Session Program – Tuesday, 24 September

# Room: North Hall

| | | | |
|---|---|---|---|
| 09:50 AM | 10:20 AM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium G - Tuesday Morning / 10:20 AM-12:10 PM** | Chair: Thomas Hammerschmidt |
| **10:20 AM** | **10:50 AM** | **Keynote Lecture: Active materials exploration and characterization with Bayesian optimization** | **Patrick Rinke** |
| 10:50 AM | 11:10 AM | Bayesian blacksmithing: Discovering thermomechanical properties and deformation mechanisms in high-entropy refractory alloys | Remi Dingreville |
| 11:10 AM | 11:30 AM | Hybrid computational approach to optimization of competing properties of multicomponent alloys | Oleg Peil |
| 11:30 AM | 11:50 AM | Bayesian optimization accelerates material discovery of bio-based foams to replace plastics | Isaac Miranda Valdez |
| 11:50 AM | 12:10 PM | **CANCELLED** | Silvia Bonfanti |
| 12:10 PM | 01:10 PM | **Lunch** | Forum Hall Foyer 2 |
| | | **Symposium G - Tuesday Afternoon / 01:10 PM-03:00 PM** | Chair: Patrick Rinke |
| **01:10 PM** | **01:40 PM** | **Keynote Lecture: Digital twins for materials science** | **Surya Kalidindi** |
| 01:40 PM | 02:00 PM | Efficient Microstructure Optimization in Ceramic Materials by Combining Microstructure Simulations and Machine Learning | Simon Pirkelmann |
| 02:00 PM | 02:20 PM | Active Learning Approach for Efficient Creation of a Surrogate Model for Crystal Growth | Lorenz Taucher |
| 02:20 PM | 02:40 PM | Novel aspects of deep learning in microstructure-property prediction for elastic homogenization | Bernhard Eidel |
| 02:40 PM | 03:00 PM | Machine learning toolkit for predicting fatigue life of structural materials trained by high-throughput micromechanical modelling | Napat Vajragupta |
| 03:00 PM | 03:30 PM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium G - Tuesday Afternoon / 03:30 PM-05:20 PM** | Chair: Napat Vajragupta |
| 03:30 PM | 03:50 PM | Training physics-based neural network surrogate models with the finite element method | Pranav Sunil |
| 03:50 PM | 04:10 PM | Descriptors of Surface Energy Based on the Crystal Structure | Yoyo Hinuma |
| 04:10 PM | 04:30 PM | A machine learning perspective on the inverse indentation problem | Quan Jiao |
| 04:30 PM | 04:50 PM | Persistent Homology for Microstructure Manifold Construction | Simon Mason |
| 04:50 PM | 05:10 PM | Success Stories in Computationally-Driven Materials Discovery | Corey Oses |
| 05:10 PM | 05:20 PM | Prediction of alloy plasticity fusing textual corpus and physical information: Information density enhancement and knowledge extraction based on MatSciBERT | Zhouran Zhang |
| **05:20 PM** | **07:20 PM** | **Poster Session 1** | **Forum Hall Foyer 3** |
| **07:20 PM** | **07:40 PM** | **Poster Award Ceremony** | **Chamber Hall** |

