

PROGRAM

The 10th International Conference on Multiscale Materials Modeling

The world's largest theoretical and computational forum on multiscale materials modeling

OCTOBER 2-7, 2022

Renaissance Harborplace Hotel
Baltimore, MD, U.S.A

<https://mmm10.jhu.edu>



Welcome to the 10th International Conference on Multiscale Materials Modeling (MMM 2022) in Baltimore, Maryland!

The biennial conference, first held in 2002 in London (UK), is a forum for researchers from academia, national laboratories, and industrial research facilities worldwide with interdisciplinary research backgrounds, including but not limited to: mechanics, materials, biomechanics, mechanobiology, advanced manufacturing, mathematics, and computational sciences.

This year's conference is hosted by Johns Hopkins University (JHU), George Mason University (GMU), Georgetown University, and the University of Maryland (UMD).

The conference will focus on both classical as well as new ground-breaking directions in the field, including:

- Mathematical and Computational Foundation of Multiscale Methods
- Probabilistic Modeling and Uncertainty Quantification
- Multiscale and Multiphysics Mechanics and Materials
- Material Classes: Biological, Soft Materials, Structural (Crystalline and Amorphous), Nuclear, Multi-functional, Interfaces, etc.
- Additive Manufacturing and Emerging Manufacturing Methods
- Materials Informatics (machine learning, data mining and artificial intelligence)
- Synergistic Coupling of Experiments with MMM modeling
- Micro and Nanostructural Evolution
- Materials by Design
- Industrial Applications

We would like to thank all the symposium organizers, sponsors, and participants for their contributions to MMM 2022. We hope you enjoy the program and your time in Baltimore.

Co-Chairs:

Jaafar El-Awady

Somnath Ghosh

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Chung Ho Woo (Hong Kong)

Sidney Yip (USA)

Michael Zaiser (Germany)

PLENARY SPEAKERS:**Julie Christodoulou**

Materials & Manufacturing Innovations, LLC, USA

“A Point of Reflection: Understanding our Progress and Challenges”

Discovery, development and implementation of advanced technologies to enable a cleaner, healthier and safer world depend on the materials systems available, understanding of which is ever more complicated and nuanced – and ever more urgently needed. Reflecting on the tools at hand to accelerate both the use of emergent materials systems and the advancement of the underlying knowledge that supports them, we find a common thread emphasizing the importance of translation: translation of understanding into terms multiple engineering disciplines can use, translation of principles from one discipline to another, translation of discovery to product/capability. Computational codes and quantitative data descriptions enable that translation. With this hypothesis, work in Integrated Computational Materials Engineering (ICME) and work toward the goals of the Materials Genome Initiative (MGI) have focused on developing the computational tools and supporting quantitative data to enable effective translation of knowledge. In this talk, we pause to assess our progress and begin to identify purposeful next steps for our community of materials science and engineering, particularly for multiscale materials modeling.

Thursday, October 6 | 8:30 - 9:30 AM

Maryland Ballroom AB&C

Norman A. Fleck

University of Cambridge, England

“The Mechanics of Multi-Phase Lattices”

Traditionally, lattice materials comprise a micro-architected lattice and intervening porosity. The mechanical properties are sensitive to the topology, relative density and the length scale, but usually much less sensitive to the degree of imperfection. But what if we fill the porosity with an inviscid, incompressible fluid? The resulting mechanical properties are sensitive to the degree to which fluid can leak from one cell into the next. The macroscopic in-plane yield surface of a hexagonal honeycomb, filled with an inviscid, incompressible fluid, has been calculated and analytical models have been obtained for the collapse modes. Numerical simulations reveal that the finite strain response is sensitive to the angle of inclination of the hexagonal cells, and to the possibility of cavitation within the liquid core. If cavitation is absent, the compressive response can display shear localisation along an inclined band (reminiscent of fibre microbuckling in composites). Alternatively, if cavitation is present, mild localisation occurs into inclined bands with unit cells that first dilate and then crush until volumetric lockup occurs and a residual shear state exists within the band. A Maxwell-line construction can be used on the unit cell response in order to determine the steady state propagation stress for both the case of no-cavitation and cavitation. Other competing collapse modes exist that exhibit strong softening but do not admit the existence of a localisation (shear) band. If time permits, some remarks will be made on the fracture of filled lattices, and on the actuation of a lattice due to induced swelling by the intercalation of a liquid phase or by Li ions.

Tuesday, October 4 | 8:30 - 9:30 AM

Maryland Ballroom AB&C

James Sethian

University of California, Berkeley, USA

“Advances in Advancing Interfaces: The Mathematics of Manufacturing of Industrial Foams, Fluidic Devices, and Automobile Painting”



Complex dynamics underlying industrial manufacturing depend in part on multiphase multiphysics, in which fluids and materials interact across orders of magnitude variations in time and space.

In this talk, we will discuss the development and application of a host of numerical methods for these problems, including Level Set Methods, Voronoi Implicit Interface Methods, implicit adaptive representations, and multiphase discontinuous Galerkin Methods. Applications for industrial problems will include modeling how foams evolve, how electro-fluid jetting devices work, and the physics and dynamics of rotary bell spray painting across the automotive industry.

