced Microcrack Initiation in the Martensitic Structure of Steel by Integration across Fracture Test, Microbeam Analysis and Atomic Simulation	Kazuki Matsubara
01:30 PM	01:50 PM	General grain boundary K-test framework for the assessment of liquid metal embrittlement at the atomic scale	Florian Brunner
02:10 PM	02:40 PM	Coffee break	Forum Hall Foyer 2
Symposium L - Monday Afternoon / 02:40 PM-04:30 PM			Chair: Coleman Alleman
02:40 PM	03:10 PM	Keynote Lecture: FFT based simulation of fracture at the microscale: application to polycrystals	Javier Segurado
03:10 PM	03:30 PM	Numerical modelling of the grain size effect on deformation properties of the 9Cr steel prepared by powder metallurgy	Luděk Stratil
03:30 PM	03:50 PM	Numerical Investigation of Fatigue and Structural Integrity in Welded High-Strength Steel Joints	Mohammad Al Khazali
03:50 PM	04:10 PM	Thermal Shock of Tungsten under Extreme Heat Flux Conditions	Mohammad Alabdullah
04:30 PM	05:00 PM	Refreshment break	Forum Hall Foyer 2
Symposium L - Monday Evening / 05:00 PM-06:50 PM			Chair: Martin Diehl
05:00 PM	05:30 PM	Keynote Lecture: HUNNY theory of porous material plasticity and ductile failure	Amine Benzerga
05:30 PM	05:50 PM	Crystallographic Orientation dependence on Intragranular Void Evolution and Failure in Aluminum Alloy: A Case Study of Coupled Phase Field Damage and Crystal Plasticity Modeling	Aashique Rezwan
05:50 PM	06:10 PM	The Micromechanics of Void Nucleation	Coleman Alleman



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Room: South Hall 3A

09:00 AM	09:30 AM	Coffee break	Forum Hall Foyer 2
Symposium E - Monday Morning / 09:30 AM-11:20 AM			Chair: Eva Zarkadoula (she/her)
09:30 AM	10:00 AM	Keynote Lecture: Atomistic modeling of ion-matter interactions for material modification	Eva Zarkadoula (she/her)
10:00 AM	10:20 AM	Molecular dynamics simulation of the formation of W-centers in silicon by Ga ion irradiation	Christos Gennetidis
10:20 AM	10:40 AM	Generative Machine Learning for Atomic-Scale Modeling of Chemically Disordered Materials: Application to (U, Pu)O ₂ Nuclear Fuels	Emeric Bourasseau
10:40 AM	11:00 AM	Irradiation effects on stress and deformations: from atomistic simulations to finite element models for reactor components	Luca Reali
11:00 AM	11:20 AM	Modelling properties of self-interstitial atoms in Fe-Ni alloys across the magnetic transition	Thomas Mainguy
11:20 AM	12:20 PM	Lunch	Forum Hall Foyer 2
Symposium E - Monday Afternoon / 12:20 PM-02:10 PM			Chair: Andrea Sand
12:20 PM	12:50 PM	Keynote Lecture: Environmentally dependent electronic energy losses in collision cascades	Andrea Sand
12:50 PM	01:10 PM	Spatially Resolved Cluster Dynamics Modelling of Irradiation Growth	Matthew Maron
01:10 PM	01:30 PM	Cationic self-diffusion coefficients modeling from atomistic-scale calculations in nuclear oxide fuels	Petra Ospital
01:30 PM	01:50 PM	Ab initio study of point defect diffusion induced by plutonium self-irradiation	Romuald Béjaud
01:50 PM	02:10 PM	Cluster dynamics simulations of the full xenon-vacancy-interstitial phase-space in irradiated UO ₂	Sophie Blondel
02:10 PM	02:40 PM	Coffee break	Forum Hall Foyer 2
Symposium E - Monday Afternoon / 02:40 PM-04:30 PM			Chair: Nasr Ghoniem
02:40 PM	03:10 PM	Keynote Lecture: Modeling Irradiation-Induced Inelastic Deformation of Zirconium	Nasr Ghoniem
03:10 PM	03:30 PM	Structure and mobility of small self-interstitials clusters in zirconium	Ludovic Thuinet
03:30 PM	03:50 PM	Multiscale modelling of nuclear fuel behavior from industry perspective	Radan Sedlacek
03:50 PM	04:10 PM	A hierarchical statistical surrogate model for collision cascade damage in zirconium	Chris Race
04:10 PM	04:30 PM	Atomic scale investigation of the structural, thermodynamic and elastic properties of hypostoichiometric Am-bearing oxides	Baptiste Labonne
04:30 PM	05:00 PM	Refreshment break	Forum Hall Foyer 2
Symposium E - Monday Evening / 05:00 PM-06:50 PM			Chair: Duc Nguyen-Manh
05:00 PM	05:30 PM	Keynote Lecture: Irradiation-driven stability of microstructure in compositionally complex materials: Multiscale modelling prediction and experimental validation	Duc Nguyen-Manh
05:30 PM	05:50 PM	Radiation-Induced Defect Evolution in FCC Single Phase Compositionally Complex Alloys	Annie Barnett
05:50 PM	06:10 PM	Implementation of Electron Temperature Model to W Damage Cascades Molecular Dynamics Simulation under Neutron Irradiation	Younggak Shin
06:10 PM	06:30 PM	Atomistic modelling of fracture and point defects in reactor pressure vessel steels	Lakshmi Shenoy