Session Program – Tuesday, 24 September

# Room: Terrace 2A

| | | | |
|---|---|---|---|
| 09:50 AM | 10:20 AM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium I - Tuesday Morning / 10:20 AM-12:10 PM** | Chair: David Srolovitz |
| **10:20 AM** | **10:50 AM** | **Keynote Lecture: Unraveling mechanics of grain boundary migration from atomistic to continuum scales** | **Brandon Runnels** |
| 10:50 AM | 11:10 AM | Modelling the effects of internal stress on microstructure evolution at the meso-scale | Qiu Caihao |
| 11:10 AM | 11:30 AM | (Non)linear elastic fields of interfacial (disclination) and bulk (dislocation) line defects | Amit Acharya |
| 11:30 AM | 11:50 AM | Extended phase-field crystal models | Maik Punke |
| 11:50 AM | 12:10 PM | Dynamics of height fluctuations for two-dimensional materials | Tapio Ala-Nissila |
| 12:10 PM | 01:10 PM | **Lunch** | Forum Hall Foyer 2 |
| | | **Symposium I - Tuesday Afternoon / 01:10 PM-03:00 PM** | Chair: Brandon Runnels |
| **01:10 PM** | **01:40 PM** | **Keynote Lecture: The enumeration of grain boundary microstates** | **Nikhil Chandra Admal** |
| 01:40 PM | 02:00 PM | Interface energy and structure anisotropy of coherent heterophase interfaces | Christian Brandl |
| 02:00 PM | 02:20 PM | Characterization of the stability of metal/metal interfaces by atomistic simulations | Reyhaneh Ghassemizadeh |
| 02:20 PM | 02:40 PM | Interface Mobility and Twin Formation in NiTi Shape Memory Alloys | Lorenzo La Rosa |
| 02:40 PM | 03:00 PM | Multiscale multiphysics model for redistribution of hydrogen within steel microstructure during martensitic transformation | Christian Posch-Peperkorn |
| 03:00 PM | 03:30 PM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium I - Tuesday Afternoon / 03:30 PM-05:20 PM** | Chair: Nikhil Chandra Admal |
| **03:30 PM** | **03:50 PM** | **Coupled-growth dynamics of lamellar patterns in eutectic grains with a crystallographic mosaicity** | **Silvere Akamatsu** |
| 03:50 PM | 04:10 PM | Multiscale characterization of nonclassical crystallization pathways for trans-stilbenes | Tesia Janicki |
| 04:10 PM | 04:30 PM | Micro-scale model for the onset of freezing in a porous medium | Michal Beneš |
| 04:30 PM | 04:50 PM | Surface-induced warping in nanowires | Jean-Marc Roussel |
| 04:50 PM | 05:10 PM | Structural transitions at emergent grain boundaries in strained thin films | Moneesh Upmanyu |
| **05:20 PM** | **07:20 PM** | **Poster Session 1** | **Forum Hall Foyer 3** |
| **07:20 PM** | **07:40 PM** | **Poster Award Ceremony** | **Chamber Hall** |

Session Program – Tuesday, 24 September

# Room: Terrace 2B

| | | | |
|---|---|---|---|
| 09:50 AM | 10:20 AM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium M - Tuesday Morning / 10:20 AM-12:10 PM** | Chair: Maxime Vassaux |
| **10:20 AM** | **10:50 AM** | **Keynote Lecture: Lagrangian Heterogeneous Multiscale Modelling of Complex Fluids** | **Marco Ellero** |
| 10:50 AM | 11:10 AM | Synchronized molecular dynamics simulation using LAMMPS: an application to the pressure-driven flows of polymer melts | Kotaro Oda |
| 11:10 AM | 11:30 AM | Synchronized molecular-dynamics simulation via lubrication approximation: Method validation testing and applications | Shugo Yasuda |
| 11:30 AM | 11:50 AM | Quantum-inspired encoding enhances stochastic sampling of soft matter systems | Francesco Slongo |
| 11:50 AM | 12:10 PM | Network Formation in Dual-Cure Resins for Direct Ink Write Carbon Fiber Composites | Michael Chandross |
| 12:10 PM | 01:10 PM | **Lunch** | Forum Hall Foyer 2 |
| | | **Symposium M - Tuesday Afternoon / 01:10 PM-03:00 PM** | Chair: Felix Weber |
| **01:10 PM** | **01:30 PM** | **Molecular dynamics simulations of the interaction of energetic atomic oxygen with carbon nanotube based composites** | **Chaitanya Deo** |
| 01:30 PM | 01:50 PM | Ice Formation in the Presence of Hydrogels | Dilip Gersappe |
| 01:50 PM | 02:10 PM | Controlling ice formation: an ab initio guided modeling framework of cellulose in water | Aakash Kumar |
| 02:10 PM | 02:30 PM | Enhanced adhesion of epoxy resin and silane-treated aluminum by H2O-assisted proton shift | Shuji Ogata |
| 02:30 PM | 02:50 PM | Multi-Physics Simulation Analysis of the Gelation Process in Rechargeable Battery Electrolytes through Electron Beam Irradiation | Woojien Lee |
| 02:50 PM | 03:00 PM | CANCELLED | Alexander Chervanyov |
| 03:00 PM | 03:30 PM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium D - Tuesday Afternoon / 03:30 PM-05:20 PM** | Chair: Thomas Schrefl |
| **03:30 PM** | **03:50 PM** | **Microstructure Mechanism for Modifying the Mechanoelectrical Behavior of Polymer-Metal Composites** | **Min Zhou** |
| 03:50 PM | 04:10 PM | Molecular Simulation-guided and Physics-informed Constitutive Modeling of Highly Stretchable Polymers with Dynamic Ionic Bonds | Hua Yang |
| 04:10 PM | 04:30 PM | In-silico study on Electroelastic Properties of Hexagonal Boron Nitride Nanosheet: combined effect of vacancy structure and temperature | Jaewon Lee |
| 04:30 PM | 04:50 PM | Modelling the effect of the grain boundary distribution, and connectivity on the diffusion of hydrogen in nickel microstructures | Jamaa Bouhattate |
| 04:50 PM | 05:10 PM | - | - |
| **05:20 PM** | **07:20 PM** | **Poster Session 1** | **Forum Hall Foyer 3** |
| **07:20 PM** | **07:40 PM** | **Poster Award Ceremony** | **Chamber Hall** |