Wednesday, October 5 | 8:30 - 9:30 AM

Maryland Ballroom AB&C

Subra Suresh

Nanyang Technological University, Singapore

“Deep Learning from Nature and Machines for Engineered and Biological Materials”



Major advances in experimental and computational tools as well as data science and deep learning, along with the convergence of hitherto disparate disciplines at the intersections of the

physical, digital and biological worlds, have provided unprecedented opportunities to design, model and characterize materials. In addition, processes, mechanisms and functions found in Nature, in concert with the latest

advances in machine learning, offer unique and novel pathways to scientific discovery, mechanistic understanding, engineering design, industrial applications, and clinical practice. In this presentation, we examine our recent results from experimental, computational modeling, and data analytics of engineered and biological materials in three broad areas: materials science, plant science, and medical science. We show through examples and case studies how the appropriate combinations of experimental observations, two-dimensional and three-dimensional computational modeling and images, as well as multi-fidelity data can be combined with physics-informed neural networks and biomimetics to improve materials design, predictions of their properties and performance, and structural integrity. For biomedical applications, novel approaches that integrate microfluidic platforms with static and dynamic data and images from clinical settings are also discussed to demonstrate how deep learning approaches can offer new possibilities to improve patient outcomes in disease diagnostics, therapeutics, and treatment. Specific cases considered here are include: metallization of nanoscale diamond for tunable electronic properties; design of plant-based materials for soft robotics and sustainability; extraction of mechanical properties of materials through instrumented nanoindentation and multi-fidelity machine learning algorithms; and artificial intelligence velocimetry to probe diabetic retinopathy and blood disorders

Monday, October 3 | 8:30 - 9:30 AM

Maryland Ballroom AB&C.

SEMI-PLENARY SPEAKERS:**Markus J. Buehler**

Massachusetts Institute of Technology, USA

“Multiscale Mechanics of Bioinspired Material Intelligence”

Digital biomaterials are designed through an integrated approach of large-scale computational modeling, material informatics, and artificial intelligence/ machine learning to optimize and leverage novel smart material manufacturing for advanced mechanical properties. Through the use of nanotechnology and additive manufacturing, and bio-inspired methods, we can now mimic and improve upon natural processes by which materials evolve, are manufactured, and how they meet changing functional needs. In this talk we show how we use mechanics to fabricate innovative materials from the molecular scale upwards, with built-in bio-inspired intelligence and novel properties, while sourced from sustainable resources, and breaking the barrier between living and non-living systems. Applied specifically to protein materials, this integrated material approach is revolutionizing the way we design and use materials, and has the potential to impact many industries, as we harness data-driven modeling and manufacturing across domains and applications. The talk will cover several case studies covering distinct scales, from spider webs and silk, to collagen, to biomineralized materials, as well as applications to food and agriculture, and focuses on mechanistic insights using scaling laws and size effect studies.

Wednesday, October 5 | 1:00 - 1:45 PM

Maryland Ballroom D

Professor Pedro Camanho

University of Porto, Portugal

“Generation of Statistical Design Allowables of Composite Laminates using Theory-Guided Machine Learning”

This work represents the first study towards the application of machine learning techniques in the prediction of statistical design allowables of polymer composite laminates used in aircraft structures. Building on data generated analytically using Finite Fracture Mechanics based models developed at the length scale of the laminate, four machine learning algorithms are used to predict the notched strength of composite laminates and their statistical distribution, associated to material and geometrical variability. Excellent representations of the design space (relative errors of around $\pm 10\%$) and very accurate representations of the distributions of notched-hole strengths and corresponding B-basis allowables are obtained. The Gaussian Processes models proved to be the most reliable, considering their continuous nature and fast training process. This work serves as basis for the prediction of first-ply failure, ultimate strength and failure mode of composite specimens based on non-linear finite element simulations, providing further reduction of the time required to virtually certify the next generation of composite aerostructures.

Monday, October 3 | 1:00 - 1:45 pm

Maryland Ballroom D

Bruce Engelmann

Hexagon Manufacturing Intelligence, USA

“Physics- and AI-Based ICME Methodologies Relying on Multi-Scale Digital Twin of Heterogeneous Materials”



Over the past several years, homogenization techniques in materials engineering have worked their way into industrial applications. The rise of computational power, parallelization methods, GPU programming and solvers have paved the way for daily usage of full-field homogenization over larger and more representative RVEs (i.e., Representative Volume Element). For example, FFT/spectral solvers have demonstrated very high performance thanks to CPU/GPU parallelization while delivering accurate material performance predictions. Problems with loss of ellipticity can be regularized by non-local formulations. However, we are still challenged with the curse of dimensionality when dealing with complex material phenomenon. A full bridging of the structural and the material/RVE scale (FE^2) is cost prohibitive. Single scale phenomenological models fitted against predictions of RVE models or semi-analytical homogenization techniques can lose some of the most valuable information leading to inaccurate or incomplete predictions. However, we have a few more tools in the toolbox that can help us here. First, the use of measurement techniques like CTscans and their associated software are delivering increasing measurement accuracy at a more affordable price allowing the direct physical measurement of material microstructure. Second, many authors have suggested using AI/ML models with synthetically and physically generated data. We will discuss our experiences combining physical modelling with data and AI/ML techniques. We believe that these elements together will

enable true multi-scale driven Integrated Computational Material Engineering (ICME) methodologies across engineering processes in product development to account for material internal structure.

Wednesday, October 5 | 1:00 - 1:45 PM

Maryland Ballroom AB&C

Giulia Galli

University of Chicago & Argonne National Laboratory, USA

“Complex Materials from First Principles: From Sustainable Energy Sources to Quantum Information Science”



This talk will discuss recent progress in gaining understanding and scoping design rules for two classes of systems: sustainable materials, namely solids and molecules that are useful to develop sustainable energy sources, and promising systems for quantum technologies. We will present results obtained by carrying out first-principles simulations, coupled with computational spectroscopic techniques and, in some cases, with advanced sampling methods. The work will show that, despite several approximations to the basic equations of quantum mechanics, insightful predictions on physical and chemical processes can be made that are not only corroborated by experiments, but inspire new ones. The talk will focus on several examples to highlight both the successes and the challenges of quantum simulations, including in the study of oxides for photoelectrodes and low power electronics, and defective semiconductors for quantum sensing applications.

