



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

Session Program – Thursday, 26 September

Room: North Hall

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium G - Thursday Morning / 09:50 AM-11:40 AM			Chair: Mariano Fonti
09:50 AM	10:10 AM	A multi-fidelity deep learning framework for designing single-phase BCC refractory multi-principal element alloys at different temperatures	Ali Shargh
10:10 AM	10:30 AM	Prediction of grain-boundary segregation of vacancies using machine learning methods	Christoph Dösinger
10:30 AM	10:50 AM	CANCELLED	Wei Xu
10:50 AM	11:10 AM	Deep learning-based surrogate model for materials under shock loading	Indrashish Saha
11:10 AM	11:30 AM	Generative machine learning model for microstructure design in dual-phase steels	Navyanth Kusampudi
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2



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Session Program – Thursday, 26 September

Room: Terrace 2B

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium D - Thursday Morning / 09:50 AM-11:40 AM			Chair: Libor Šmejkal
09:50 AM	10:20 AM	Keynote Lecture: Multiscale quantitative calculation of thermal properties in magnetic materials	Joseph Barker
10:20 AM	10:50 AM	Keynote Lecture: Magnetic Shape Memory Effects in Heusler Alloys- From Macroscopic Description to Nanoscale	Oleg Heczko
10:50 AM	11:10 AM	Temperature-dependent domain wall width and free energy in BaTiO ₃ determined via molecular dynamics simulation	Hikaru Azuma
11:10 AM	11:30 AM	Functionalized-nanopore graphene as potent membrane for H ₂ /CO ₂ and H ₂ /CH ₄ mixtures separation: A hybrid-functional DFT-D4 investigation	Atyeh Rahmanzadeh
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2



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Session Program – Thursday, 26 September

Room: South Hall 2A

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium N - Thursday Morning / 09:50 AM-11:40 AM			Chair: Yue Fan
09:50 AM	10:20 AM	Keynote Lecture: Investigations of Solute Clustering Kinetics during Quenching and Aging of Al-Mg-Zn alloys	Liang Qi
10:20 AM	10:40 AM	Exotic chemical ordering in Co-Ni-Pt medium entropy nanoalloys	Pamela Camilos
10:40 AM	11:00 AM	Integrated Unified Phase-field modeling of dual-phase precipitation pinning induced by dislocation and grain boundary in recrystallization	Yu-Hong Zhao
11:00 AM	11:20 AM	-	-
11:20 AM	11:40 AM	-	-
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2



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Session Program – Thursday, 26 September

Room: South Hall 2B

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium A - Thursday Morning / 09:50 AM-11:40 AM			Chair: Martin Friak
09:50 AM	10:10 AM	Shape-dependence of optical properties of coinage-metal nanoparticles	Wei Zhao
10:10 AM	10:30 AM	Atomistic simulation of olfaction-receptor functionalized graphene for body odor volatiles detection	Chen Li
10:30 AM	10:50 AM	Diffusion modelling of H isotopes through the W/Cu interface	Yosvany Silva Solis
10:50 AM	11:10 AM	QM/MM Style Potential Coupling to Accelerate Simulations	Fraser Birks
11:10 AM	11:30 AM	-	-
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2



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Session Program – Thursday, 26 September