Session Program – Tuesday, 24 September

# Room: South Hall 2A

| | | | |
|---|---|---|---|
| 09:50 AM | 10:20 AM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium K - Tuesday Morning / 10:20 AM-12:10 PM** | Chair: Jan Wróbel |
| **10:20 AM** | **10:50 AM** | **Keynote Lecture: Neural network of defect kinetics for multi-principal element alloys** | **Penghui Cao** |
| 10:50 AM | 11:10 AM | Large-scale atomistic modelling of high-entropy alloys with machine-learned potentials | Jesper Byggmästar |
| 11:10 AM | 11:30 AM | Deep Potential-Based Large Atomic Models and Evaluation Workflow in the Field of Alloys | Jiawei Huang |
| 11:30 AM | 11:50 AM | A machine learning interatomic potential for high entropy alloys | Teng Li |
| 11:50 AM | 12:10 PM | - | - |
| 12:10 PM | 01:10 PM | Lunch | Forum Hall Foyer 2 |
| | | **Symposium K - Tuesday Afternoon / 01:10 PM-03:00 PM** | Chair: Jörg Neugebauer |
| **01:10 PM** | **01:40 PM** | **Keynote Lecture: Nonequilibrium chemical short-range order in metallic alloys** | **Rodrigo Freitas** |
| 01:40 PM | 02:00 PM | Thermodynamics and kinetics of long-range ordering in FCC Ni-Cr-Fe alloys: insights from atomic scale modeling | Liangzhao Huang |
| 02:00 PM | 02:20 PM | Molecular Dynamics simulations of deformation-induced mixing of a CoFeNi powder blend | Marie Charrier |
| 02:20 PM | 02:40 PM | Phase-Field Modeling of Dislocations in High Entropy Alloys | Xin Liu |
| 02:40 PM | 03:00 PM | - | - |
| 03:00 PM | 03:30 PM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium K - Tuesday Afternoon / 03:30 PM-05:20 PM** | Chair: Mikko Alava |
| **03:30 PM** | **04:00 PM** | **Keynote Lecture: Computational microstructural engineering for multi-phase HEAs** | **Yunzhi Wang** |
| 04:00 PM | 04:20 PM | **CANCELLED** | Stefan Hiemer |
| 04:20 PM | 04:40 PM | - | - |
| 04:40 PM | 05:00 PM | - | - |
| 05:00 PM | 05:20 PM | - | - |
| **05:20 PM** | **07:20 PM** | **Poster Session 1** | **Forum Hall Foyer 3** |
| **07:20 PM** | **07:40 PM** | **Poster Award Ceremony** | **Chamber Hall** |