Tuesday, October 4 | 1:00 - 1:45 PM

Maryland Ballroom AB&C

Elizabeth A. Holm

Carnegie Mellon University, USA

“Quantity or Quality? Capitalizing on Small but Rich Materials Data Sets”

The process of scientific inquiry involves observing a signal (data) and interpreting it to generate information (knowledge). Artificial intelligence (AI) – a broad term comprising data science, machine

learning (ML), neural network computing, computer vision, and other technologies – opens new avenues for extracting information from materials data by uncovering highdimensional trends that are hard to identify by conventional analysis. Thus, the key to all AI methods is data. However, for many AI applications, the quantity and quality of data required for optimal outcomes is not understood. One solution is to err on the side of data quantity, amassing large, homogeneous data sets. While this may be viable in the social media realm, it is less feasible for physical science and engineering problems where the data is expensive and often heterogeneous. Fortunately, physical data collected by scientists have several advantages: They are selected for their known relevance to the problem, bounded by a physical basis, expertly acquired, and rich in information. Using examples from microstructural characterization, we will survey the factors that should be considered when designing a materials science data set for AI analysis. We will evaluate the relative importance of data size, data type, and data quality. One encouraging observation is that the richness of materials data often enables excellent AI outcomes with surprisingly small data sets.

Thursday, October 6 | 1:00 - 1:45 PM

Maryland Ballroom AB&C

David L. McDowell

Georgia Institute of Technology, USA

“Model Form and Parameter Uncertainty in Multiscale Mesoscopic Dislocation Plasticity”

We consider crystal plasticity model constructs with complexity arising from multiple phases at micron scale and/or many body dislocation interactions. For alpha-beta Titanium colony microstructures, a three-step strategy is employed using Gaussian Process Regression as a rapid emulator with Bayesian inference and Markov Chain Monte Carlo sampling to consider the likelihood of one model form versus another in light of available spherical indentation data. For the most likely constitutive framework, it is demonstrated using this strategy that certain slip transfer parameters are more likely than others to describe the available experimental data. We close by considering the efficacy of bridging from atomistic simulations to inform the rate-dependent flow rule of crystal plasticity for bcc Fe based on coordinated kink pair formation on screw dislocations, introducing the need for a model discrepancy layer to inject the role of sources.

Tuesday, October 4 | 1:00 - 1:45 PM

Maryland Ballroom D

Shigenobu Ogata

Osaka University, Japan

“Atomistic Modeling of The Impact of Hydrogen on Metals”

The impacts of hydrogen on the mechanical behavior of metals have been studied for many years, and many models and theories have been proposed. However, many issues remain open due

to the difficulty in the direct observation of hydrogen behavior in materials. Therefore, atomistic modeling and simulation are promising tools that can directly examine the hydrogen behavior and its impacts on the mechanical behavior of metals, such as plasticity, defect growth, and fracture. Therefore, a vast number of atomistic simulations have also been performed. However, the lack of reliable atomic interactions has limited atomic simulations to small-scale density functional theory (DFT) calculations or qualitative molecular dynamics (MD) calculations. To overcome this problem, we recently constructed a general-purpose artificial neural network interatomic potential (ANNIP) for the iron-hydrogen binary system based on a DFT-based training dataset. The ANNIP was successfully applied to quantitatively simulate and understand the essential phenomena dominating the hydrogen-induced degradation of metals, such as hydrogen diffusion at defects, hydrogen trapping/desorption at defects, hydrogen-assisted cracking at the grain boundary, hydrogen-accelerated defect motion, and so on.

Thursday, October 6 | 1:00 - 1:45 PM

Maryland Ballroom D

Peter W. Voorhees

Northwestern University, USA

“Additive Manufacturing: From Nonequilibrium Interfaces to Strange Grains”



Additive manufacturing (AM) has emerged as a promising technique for the fabrication of complex metallic parts. Under AM processing conditions the resulting microstructures can be very complex due to a combination of factors such as the alloy powder being processed, the AM technique, the heat

source power and speed and the resulting shape of the melt pool, and the scan strategy employed by the build, to name a few examples. The microstructures and the resulting properties of the part can differ significantly from those observed through traditional solidification processes due to fast solidification rates (10^{-3} - 1 m/s) and large thermal gradients (10^5 - 10^7 K/m). Simulation plays a critical role in understanding the link between the processing conditions and the resulting microstructure. A phase field model for the development of grain structure during powder bed AM will be discussed. Using the parameters from molecular dynamics simulations, these three-dimensional phase field simulations of the morphological development of grains illustrate the complicated interaction between interfacial mobility anisotropy, weld pool shape, laser scan strategy and multiple powder layers on the resulting grain morphology. The large solidification velocities of AM require a phase field model with the flexibility to incorporate a wide range of models for non-equilibrium solid-liquid interfaces. A phase-field model in which non-equilibrium effects such as solute trapping, solute drag, and interface kinetics can be introduced in a controlled manner while at the same time using interface widths that permit calculations at experimentally accessible length scales will be discussed.

Monday, October 3 | 1:00 - 1:45 PM

Maryland Ballroom AB&C

THE 2022 MMM COMMUNITY AWARD RECIPIENTS

MMM Distinguished Career Achievement Award

William A. Curtin Jr.



Professor Curtin earned a 4 yr. ScB/ScM degree in Physics from Brown University in 1981 and a PhD in theoretical physics from Cornell University in 1986. He worked as staff researcher at British Petroleum until 1993 when he joined Virginia Tech. In 1998 he returned to Brown as Full Professor in the Solid Mechanics

group, and was appointed Elisha Benjamin Andrews Professor in 2006. He joined Ecole Polytechnique Federale de Lausanne as the Director of the Institute of Mechanical Engineering in 2011 and officially as Full Professor in 2012. He will rejoin Brown as Full Professor in 2023. His research successes include predictive theories of hydrogen storage in amorphous metals, strength and toughness of fiber composites, dynamic strain aging and ductility in lightweight Al and Mg metal alloys, solute strengthening of metal alloys including high entropy alloys, and hydrogen embrittlement of metals, along with innovative multiscale modeling methods to tackle many of these problems. Professor Curtin was a Guggenheim Fellow in 2005-06, was Editor-in-Chief of “Modeling and Simulation in Materials Science and Engineering” from 2006-2016, has published over 300 journal papers that have received nearly 23500 citations with an h-index of 82 (Google Scholar), and has been the Principal Investigator on over \$36M of funded research projects.