Room: South Hall 3A

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium E - Thursday Morning / 09:50 AM-11:40 AM			Chair: Ghiath Monnet
09:50 AM	10:20 AM	Keynote Lecture: A multiscale approach for the prediction of the ductile-brittle transition temperature in irradiated low alloy steels	Ghiath Monnet
10:20 AM	10:40 AM	Complex dislocation loop networks as natural extensions of the sink efficiency of saturated grain boundaries in irradiated metals	Sicong He
10:40 AM	11:00 AM	Structure and mobility of small self-interstitials clusters in zirconium	Ludovic Thuinet
11:00 AM	11:20 AM	CANCELLED	Huiqiu Deng
11:20 AM	11:40 AM	-	-
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2
Symposium E - Thursday Afternoon / 12:40 PM-02:30 PM			Chair: Christophe Domain
12:40 PM	01:10 PM	Keynote Lecture: From statistical analysis of isolated displacement cascades in metals to cascade accumulation and microstructure evolution under irradiation	Christophe Domain
01:10 PM	01:30 PM	Grain boundary morphology evolution under irradiation	Ian Chesser
01:30 PM	01:50 PM	Simulating Dark-Field X-ray Microscopy Images of Complex Discrete Dislocation Structures	Yifan Wang
01:50 PM	02:10 PM	-	-
02:10 PM	02:30 PM	-	-
02:30 PM	03:00 PM	Refreshment break	Forum Hall Foyer 2
Symposium E - Thursday Afternoon / 03:00 PM-04:50 PM			Chair: Daniel Mason
03:00 PM	03:30 PM	Keynote Lecture: Validating multiscale models of highly irradiated metals: from thermal desorption spectroscopy to transmission electron microscopy	Daniel Mason
03:30 PM	03:50 PM	Crack tip plasticity at the scale of dislocation microstructure	Anter El-Azab
03:50 PM	04:10 PM	Mobility of a $1/2 \{110\}$ edge dipole in alpha-iron due to collisional cascades: a molecular dynamics study	Cristian Denton
04:10 PM	04:30 PM	-	-
04:30 PM	04:50 PM	-	-



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Room: South Hall 3B

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium F - Thursday Morning / 09:50 AM-11:40 AM			Chair: Chantal Valeriani
09:50 AM	10:20 AM	Keynote Lecture: Sub-THz acoustic excitation of protein motion	Matej Praprotnik
10:20 AM	10:40 AM	Controlling Polyelectrolyte Interactions and Electrophoretic Mobility in Aqueous Environments via Salt	Hossein Vahid Dastjerdi
10:40 AM	11:00 AM	Discovering dynamic laws from observations: The case of self-propelled, interacting colloids	Chantal Valeriani
11:00 AM	11:20 AM	Quantitative Model of Solvation Shell Dynamics and Energetics in Electron Transfer Reactions via Molecular Dynamics Simulations	Zhenyu Wang
11:20 AM	11:40 AM	Learning macroscopic dynamic laws from dissipative particle dynamics simulations of fluids	Tilen Potisk
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2
Symposium F - Thursday Afternoon / 12:40 PM-02:30 PM			Chair: Matej Praprotnik
12:40 PM	01:10 PM	Keynote Lecture: Open-Boundary Molecular Dynamics Simulations with the Adaptive Resolution Method	Robin Cortes-Huerta
01:10 PM	01:30 PM	Development of Coarse Grain Models for Molecular Simulations by Score Matching	Alain Dequidt
01:30 PM	01:50 PM	Dynamically Consistent Coarse-Graining with Koopman Operators	Feliks Nueske
01:50 PM	02:10 PM	-	-
02:10 PM	02:30 PM	-	-
02:30 PM	03:00 PM	Refreshment break	Forum Hall Foyer 2



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Session Program – Thursday, 26 September