Session Program – Tuesday, 24 September

# Room: South Hall 2B

| | | | |
|---|---|---|---|
| 09:50 AM | 10:20 AM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium A - Tuesday Morning / 10:20 AM-12:10 PM** | Chair: David Holec |
| **10:20 AM** | **10:50 AM** | **Keynote Lecture: Point defect induced omega phase fluctuations in bcc Ti and Zr** | **Celine Varvenne** |
| 10:50 AM | 11:10 AM | The impact of spin-polarization, atomic ordering and charge transfer on the stability of medium-entropy CoCrNi alloy | Pavel Papež |
| 11:10 AM | 11:30 AM | Quantum-mechanical study of phonon contributions to stability of Pb-Sn alloys | Petr Čípek |
| 11:30 AM | 11:50 AM | Metastable defect phase diagrams as roadmap to tailor chemically driven defect formation | Ali Tehranchi |
| 11:50 AM | 12:10 PM | Materials properties of defect-stabilized off-stoichiometric τ-phase Al2Ge2Mg | Martin Friak |
| 12:10 PM | 01:10 PM | **Lunch** | Forum Hall Foyer 2 |
| | | **Symposium A - Tuesday Afternoon / 01:10 PM-03:00 PM** | Chair: Ali Tehranchi |
| **01:10 PM** | **01:40 PM** | **Keynote Lecture: Stability and magnetic properties of grain boundaries in the inverse Heusler phase Fe2CoGa and in bcc Fe** | **Daniel Urban** |
| 01:40 PM | 02:00 PM | Segregation to grain boundaries in disordered systems: an application to a Ni-based superalloy | David Holec |
| 02:00 PM | 02:20 PM | Revisiting the nucleation mechanism of the GP zones and precipitates in Al-Zn-Mg alloy | Liu Sha |
| 02:20 PM | 02:40 PM | Insight into the decomposition of cubic Ti1-xAlxN by activation energy and vacancy formation envelopes | Ganesh K Nayak |
| 02:40 PM | 03:00 PM | Exploring the γ/γ'' interfaces in Ni-based superalloy: a systematic first-principles study | Ziyi Xiong |
| 03:00 PM | 03:30 PM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium A - Tuesday Afternoon / 03:30 PM-05:20 PM** | Chair: Daniel Urban |
| 03:30 PM | 03:50 PM | First-principles study of the vacancy-enhanced formation of deformation twins in Cu-In alloys | Eun-Ae Choi |
| 03:50 PM | 04:10 PM | First-Principles Calculation Aided Design of High-Strength Cu-Ni-Si Alloy with Grain Boundary Phases | Seung Zeon Han |
| **04:10 PM** | **04:40 PM** | **Keynote Lecture: Multiscale approaches for the hydrogen redistribution in metallic microstructures** | **Ali Tehranchi** |
| 04:40 PM | 05:00 PM | Deciphering Hydrogen Embrittlement: A Multi-Scale Approach to Thermal Desorption Spectroscopy Analysis | Osamu Waseda |
| 05:00 PM | 05:20 PM | Accurate Gibbs energy of planar defects in Ni3Al at high temperatures | Xiang Xu |
| **05:20 PM** | **07:20 PM** | **Poster Session 1** | **Forum Hall Foyer 3** |
| **07:20 PM** | **07:40 PM** | **Poster Award Ceremony** | **Chamber Hall** |