MMM Early Career Investigator Award

Yinan Cui



Yinan Cui is an associate professor at Tsinghua University. She received her PhD from Tsinghua University in 2015, and then worked as a postdoc at the University of California, Los Angeles (UCLA) until June 2019. Yinan is primarily engaged in the field of mechanics of materials under severe environments. Her research

is focused on developing unique multiscale and multi-physics coupled simulation methods, and disclosing the microscopic physical origins of material deformation and failure. Her work aims to guide the design of more resilient materials used in future energy and power technologies. She has authored more than 50 SCI papers, two academic books, and is a member of the editorial board of Tungsten and the International Journal of Plasticity. She won the 2022 National Nature Science Foundation of China’s Excellent Young Excellent Young Scientists Fund, the 2021 Emerging Leader of Modelling and Simulation in Materials Science and Engineering, and the 2016 Springer Outstanding PhD Thesis Award.

NSF Mechanics of Materials & Structures (MoMS) Outreach at MMM10

Monday, October 3 (12-1pm):

NSF MoMS Program Directors will present opportunities for the Mechanics community at large (~30 minutes). It will be followed by Q/A (Open to all.)

Bring your boxed lunch and curiosities. *Baltimore A*

Tuesday, October 4 (12-1pm):

Join NSF MoMS Program Directors for a lunch. Bring your boxed lunch and curiosities! (Open to all, no sign up needed, but there might be limited seating.)

James Room (6th floor)

Tuesday, October 4 (2-5:30pm):

One-on-one PI meetings with NSF MoMS program directors, please come prepared with your talking point. (15 minutes per meeting slot, sign up required at the registration desk. For US-affiliated PIs only.)

The Technical Program

SYMPOSIA

1. Advances in Methods for Bridging Spatiotemporal Scales in Soft Matter, Polymer and Network Materials
2. Bridging Scales in the Microstructure Modeling of Nuclear Materials
3. Computer Modeling of Laser and Ion Beam Interactions with Materials
4. Contact, Friction, Adhesion: Mechanics of Interfaces across Scales
5. Data-Driven and Physics-Informed Multiscale Materials Modelling
6. Defects and Microstructure Complexity in Materials: Experiments and Multiscale Modeling
7. Dislocations, Twinning, Phase Transformation, Phonon, Diffusion, and Their Interactions in Materials Manufacturing, Processing, and Testing
8. Fatigue and Fracture of Materials: from Micro to Macroscale Modeling and Experimentation
9. Integrated Multiscale/Multiphysics Modeling of Structural Materials
10. Interface-driven Phenomena in Condensed Matter Systems: Thermodynamics, Kinetics, and Chemistry
11. Multiscale Material Modeling of Microelectronics
12. Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem
13. Mechanics and Physics of Material Failure
14. Metals at the Nanoscale and Metals-Based Nanoparticles: Environmental, Mechanical and Kinetic Properties
15. Modeling and Design of Architected Materials
16. Modeling and Experimental Measurements for Metal Additive Manufacturing
17. Multiscale and Multifield Modeling of Composites: from Atomic to Continuum Scale
18. Multiscale Materials Modeling using Ab-initio Accuracy Methods
20. Multiscale Modeling of Battery Materials
21. Multiscale Modeling of Glasses and Structurally Disordered Materials
22. Multiscale Solidification Modeling
23. Scale Bridging in Materials Science
24. Stochastic Methods in Materials Simulation
25. Uncertainty Quantification, Sensitivity Analysis, and Machine Learning in Materials Modeling
27. The Physics of Metal Plasticity: A memorial symposium in honor of Professor Hussein Zbib

Monday Morning, October 3 / TECHNICAL PROGRAM**HOST WELCOME / 8:20 AM****PLENARY LECTURE / 8:30 – 9:30 AM****Prof. Subra Suresh****“Deep Learning from Nature and Machines for Engineered and Biological Materials”****Chair: Somnath Ghosh**