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Room: South Hall 3B

09:00 AM	09:30 AM	Coffee break	Forum Hall Foyer 2
Symposium B - Monday Morning / 09:30 AM-11:20 AM			Chair: Ronan Madec
09:30 AM	9:50 AM	Ladislav Kubin, a visionary	Yves Brechet
09:50 AM	10:20 AM	Keynote Lecture: Mesoscale modeling of plasticity in random alloys	David Rodney
10:20 AM	10:40 AM	Interaction between solutes and dislocations in anisotropic elastic media : application to the dynamic strain aging	Florian Billon
10:40 AM	11:00 AM	Nano-indentation as a tool to question the impact of hydrogen on the plasticity of fcc metals and alloys	Xavier Feaugas
11:00 AM	11:20 AM	Dynamic Evolution of Near-Surface Microstructures in FCC Alloys under Extreme Sliding Velocities	Stefan J. Eder
11:20 AM	12:20 PM	Lunch	Forum Hall Foyer 2
Symposium B - Monday Afternoon / 12:20 PM-02:10 PM			Chair: David Rodney
12:20 PM	12:50 PM	Keynote Lecture: Continuum dislocation models of dislocation patterning in uni-axial and cyclic deformation	Michael Zaiser
12:50 PM	01:10 PM	Early stages of deformation induced dislocation patterning	Grethe Winther
01:10 PM	01:30 PM	A graph database for feature characterization of dislocation networks	Balduin Katzer
01:30 PM	01:50 PM	Application of field dislocation mechanics and fast Fourier transforms to electron microscopy	Vincent Taupin
01:50 PM	02:10 PM	CS-UNet: A Flexible Segmentation Algorithm for Microscopy Images	Amir Kordijazi
02:10 PM	02:40 PM	Coffee break	Forum Hall Foyer 2
Symposium B - Monday Afternoon / 02:40 PM-04:30 PM			Chair: Marc Fivel
02:40 PM	03:10 PM	Keynote Lecture: Continuous modeling of dislocation in concentrated random alloys: dislocation roughness, depinning and thermal activation	Pierre-Antoine Geslin
03:10 PM	03:30 PM	Strain localization in an expanding metal ring: polycrystal plasticity approach	Jean-Lin Dequiedt
03:30 PM	03:50 PM	Connecting Continuum and Quantum Mechanical Electromigration Theories at Mesoscale using Phase Field Crystal Method	Nan Wang
03:50 PM	04:10 PM	Exploring the potential of dislocation density fields for bridging length scales in nanomechanics	Julien Guérolé
04:10 PM	04:30 PM	A nonlinear variational model of cracks and dislocations	Godefroy Engrand
04:30 PM	05:00 PM	Refreshment break	Forum Hall Foyer 2
Symposium B - Monday Evening / 05:00 PM-06:50 PM			Chair: Dan Mordehai
05:00 PM	05:30 PM	Keynote Lecture: Computational and experimental high-resolution micro-plasticity in advanced steels	Marc Geers
05:30 PM	05:50 PM	Microstructure and kinetics of the alpha-epsilon transformation in iron under dynamical loading	Rémi Lemaire
05:50 PM	06:10 PM	Multi-phase-field simulation of microstructure evolution during austenite-to-ferrite transformation in Fe-C-Mn alloy using machine learning and Bayesian inference	Taiki Suzuki
06:10 PM	06:30 PM	CANCELLED	-
06:30 PM	06:50 PM	Generalized Granular Micromechanics Approach to Obtain Injective Mapping Between Material State Variables and Mesoscale and Macroscopic Field Variables	Abhinav Ramkumar