Session Program – Tuesday, 24 September

## Room: 221 + 222

| | | | |
|---|---|---|---|
| 09:50 AM | 10:20 AM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium L - Tuesday Morning / 10:20 AM-12:10 PM** | Chair: Coleman Alleman |
| **10:20 AM** | **10:50 AM** | **Keynote Lecture: Coupled Dislocations and Fracture dynamics at finite deformation** | **Amit Acharya** |
| 10:50 AM | 11:10 AM | Screw Dislocations and Crack-Tip Plasticity in Tungsten | Erik Bitzek |
| 11:10 AM | 11:30 AM | Alloying Effects on Grain Boundary Kinetics and Disconnection Behavior | Jason Trelewicz |
| 11:30 AM | 11:50 AM | Grain boundary misorientation informed numerical framework for stress corrosion cracking in polycrystalline materials | Siladitya Pal |
| 11:50 AM | 12:10 PM | Analytical and Numerical Implementation of Microelement Plastic Strain Accumulation Model for Rotating Bending Fatigue Life Prediction | Vignesh Kumar Gopalakrishnan |
| 12:10 PM | 01:10 PM | **Lunch** | Forum Hall Foyer 2 |
| | | **Symposium L - Tuesday Afternoon / 01:10 PM-03:00 PM** | Chair: Coleman Alleman |
| **01:10 PM** | **01:40 PM** | **Keynote Lecture: Atomistically informed void nucleation in ductile fracture modeling** | **Ryan Sills** |
| 01:40 PM | 02:00 PM | The Atomistic Origin of Fracture Toughness in Amorphous Silica | Gergely Molnár |
| 02:00 PM | 02:20 PM | Stability of nanoscale intergranular vacancy clusters : Monte Carlo simulations and elastic calculations | Döme Tanguy |
| 02:20 PM | 02:40 PM | Atomistic Insights: Shattering Expectations in Crack Dynamics | Fraser Birks |
| 02:40 PM | 03:00 PM | Experiment and multiscale modelling of stress redistribution and damage in Titanium dwell fatigue, and its temperature sensitivity | Fionn Dunne |
| 03:00 PM | 03:30 PM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium L - Tuesday Afternoon / 03:30 PM-05:20 PM** | Chair: Ryan Sills |
| **03:30 PM** | **04:00 PM** | **Keynote Lecture: Hybrid FE-laminographic Analysis of Damage Mechanism in Biaxial Experiments on Aluminum 2198-T8R** | **Dirk Mohr** |
| 04:00 PM | 04:20 PM | Microstructural Induced Failure Modes in Crystalline Materials | Mohammed Zikry |
| 04:20 PM | 04:40 PM | Modelling fracture in EUROFER97 steel | Andris Freimanis |
| 04:40 PM | 05:00 PM | Phase field modeling of fracture in dual phase microstructures | Tuncay Yalcinkaya |
| 05:00 PM | 05:20 PM | CANCELLED | Afzaal Ahmed |
| **05:20 PM** | **07:20 PM** | **Poster Session 1** | **Forum Hall Foyer 3** |
| **07:20 PM** | **07:40 PM** | **Poster Award Ceremony** | **Chamber Hall** |