Maryland Ballroom AB&C

10:00 AM	10:30 AM	10:50 AM	11:10 AM	11:30 AM
5th Floor Guilford Room	Symposium 1	Advances in Methods for Bridging Spatiotemporal Scales in Soft Matter, Polymer and Network Materials, Chair(s): Wenjie Xia		
Keynote presentation: Effects of Additive Molecules on Shape Memory Effect in Polymers: A Combined Experimental and Computer Simulation Study <i>Fathollah Varnik*, Gunther Eggeler, Yucen Shen, Hakan Dumlu, Elias M. Zirdehi</i>	Thermal Transport in Polymers: Intra- versus Intermolecular Energy Transport <i>Louis Pigard, Debashish Mukherji, Joerg Rottler*, Marcus Mueller</i>	A Statistical Mechanics Framework for Polymer Chain Scission, Based on the Concepts of Distorted Bond Potential and Asymptotic Matching <i>Jason Mulderrig*, Brandon Talamini, Nikolaos Bouklas</i>	Implicit Finite Element Analysis of the Polymer Physics-Based Multi-Scale Visco-Hyperelastic Constitutive Model <i>Jiwon Jung*, Gun Jin Yun</i>	Coarse-Grained Molecular Dynamics Simulation of Poly(dimethyl-co-diphenyl) Siloxane: Chain Dynamics of Unentangled and Entangled Melts <i>Weikang Xian*, Ying Li</i>
5th Floor Maryland Ballroom F	Symposium 2	Bridging Scales in the Microstructure Modeling of Nuclear Materials, Chair(s): Luca Messina		
Keynote presentation: Damage Induced in Irradiated Tungsten: Modeling and Experimental Validation <i>Marie-France Barthe*, Zhiwei Hu, Cécile Genevois, Brigitte Decamps, Pierre Desgardin, Robin Schäublin, Qigui Yang, Pär Olsson, Andrée De Backer, Christophe Domain, Charlotte S. Becquart</i>	Effects of Stress-Irradiation Coupling on the Formation and Partition of Various Types of Defects <i>Miao He*, Yue Fan</i>	Modelling the Spatial Distribution of Primary Radiation Damage in Heterogeneous Materials <i>Matthew Brand*, Patrick Burr, Edward Obbard, Bernd Gludovatz, Jack Astbury, Christopher Wilson, Colin Windsor</i>	Statistical Analysis of Displacement Cascades in Metals – from Atypic Cascades to Outlier Analysis and Microstructure Evolution Under Irradiation <i>Christophe Domain*, Andrée de Backer, Adithya Nair, Charlotte S Becquart</i>	High-Dose Accumulation of Defects in Fusion Relevant Materials Under Irradiation <i>Fredric Granberg*, Jintong Wu, Daniel Mason, Jesper Byggmästar</i>
5th Floor Baltimore Ballroom B	Symposium 4	Contact, Friction, Adhesion: Mechanics of Interfaces Across Scales, Chair(s): Tevis Jacobs		
Multiscale Approach for Solid Lubrication, Friction and Wear <i>Hitoshi Washizu*, Natsuko Sugimura, Le Van Sang</i>	A Multiscale Perspective on the Effective Relaxation Behavior of Confined Fluids <i>Hannes Holey*, Peter Gumbsch, Lars Pastewka</i>	Friction Prediction in EHL Contact Under Severe Conditions <i>Ruibin XU*, Nicolas Fillot, Laetitia Martinie</i>	Morphology, Concentration, Potential: Parametric Probing of Adsorption Film Friction with Molecular Dynamics <i>Johannes L. Hörmann*, Lars Pastewka</i>	Computational Simulations of Leukocyte Rolling, Adhesion and Bond Formation on Surface Coated with Varying P-Selectin Density <i>Grishma Prabhukhot*, Andrew Kowalewski, Charles Eggleton, Rohan Banton</i>

Monday Morning, October 3 / TECHNICAL PROGRAM

10:00 AM	10:30 AM	10:50 AM	11:10 AM	11:30 AM
5th Floor Homeland Room Keynote presentation: Large Molecular Dynamics Simulations of Fatigue Crack Growth in Face Centered Cubic Metals <i>Eyouileki Awi, Laurent Van Brutzel*, Maxime Sauzay</i>	Symposium 8 Machine Learning-Based Prediction of Small Fatigue Crack Growth in Ti-6Al-4V Alloys <i>Samuel Alfred*, Mehdi Amiri</i>	Fatigue and Fracture of Materials: from Micro to Macroscale Modeling and Experimentation, Chair(s): Mehdi Amiri Accelerating Microstructurally Small Crack Growth Predictions in Three-Dimensional Microstructures Using Deep Learning A phase-field model of quasi-brittle fracture for pressurized cracks: Application to nuclear fuel microstructure fragmentation Multi-Scale Modeling Platform for Performance and Failure Analysis of Cold Spray Formed Materials <i>Vignesh Babu Rao*, Brian Phung, Ashley Spear</i> <i>Wen Jiang*, Tianchen Hu, Larry Aagesen, Sudipta Biswas, Kyle Gamble</i>		
6th Floor Kent Room Keynote presentation: Multiscale Modelling and in Situ Characterization Strategies at IMDEA Materials Institute: Roadmaps for Virtual Processing and Virtual Testing of Metallic Alloys <i>Javier LLorca*, Damien Touret, Javier Segurado, Ignacio Romero, Jon Molina-Aldareguia, Federico Sket</i>	Symposium 9 Integrated Computational Materials Engineering Toolkit to Understand Process-Structure-Property Relationships of Additively Manufactured Metals <i>Napat Vajragupta*, Tatu Pinomaa, Matti Lindroos, Abhishek Biswas, Mohammadreza Yaghoobi, David Montiel Taboada, Tom Andersson, Anssi Laukkanen</i>	Integrated Multiscale/Multiphysics Modeling of Structural Materials, Chair(s): John Allison Phase Field Modeling of Precipitate Evolution Under Magnetic Fields Relating Polyurea Mechanical Behavior to Microstructure by Modeling Domains as Explicit Geometries in Finite Element Simulations <i>Efrain Hernandez-Rivera*, Heather Murdoch, Anit Giri, Daniel Field</i> <i>Steven Yang*, Meredith Silberstein</i>		
5th Floor Maryland Ballroom D Keynote presentation: Continuum Theory of Defects as a Framework for Predictive Modeling of Radiation Effects in Crystalline Solids <i>Anter El-Azab*</i>	Symposium 12 Handling Conditional Convergence in Point Defect Calculations <i>Celine Varvenne*, Thomas Jourdan, Emmanuel Clouet</i>	Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem, Chair(s): Giacomo Po H-Dislocation Interaction in Iron: Consequence for Hydrogen Embrittlement Plastic Strain Localization Mechanisms in Polycrystals Interaction Between Dislocation and Vacancies in Magnesium Oxide <i>Varun Shah, Gábor Csányi, Erik van der Giessen, Francesco Maresca*</i> <i>Baptiste Joste*, Benoit Devincere, Riccardo Gatti, Henry Proudhon</i> <i>Philippe Carrez*, Marie Landeiro dos Reis, Pierre Hirel, Patrick Cordier</i>		
5th Floor Fells Point Room Keynote presentation: Micromechanical fatigue experiments for validation of microstructure-sensitive fatigue simulation models <i>Peter Gumbsch*, Ali Riza Durmaz, Erik Natkowski, Thomas Straub, Chris Eberl</i>	Symposium 13 Damage accumulation during creep in metals: the role of microstructure <i>Laurent Capolungo*, Ricardo Lebensohn, Andrea Rovinelli</i>	Mechanics and Physics of Material Failure, Chair(s): Coleman Alleman Machine learning predictive modeling of creep rupture time in high temperature alloys Interaction based Damage Model for Brittle Solids under High-Rate Compression Statistics evaluation of nucleation conditions using physics-based ductile damage modelling <i>Madison Wenzlick*, M.F.N. Taufique, Ram Devanathan, Kelly Rose, Keerti Kappagantula</i> <i>Sakshi Braroo*, K. T. Ramesh</i> <i>Curt Bronkhorst*, Robert Argus, Nan Chen, Noah Schmelzer</i>		