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Session Program

Room: South Hall 3C

09:00 AM	09:30 AM	Coffee break	Forum Hall Foyer 2
Symposium C - Monday Morning / 09:30 AM-11:20 AM			Chair: Katrin Schulz
09:30 AM	10:00 AM	Keynote Lecture: Crystal plasticity simulations of deformation and damage in metallic polycrystals including the effect of grain boundaries	Javier Llorca
10:00 AM	10:20 AM	A multiscale CPFE approach for modelling the flow stress response of an austenitic stainless steels under high temperature cyclic loading conditions	Miguel Espadero Sanchez-Crespo
10:20 AM	10:40 AM	Parametric investigation for rolling texture formation of stainless steels	Takayuki Otsuka
10:40 AM	11:00 AM	CANCELLED	
11:00 AM	11:20 AM	Bridging Electronic and Large-Scale Simulations with Machine-Learning Potentials: Investigating the Yield Stress Anomaly in L12 Intermetallics	Xiang Xu
11:20 AM	12:20 PM	Lunch	Forum Hall Foyer 2
Symposium C - Monday Afternoon / 12:20 PM-02:10 PM			Chair: Javier Llorca
12:20 PM	12:50 PM	Keynote Lecture: Influence of intermetallics and pores on the fatigue behavior of cast aluminum alloys: A crystal plasticity study	Martin Diehl
12:50 PM	01:10 PM	A data-driven quantification of damage caused by voids in polycrystalline materials	David Montes De Oca Zapiain
01:10 PM	01:30 PM	Incorporation of temperature dependent coefficients of Voce hardening law in viscoplastic self-consistent model (VPSC) for multiple slip systems implemented in a FEM framework	Leo Schwarzmeier
01:30 PM	01:50 PM	From continuum dislocation dynamics to crystal plasticity: Modelling the fatigue behaviour of a γ' Nickel-Based Superalloy	Miguel Espadero Sanchez-Crespo
01:50 PM	02:10 PM	Quantitative Comparison between Experiment and Crystal Plasticity simulations using Microstructure Clones	Hojun Lim
02:10 PM	02:40 PM	Coffee break	Forum Hall Foyer 2
Symposium C - Monday Afternoon / 02:40 PM-04:30 PM			Chair: Nicolas Bertin
02:40 PM	03:10 PM	Keynote Lecture: Peierls-Nabarro Modeling of Dislocations in Complex Alloys	William A. Curtin
03:10 PM	03:30 PM	Effects of Short Range Ordering on the Generalized Stacking Fault Energy and Deformation Mechanisms in FCC Multiprincipal Element Alloys	Lingyu Zhu
03:30 PM	03:50 PM	CANCELLED	
03:50 PM	04:10 PM	Structure of dislocations in high-entropy alloys	Hoa Le
04:10 PM	04:30 PM	Investigating the dynamical response of metals within a polyphase thermomechanical framework	Nicolas Bruzy
04:30 PM	05:00 PM	Refreshment break	Forum Hall Foyer 2
Symposium C - Monday Evening / 05:00 PM-06:50 PM			Chair: William A. Curtin
05:00 PM	05:20 PM	Influence of elastic modulus mismatch on lattice distortion and strengthening in random alloys	Pierre-Antoine Geslin
05:20 PM	05:40 PM	Discrete dislocation dynamics study of dislocation avalanche statistics in high entropy alloy	Hengxu Song
05:40 PM	06:00 PM	Investigation on the energy landscape of grain boundary-mediated plasticity in high entropy alloys	Xiao-Zhi Tang
06:00 PM	06:20 PM	AI-assisted atomistic simulations of defects in Ti and Ti-Al from solid solutions to intermetallics	Wen Tongqi
06:20 PM	06:40 PM	Solute effects on softening/strengthening of prismatic slip in Mg	Masoud Rahbarniazi



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Room: Chamber Hall

09:00 AM	09:30 AM	Coffee break	Forum Hall Foyer 2
Symposium H - Monday Morning / 09:30 AM-11:20 AM			Chair: Roman Gröger
09:30 AM	10:00 AM	Keynote Lecture: A mechanism of the electroplastic effect	Adrian Sutton
10:00 AM	10:20 AM	Modeling of defects using atomic cluster expansion	Matous Mrovec
10:20 AM	10:40 AM	Atomic cluster expansion for hydrogen embrittlement in iron	Aleksei Egorov
10:40 AM	11:00 AM	Development of Machine-Learning Potentials for Atomistic Modeling of Mechanical Behaviors at Interfaces	Daisuke Matsunaka
11:00 AM	11:20 AM	Modelling precipitation kinetics in Ni-based superalloys using machine learned interatomic potentials	Adam Fisher
11:20 AM	12:20 PM	Lunch	Forum Hall Foyer 2
Symposium H - Monday Afternoon / 12:20 PM-02:10 PM			Chair: Adrian Sutton
12:20 PM	12:50 PM	Keynote Lecture: The Grain Boundary Ratchet: directional grain boundary migration & its implications	David Srolovitz
12:50 PM	01:10 PM	Modeling and prediction of interface structures by number-theoretical approach	Kazutoshi Inoue
01:10 PM	01:30 PM	Realistic Grain Boundaries in Nanocrystalline Thin Films	Ankit Yadav
02:10 PM	02:40 PM	Coffee break	Forum Hall Foyer 2
Symposium H - Monday Afternoon / 02:40 PM-04:30 PM			Chair: Matous Mrovec
02:40 PM	03:10 PM	Keynote Lecture: Vasek Vitek and Disordered Materials	Takeshi Egami
03:10 PM	03:30 PM	Identifying and Characterizing Deformation Elements in Metallic Glasses through Molecular Dynamics	Yoshinori Shiihara
03:30 PM	03:50 PM	Mechanical properties of Mg ₂ SiO ₄ glasses	Philippe Carrez
03:50 PM	04:10 PM	Effect of vacancies and impurities on properties of MoSi ₂ /TiSi ₂ disilicide nanocomposites	Mojmir Sob
04:10 PM	04:30 PM	Structural Transition in Grain Boundary: The Effect of Impurities	Qian Chen
04:30 PM	05:00 PM	Refreshment break	Forum Hall Foyer 2