Session Program – Tuesday, 24 September

# Room: South Hall 3A

| | | | |
|---|---|---|---|
| 09:50 AM | 10:20 AM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium E - Tuesday Morning / 10:20 AM-12:10 PM** | Chair: Maylise Nastar |
| **10:20 AM** | **10:50 AM** | **Keynote Lecture: Phase-field model of non-coherent thermal composition fluctuations and radiation-induced spinodal decomposition in INVAR Fe-Ni alloys** | **Maylise Nastar** |
| 10:50 AM | 11:10 AM | Phase-field modelling of grain boundary segregation at equilibrium and under irradiation | Yanis Calbert |
| 11:10 AM | 11:30 AM | Phase-field modeling predicting three-dimensional microstructural defect evolution in ferrous alloy under irradiation condition | Ilhyun Cho |
| 11:30 AM | 11:50 AM | Phase-field modelling of extended defects in metals under extreme conditions | Antoine Ruffini |
| 11:50 AM | 12:10 PM | Kinetics of segregation and precipitation in Fe-Cr alloys under irradiation: strain/stress effects | Frédéric Soisson |
| 12:10 PM | 01:10 PM | **Lunch** | Forum Hall Foyer 2 |
| | | **Symposium E - Tuesday Afternoon / 01:10 PM-03:00 PM** | Chair: Osman El Atwani |
| **01:10 PM** | **01:40 PM** | **Keynote Lecture: Multiscale Material Studies on Innovative Materials for Fusion Power** | **Osman El Atwani** |
| 01:40 PM | 02:00 PM | Impact of Interface Roughness and Alignment on the Deformation Mechanisms in Al-Ti Bimetallic Microstructures | John Carpenter |
| 02:00 PM | 02:20 PM | Cascade damage in mechanically loaded materials | Antoine Clement |
| 02:20 PM | 02:40 PM | Point defect properties in Fe-Cr-He alloys using DFT-based machine learning potential | Jan Wróbel |
| 02:40 PM | 03:00 PM | - | - |
| 03:00 PM | 03:30 PM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium E - Tuesday Afternoon / 03:30 PM-05:20 PM** | Chair: Chenyang Lu |
| **03:30 PM** | **04:00 PM** | **Keynote Lecture: Distinct defect properties and enhanced radiation resistance of NbZrTi-based refractory multi-principal element alloys** | **Chenyang Lu** |
| 04:00 PM | 04:20 PM | Modeling SISF nucleation and shearing mechanisms in Ni-based superalloys | Inam Iqbal Lalani |
| 04:20 PM | 04:40 PM | Sensitivity analysis and optimization of multi-scale models for microstructural evolution in metal materials under neutron irradiation | Shaoting Wan |
| 04:40 PM | 05:00 PM | Multiscale modeling of the synergistic evolution of transmutation elements and irradiation defects in tungsten | Hong-Bo Zhou |
| 05:00 PM | 05:20 PM | - | - |
| **05:20 PM** | **07:20 PM** | **Poster Session 1** | **Forum Hall Foyer 3** |
| **07:20 PM** | **07:40 PM** | **Poster Award Ceremony** | **Chamber Hall** |

Session Program – Tuesday, 24 September

# Room: South Hall 3B

| | | | |
|---|---|---|---|
| 09:50 AM | 10:20 AM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium B - Tuesday Morning / 10:20 AM-12:10 PM** | Chair: Ryan Sills |
| **10:20 AM** | **10:50 AM** | **Keynote Lecture: Strain gradient crystal plasticity modelling of kinematic hardening inspired from discrete dislocation dynamics** | **Marc FIVEL** |
| 10:50 AM | 11:10 AM | Simulation of plastic strain localisation in polycrystals by Discrete Dislocation Dynamics and crystal plasticity | Riccardo Gatti |
| 11:10 AM | 11:30 AM | On the role of collinear annihilation and cross-slip in dynamic recovery | Ronan Madec |
| 11:30 AM | 11:50 AM | Unraveling dislocation microstructures via surrogate modelling of continuum dislocation dynamics simulations | Katrin Schulz |
| 11:50 AM | 12:10 PM | On qualitative aspects of parametric dislocation dynamics model by means of evolving curves | Miroslav Kolar |
| 12:10 PM | 01:10 PM | **Lunch** | Forum Hall Foyer 2 |
| | | **Symposium B - Tuesday Afternoon / 01:10 PM-03:00 PM** | Chair: Pierre-Antoine Geslin |
| **01:10 PM** | **01:40 PM** | **Keynote Lecture: Integration of Atomistically-Derived Dislocation Behavior into Discrete Dislocation Dynamics Simulations** | **Douglas Spearot** |
| 01:40 PM | 02:00 PM | High-speed mobility law of dislocations in anisotropic crystals : theory vs. atomistic simulations | Yves-Patrick Pellegrini |
| 02:00 PM | 02:20 PM | Development of an irradiation hardening model based on multi-scale numerical simulations. Application to zirconium | Pascal Noirot |
| 02:20 PM | 02:40 PM | Physical insights into dislocation avalanche statistics in Cu through Dislocation Dynamics simulations | Sylvain Queyreau |
| 02:40 PM | 03:00 PM | Dislocation Dynamics investigation of dislocation avalanches and confrontation with experiments | Aissaoui Missipsa |
| 03:00 PM | 03:30 PM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium B - Tuesday Afternoon / 03:30 PM-05:20 PM** | Chair: Douglas Spearot |
| **03:30 PM** | **04:00 PM** | **Keynote Lecture: From Pure Metals to Multi-Principal Element Alloys – A Dislocation-Based Data-Driven Approach for Predicting the Stress-Strain Curves FCC Metals** | **Jaafar El-Awady** |
| 04:00 PM | 04:20 PM | Multiscale modelling of stochastic dislocation mechanisms – cross-slip and dislocation nucleation | Dan Mordehai |
| 04:20 PM | 04:40 PM | The role of surface nucleation in bcc micropillar plasticity | Yang Li |
| 04:40 PM | 05:00 PM | Mechanical properties of small nanoparticles: ultra high strength, shape dependence and uncommon plasticity mechanisms | Laurent pizzagalli |
| 05:00 PM | 05:20 PM | On the relation between dislocation microstructures and the densification of nanoporous Au nanoparticles | Santhosh Mathesan |
| **05:20 PM** | **07:20 PM** | **Poster Session 1** | **Forum Hall Foyer 3** |
| **07:20 PM** | **07:40 PM** | **Poster Award Ceremony** | **Chamber Hall** |