Monday Morning, October 3 / TECHNICAL PROGRAM

10:00 AM	10:30 AM	10:50 AM	11:10 AM	11:30 AM
6th Floor Gibson Room	Symposium 14	Metals at the Nanoscale and Metals-Based Nanoparticles: Environmental, Mechanical and Kinetic Properties, Chair(s): Eugen Rabkin		
<p>Keynote presentation: Minimum Free-Energy Shapes and Transformations of Metal Nanoclusters Using Replica-Exchange Molecular Dynamics</p> <p><i>Kristen Fichthorn*</i></p>	<p>Ni-Ti Core-Shell Nanoparticles for Self-Propagating Reactions</p> <p><i>Miroslav Cieslar*, Lucia Bajtošová, Jan Hanuš, Jan Fikar, Barbora Krivská, Rostislav Králík</i></p>	<p>From Core-Shell To Intermixing And Eventually Ordering In Pt-Ag Nanoparticles</p> <p><i>Fabienne Berthier, Diana Nelli, Caroline Andrezza-Vignolle, Pascal Andrezza, Riccardo Ferrando, Christine Mottet*</i></p>	<p>When more is less: the effect of grain boundaries on the mechanical properties of metal nanoparticles</p> <p><i>Jonathan Amodeo*, Amit Sharma, Nimrod Gazit, Yuanshen Qi, Olivier Thomas, Eugen Rabkin</i></p>	
5th Floor Pride of Baltimore Room	Symposium 15	Modeling and Design of Architected Materials, Chair(s): Stavros Gaitanaros		
<p>Keynote presentation: Mechanics of Architected Material Systems Based on Topological Interlocking</p> <p><i>Thomas Siegmund*</i></p>	<p>Exploring the Design Space of Cubic Elastic Architected Materials</p> <p><i>Pai Wang*, Yunya Liu, Christian Kern</i></p>	<p>Data-Based Techniques for Structure-Property Correlation in Periodic and Aperiodic Metamaterials</p> <p><i>Shengzhi Luan*, Enze Chen, Stavros Gaitanaros</i></p>	<p>Design of Failure-resistant Architected Materials via Distributed Agents</p> <p><i>Jiakun Liu*, Xiaoheng Zhu, Walker Gosrich, Mark Yim, Jordan Raney</i></p>	
5th Floor Federal Hill Room	Symposium 21	Multiscale Modeling of Glasses and Structurally Disordered Materials, Chair(s): Michael Falk		
<p>Keynote presentation: Plasticity in Amorphous Solids from Local Shear Transformations</p> <p><i>Tristan Albaret*, David Rodney</i></p>	<p>Disentangling the structural and elastoplastic components of dynamical facilitation</p> <p><i>Rahul Chacko*, François Landes, Giulio Biroli, Olivier Dauchot, Andrea Liu, David Reichman</i></p>	<p>Characterizing the Local Yield Surface in Simulated Glasses</p> <p><i>Spencer Fajardo*, Bin Xu, Dihui Ruan, Rahul Meena, Michael Shields, Thomas Hardin, Michael Chandross, Michael Falk</i></p>	<p>Systematic Manipulation of Disorder for Extraordinary Functionality in Materials</p> <p><i>Varda F. Hagh*, Sidney Nagel, Andrea Liu, Lisa Manning, Eric Corwin</i></p>	<p>Keynote presentation: Irreversibility Transition in Mesoscopic Models Under Cyclic Shear</p> <p><i>Damien Vandembroucq*</i></p>
5th Floor Baltimore Ballroom A	Symposium 22	Multiscale Solidification Modeling, Chair(s): Joel Berry		
<p>Keynote presentation: Measuring and modelling crystal formation and growth, flow, and defect formation in solidifying metals</p> <p><i>Patrick Grant*, Insung Han, Shikang Feng, Enzo Liotti</i></p>	<p>Permeability Prediction for Flow of Interdendritic Liquid by Phase-field and Lattice Boltzmann Methods</p> <p><i>Tomohiro Takaki*</i></p>	<p>Floating and Anisotropy-driven Dynamics of Tilted Lamellar Eutectic Solidification Patterns</p> <p><i>Silvère Akamatsu*, Sabine Bottin-Rousseau</i></p>	<p>Multiscale Simulations of Directional Ice Crystal Growth in Sugar Solutions</p> <p><i>Ruud van der Sman*</i></p>	

Monday Morning, October 3 / TECHNICAL PROGRAM

10:00 AM	10:30 AM	10:50 AM	11:10 AM	11:30 AM
5th Floor Maryland Ballroom E	Symposium 24	Stochastic Methods in Materials Simulation, Chair(s): Steve Fitzgerald		
Keynote presentation: Analysis of noise in phase field models <i>Qianran Yu, Nicholas Julian, Jaime Marian, Enrique Martinez*</i>	Dynamical minimum action paths and non-equilibrium transitions <i>Amanda Bailey Hass*, Steve Fitzgerald, Andrew Archer, Grisell Diaz Leines, Stuart Thomson</i>	First Passage Densities from Stochastic Path Integrals <i>Tom Honour*, Steve Fitzgerald</i>	Evaluation of microstructural development of W-Re transmutation using Phase-field modeling <i>Hyeonho Kim*, Kunok Chang</i>	A parallel discrete dislocation dynamics/kinetic Monte Carlo method to study coalescence dynamics of dislocation loops due to vacancy supersaturation <i>Cameron McElfresh*, Jaime Marian</i>