Room: South Hall 3C

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium C - Thursday Morning / 09:50 AM-11:40 AM			Chair: Péter Dusán Ispánovity
09:50 AM	10:20 AM	Keynote Lecture: High-temperature plasticity in bcc micropillars	Giacomo Po
10:20 AM	10:40 AM	Investigation of the influence of sample initial misalignment on slip system activity during nanoindentation in bcc tungsten	Tevfik Ozan Fenercioğlu
10:40 AM	11:00 AM	Influence of surface roughness and oxidation on the mechanics of nano-objects	Jonathan Amodeo
11:00 AM	11:20 AM	Size dependent scaling law of plastic flow in FCC Nanolattices: A Dislocation Dynamics Study	I'll Ryu
11:20 AM	11:40 AM	The effect of crack tip dislocation emission and blunting: A discrete dislocation dynamics study	Lei Zhang
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2
Symposium C - Thursday Afternoon / 12:40 PM-02:30 PM			Chair: Zhaoxuan Wu
12:40 PM	01:10 PM	Keynote Lecture: Understanding Strain Hardening of Face-Centered Cubic Metals using Dislocation Dynamics	Wei Cai
01:10 PM	01:30 PM	Simulating plastic flow in highly constrained bicrystals with a nodal dislocation dynamics framework	Mujan Seif
01:30 PM	01:50 PM	Edge dislocation annihilation in FCC during fatigue	Jan Fikar
01:50 PM	02:10 PM	Numerical simulation of dislocation multiple cross-slip	Petr Pauš
02:10 PM	02:30 PM	Dynamic grain refinement of metal microparticles during high-velocity impact	Marisol Koslowski
02:30 PM	03:00 PM	Refreshment break	Forum Hall Foyer 2
Symposium C - Thursday Afternoon / 03:00 PM-04:50 PM			Chair: Wei Cai
03:00 PM	03:30 PM	Keynote Lecture: On incorporating strain avalanches in coarse grained descriptions of plasticity	Péter Dusán Ispánovity
03:30 PM	03:50 PM	Spatio-temporal averaging of three-dimensional Discrete Dislocation Dynamics (DDD) data	Bernhard Heiningger
03:50 PM	04:10 PM	Plasticity theory based on the statistical properties of dislocations	Istvan Groma
04:10 PM	04:30 PM	A data-based derivation of the internal stress in the discrete-continuum transition regime for dislocation-based plasticity	Sing-Huei Lee
04:30 PM	04:50 PM	Interpretation of plastic deformation of copper particles in silver	Václav Paidar



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Session Program – Thursday, 26 September

Room: Chamber Hall

09:20 AM	09:50 AM	Coffee break	Forum Hall Foyer 2
Symposium O - Thursday Morning / 09:50 AM-11:40 AM			Chair: Daniel Weisz-Patrault
09:50 AM	10:20 AM	Keynote Lecture: Multiphysics-multiscale simulations of process-microstructure-property relation of additive manufactured Fe-Ni permalloy	Bai-Xiang Xu
10:20 AM	10:40 AM	Scaling laws and a homogenized plasticity model of additively manufactured lattice structures under large deformations	Zhi Chen
10:40 AM	11:00 AM	Utilizing the Coupled Crystal Plasticity Phase-Field Method for Investigating Microstructural Evolutions during Rapid Solidification Processes of Inconel Alloy 617 in Additive Manufacturing	Benhour Amirian
11:00 AM	11:20 AM	Phase field modelling of microstructure evolution during AM thermal cycles : application to martensitic steels	Jules L'Hostis
11:20 AM	11:40 AM	Intergranular stress and plastic strain formation during lasering of an additively manufactured stainless steel: an experimentally-driven thermomechanical simulation study	Manas Upadhyay
11:40 AM	12:40 PM	Lunch	Forum Hall Foyer 2
Symposium O - Thursday Afternoon / 12:40 PM-02:30 PM			Chair: Chinnapat Panwisawas
12:40 PM	01:00 PM	Modeling of failure in additive manufacturing: from fracture in monolithic to functionally graded samples	Allison Beese
01:00 PM	01:20 PM	Influence of material structure on fatigue life of AISI P20+Ni steel with laser clad functional aluminium bronze layers	Pavel Doubek
01:20 PM	01:40 PM	Efficient texture prediction for additive manufacturing	Xiaohui Liang
01:40 PM	02:00 PM	Multi-fidelity framework to predict the melt pool characteristics for laser powder bed fusion of Inconel 718	Abdul Khalad
02:00 PM	02:20 PM	-	-
02:30 PM	03:00 PM	Refreshment break	Forum Hall Foyer 2