Session Program – Tuesday, 24 September

# Room: South Hall 3C

| | | | |
|---|---|---|---|
| 09:50 AM | 10:20 AM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium C - Tuesday Morning / 10:20 AM-12:10 PM** | Chair: Abigail Hunter |
| **10:20 AM** | **10:50 AM** | **Keynote Lecture: A creep model controlled by the interdependent dynamics of point defect, dislocation, grain boundary, and void** | **Yinan Cui** |
| 10:50 AM | 11:10 AM | Multi-scale Anisotropic Study of Primary Creep Deformation of Heterogeneous SAC Solder Crystals | Abhijit Dasgupta |
| 11:10 AM | 11:30 AM | Anomalous entropy-driven kinetics of dislocation nucleation | Danny Perez |
| 11:30 AM | 11:50 AM | Activation entropy of dislocation glide from atomistic simulations | Arnaud Allera |
| 11:50 AM | 12:10 PM | Mobility of dislocations in body-centered cubic transition metals | Emmanuel Clouet |
| 12:10 PM | 01:10 PM | **Lunch** | Forum Hall Foyer 2 |
| | | **Symposium C - Tuesday Afternoon / 01:10 PM-03:00 PM** | Chair: Yinan Cui |
| **01:10 PM** | **01:40 PM** | **Keynote Lecture: Mesoscale Investigations of deformation mechanisms in metals and alloys using Phase Field Dislocation Dynamics (PFDD)** | **Abigail Hunter** |
| 01:40 PM | 02:00 PM | Coarse-Grained Phase-Field Crystal Model of Dislocations in Quasicrystals | Marcello De Donno |
| 02:00 PM | 02:20 PM | Energetic and structusral analyses of affecting factors for dislocation nucleation and transmission at grain boundary in metals and alloys | Masato Wakeda |
| 02:20 PM | 02:40 PM | Bridging Atomistic and Continuum Mechanics for describing Crystal Defects and Grain Boundary Excess Energy | Houssam Kharouji |
| 02:40 PM | 03:00 PM | Energy-based Stopping Criteria for FFT-based Computational Homogenization | Martin Ladecký |
| 03:00 PM | 03:30 PM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium C - Tuesday Afternoon / 03:30 PM-05:20 PM** | Chair: Emmanuel Clouet |
| 03:30 PM | 03:50 PM | Frank Dislocations at a Twin Boundary as Efficient Dislocation Sources | Daren Liu |
| 03:50 PM | 04:10 PM | Analysis of twinning propagation and thickening in 3D | Filip Siska |
| 04:10 PM | 04:30 PM | Exploring Plastic Deformation Behavior in Nanotwinned Metals under High Quasi-hydrostatic Pressure: A Molecular Dynamics Insight | Ruoqi Dang |
| 04:30 PM | 04:50 PM | Micro-twinning induced plasticity in solid-solid reconstructive phase transformation | Kanka Ghosh |
| 04:50 PM | 05:10 PM | TRIP effect in Zirconia: atomistic simulations based on a Neural Network potential compared to in-situ experiments | Gaël Huynh |
| **05:20 PM** | **07:20 PM** | **Poster Session 1** | **Forum Hall Foyer 3** |
| **07:20 PM** | **07:40 PM** | **Poster Award Ceremony** | **Chamber Hall** |