Monday Afternoon, October 3 / TECHNICAL PROGRAM

SEMI-PLENARY LECTURES / 1:00 – 1:45 PM

Prof. Peter W. Voorhees

“Additive Manufacturing: From Nonequilibrium Interfaces to Strange Grains”

Chair: Yuri Mishin

Maryland Ballroom AB&C

Prof. Pedro Camanho

“Generation of Statistical Design Allowables of Composite Laminates using Theory-Guided Machine Learning”

Chair: Javier Llorca

Maryland Ballroom D

1:45 PM	2:15 PM	2:35 PM	2:55 PM	3:15 PM
5th Floor Guilford Room	Symposium 1	Advances in Methods for Bridging Spatiotemporal Scales in Soft Matter, Polymer and Network Materials, Chair(s): Pratyush Tiwary		
<p>Keynote presentation: Potential of Mean Force Based Coarse-Graining for Polymer Grafted Nanoparticles</p> <p><i>Sinan Keten*</i></p>	<p>Effects of Coarse-Graining on Molecular Simulations of Glassy Polymer Mechanics</p> <p><i>Ting Ge*, Jiuling Wang, Pieter in't Veld, Mark Robbins</i></p>	<p>Energy Renormalization for Temperature Transferable Coarse-Grained Modeling of Polymers</p> <p><i>Wenjie Xia*, Zhaofan Li</i></p>	<p>Coarse-Grained Models of Polymer Melts Using Dissipative Potentials: Analysis of Consistent Friction Parametrization Measures</p> <p><i>Lilian Johnson*, Frederick Phelan</i></p>	<p>The Crucial Role of Solvation Forces in Inter-Nanoplatelet Interactions and Stack Formation</p> <p><i>Nanning Petersen*, Martin Girard, Andreas Riedinger, Omar Valsson</i></p>
5th Floor Maryland Ballroom F	Symposium 2	Bridging Scales in the Microstructure Modeling of Nuclear Materials, Chair(s): Marie-France Barthe		
<p>Keynote presentation: Informing Fuel Performance Through Simulations of Irradiation-Enhanced Diffusion in Ceramic Nuclear Fuels</p> <p><i>Michael Cooper*, Christopher Matthews, Vancho Kocevski, Christopher Stanek, Antoine Claisse, Kyle Gamble, Giovanni Pastore, Yifeng Che, Koroush Shirvan, David Andersson</i></p>	<p>Equilibrium point-defect disorder and vibrational entropy of defects in ThO₂ and (U,Th)O₂</p> <p><i>Maniesha Singh*, Anter El-Azab, Tomohisa Kumagai</i></p>	<p>A Monte-Carlo Solution of the Boltzmann Transport Equation for Phonons in Thorium Dioxide and the Effect of Irradiation Induced Defects on Thermal Transport</p> <p><i>W. Ryan Deskins, Jie Peng, Anter El-Azab, Sanjoy K. Mazumder*</i></p>	<p>Exploring uranium-zirconium alloys through ab initio molecular dynamics</p> <p><i>Benjamin Beeler*, Ahmed Aly, Shehab Shousha</i></p>	<p>Ab initio study of tungsten-based alloys under fusion power-plant conditions</p> <p><i>Yichen Qian, Mark Gilbert, Lucile Dezerald, Duc Nguyen, David Cereceda*</i></p>

Monday Afternoon, October 3 / TECHNICAL PROGRAM

1:45 PM	2:15 PM	2:35 PM	2:55 PM	3:15 PM
5th Floor Baltimore Ballroom B				
Symposium 4				
Contact, Friction, Adhesion: Mechanics of Interfaces Across Scales, Chair(s): Lucas Frerot				
<p>Keynote presentation: The Origin of Pressure-Dependent Adhesion in Nanoscale Contacts</p> <p><i>Tevis D. B. Jacobs*, Andrew J. Baker, Sai Bharadwaj Vishnubhotla, Rimei Chen</i></p>	<p>Exploiting Interface Patterning for Adhesion Control</p> <p><i>Ranny Zhao, Kevin Turner, John Bassani*</i></p>	<p>Triboeopitaxy: Selective Crystal Growth Exploiting Shear-Induced Phase Transitions</p> <p><i>Thomas Reichenbach*, Gianpietro Moras, Lars Pastewka, Michael Moseler</i></p>	<p>The Degraded Surface Layer of a Tire Tread: A Numerical Model Combining Discrete and Continuum Approaches</p> <p><i>Kévin Daigne*, Guilhem Mollon, Nicolas Fillot, Sylvie Descartes, Romain Jeanneret-Dit-Grosjean, Frederic Biesse, Antoine Perriot</i></p>	
6th Floor Kent Room				
Symposium 9				
Integrated Multiscale/Multiphysics Modeling of Structural Materials, Chair(s): Javier Llorca				
<p>Keynote presentation: The PRISMS Framework: An Integrated Open-Source Multi-Scale Capability for Accelerated Predictive Materials Science</p> <p><i>John Allison*</i></p>	<p>Calculation of thermodynamic and kinetic properties of Mg alloys using CASM</p> <p><i>Brian Puchala*, Anirudh Natarajan, Anton Van der Ven</i></p>	<p>Integration of the PRISMS Phase-field Modeling Framework with Other PRISMS Computational Tools</p> <p><i>David Montiel*, Yanjun Lyu, Mohammadreza Yaghoobi, Katsuyo Thornton, John Allison</i></p>	<p>Effects of Segregated Solute Atoms and Clusters on Grain Boundary Properties in Magnesium Alloys.</p> <p><i>Vaidehi Menon*, Liang Qi</i></p>	<p>PRISMS-Plasticity and PRISMS-Fatigue: ICME Frameworks to Advance Boundaries of High-Fidelity Simulations</p> <p><i>Mohammadreza Yaghoobi*, Krzysztof S. Stopka, Aaditya Lakshmanan, Duncan Greeley, Zhe Chen, David L. McDowell, John E. Allison, Veera Sundararaghavan</i></p>
5th Floor Maryland Ballroom D				
Symposium 12				
Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem, Chair(s): Anter El-Azab				
<p>Keynote presentation: Computer Simulations of Plasticity During Concurrent Mechanical Deformation and Irradiation</p> <p><i>Nasr Ghoniem*, Yang Li, Giacomo Po</i></p>	<p>About the formation of vacancy clusters in fcc metals: an atomistic approach of the impact of hydrogen</p> <p><i>Marie Landeiro Dos Reis*, Abdelali Oudriss, Xavier Feaugas</i></p>	<p>Linear Complexions Provide Extreme Strengthening in Face Centered Cubic Alloys</p> <p><i>Divya Singh*, Timothy Rupert, Daniel Gianola</i></p>	<p>Diffusion of C in Fe in the presence of defects</p> <p><i>Sebastián Echeverri Restrepo*, Predrag Andric, Anthony Paxton</i></p>	<p>Discrete Dislocation Plasticity-Based Modelling of <a>-type Irradiation Loops in Zirconium</p> <p><i>Rakesh Kumar*, Daniel Hortelano Roig, Edmund Tarleton, Daniel S. Balint</i></p>
5th Floor Fells Point Room				
Symposium 13				
Mechanics and Physics of Material Failure, Chair(s): Laurent Capolungo				
<p>Keynote presentation: Effect of Local Structure and Stoichiometry on the Dynamic Behavior of Bi-Metal Interfaces</p> <p><i>Saryu Fensin*, Jie Chen</i></p>	<p>Modeling Failure of Nano-Metallic Laminates Using a FFT-based Strain Gradient Crystal Plasticity</p> <p><i>Miroslav Zecevic*, Ricardo Lebensohn, Laurent Capolungo</i></p>	<p>Void Growth and Coalescence in Porous Plastic Solids with Sigmoidal Hardening</p> <p><i>Showren Datta*, Hoang Nguyen, Shailendra Joshi</i></p>	<p>Biaxial tensile testing of composite solid propellant</p> <p><i>Rajeev Ranjan*, Murthy H.</i></p>	