Session Program – Tuesday, 24 September

# Room: Chamber Hall

| | | | |
|---|---|---|---|
| 09:50 AM | 10:20 AM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium H - Tuesday Morning / 10:20 AM-12:10 PM** | Chair: Takeshi Egami |
| **10:20 AM** | **10:50 AM** | **Keynote Lecture: A model of thermodynamic stabilization of nanocrystalline grain boundaries in alloy systems** | **Yuri Mishin** |
| 10:50 AM | 11:10 AM | Multiscale model predicting brittle fracture of nanocomponents | Miroslav Černý |
| 11:10 AM | 11:30 AM | The Energetics of Disconnection Nucleation and Glide in Symmetric Tilt Grain Boundaries | Himanshu Joshi |
| 11:30 AM | 11:50 AM | Capabilities and improvement ability of classical many-body potentials: application to hcp-Zr | Alessandra Del Masto |
| 11:50 AM | 12:10 PM | Insights into Shear-Coupled Twin Boundary Migration: A Comprehensive Analysis | Ritu Verma |
| 12:10 PM | 01:10 PM | **Lunch** | Forum Hall Foyer 2 |
| | | **Symposium H - Tuesday Afternoon / 01:10 PM-03:00 PM** | Chair: Yuri Mishin |
| **01:10 PM** | **01:40 PM** | **Keynote Lecture: Atomistic simulations in multi-principal-component FCC materials** | **Diana Farkas** |
| 01:40 PM | 02:00 PM | Phase Pattern Formation in Grain Boundaries | Ian Winter |
| 02:00 PM | 02:20 PM | Revealing and Controlling of Dislocation Plasticity, Twinning and Fracture in BCC Transition Metals and Alloys | Zhaoxuan Wu |
| 02:20 PM | 02:40 PM | Investigation of Impacts of Spin Inhomogeneity on Screw Dislocation Mobility in BCC Iron | Hideki Mori |
| 02:40 PM | 03:00 PM | Revisiting Franks Theory for the creation of open-core screw dislocations in 4H-SiC by molecular dynamics simulation | Georg Holub |
| 03:00 PM | 03:30 PM | **Coffee break** | Forum Hall Foyer 2 |
| | | **Symposium H - Tuesday Afternoon / 03:30 PM-05:20 PM** | Chair: Diana Farkas |
| **03:30 PM** | **03:50 PM** | **Atomistic Mechanisms of Ring Formation During Catalyzed Carbon Nanotube Growth** | **Wang Rui** |
| 03:50 PM | 04:10 PM | Relating Shear Transformations in a Model Glass to Features of the Two-Dimensional Local Yield Surface | Spencer Fajardo |
| 04:10 PM | 04:30 PM | Integrating Newton's Equations of Motion in the Reciprocal Space as a Novel Materials Modeling Technique | Miljan Dašić |
| 04:30 PM | 04:50 PM | Pseudo-twin boundary improves flow stress and fatigue resistance of TiAl single crystal: atomistic simulations | Prof. Dr. Min Yi |
| 04:50 PM | 05:10 PM | - | - |
| **05:20 PM** | **07:20 PM** | **Poster Session 1** | **Forum Hall Foyer 3** |
| **07:20 PM** | **07:40 PM** | **Poster Award Ceremony** | **Chamber Hall** |