Monday Afternoon, October 3 / TECHNICAL PROGRAM

1:45 PM	2:15 PM	2:35 PM	2:55 PM	3:15 PM
6th Floor Gibson Room	Symposium 14	Metals at the Nanoscale and Metals-Based Nanoparticles: Environmental, Mechanical and Kinetic Properties, Chair(s): Jonathan Amodeo		
<p>Keynote presentation: Structure and Properties of Non-Ideal Coherent Interfaces in Alloys</p> <p><i>Christian Brandl*</i></p>	<p>Bimetals at the Nanoscale: Interdiffusion-Induced Bending of Bimetallic Nanowhiskers</p> <p><i>Eugen Rabkin*, Yuanshen Qi, Anuj Bisht, Gunther Richter, Eylül Suadiye, Michael Kalina</i></p>	<p>Shape-dependence of optical properties of coinage-metal nanoparticles</p> <p><i>Wei Zhao*, Robert Jones, Roberto D'Agosta, Francesca Baletto</i></p>		
5th Floor Pride of Baltimore Room	Symposium 15	Modeling and Design of Architected Materials, Chair(s): Baoxing Xu		
<p>Keynote presentation: Load-Bearing Origami-Inspired Metamaterials</p> <p><i>Damiano Pasini*</i></p>	<p>3D Printed Tubular Metamaterials with Enhanced Mechanical Properties</p> <p><i>Huan Jiang*, Yanyu Chen</i></p>	<p>Development of One-Dimensional Hierarchical Beams for Truss Lattice Materials</p> <p><i>Andrew Gross*, Fakhreddin Emami</i></p>	<p>Design of Architected Nanoporous Silicon Nitride Membranes with Tunable Mechanical Properties: A Combined Simulation, Deep Learning, and Experimental Investigation</p> <p><i>Ali K. Shargh*, Gregory R. Madejski, James L. McGrath, Niaz Abdolrahim</i></p>	
5th Floor Federal Hill Room	Symposium 21	Multiscale Modeling of Glasses and Structurally Disordered Materials, Chair(s): Douglas Durian		
<p>Keynote presentation: Avalanches in Sheared and Active Granular Systems</p> <p><i>M. Lisa Manning*, David Richard, Ahmed Elgailani, Damien Vandembroucq, Craig E. Maloney</i></p>	<p>Characterizing Co-Existent Amorphous and Crystalline Phases of H₂O at Room Temperature by Integrating MD Simulation to Experiments</p> <p><i>Ali K. Shargh*, Aude Picard, Rostislav Hrubyak, Dongzhou Zhang, Russel Hemley, Shanti Deemyad, Niaz Abdolrahim, Saveez Saffarian</i></p>	<p>Avalanche phase diagram for the yielding transition of warm amorphous solids</p> <p><i>Daniel Korchinski*, Jörg Rottler</i></p>	<p>Stressful situations: modeling brittle fragmentation and granular compaction</p> <p><i>Joel Clemmer*</i></p>	<p>Numerical study of the mechanical properties of Mg₂SiO₄ glasses</p> <p><i>Valentin Delbecq*, Tristan Albaret, Philippe Carrez, Patrick Cordier, Jean-François Paul, Silvio Pipolo</i></p>
5th Floor Baltimore Ballroom A	Symposium 22	Multiscale Solidification Modeling, Chair(s): Jean-Luc Fattebert		
<p>Keynote presentation: Phase-Field Modeling of Solute Trapping in Rapid Solidification: Where do we Stand?</p> <p><i>Mathis Plapp*</i></p>	<p>Rapid solidification analysis of tungsten</p> <p><i>Tatu Pinomaa*, Jukka Aho, Matias Haapalehto, Joni Kaipainen, Paul Jreidini, Lei Wang, Nikolas Provatas, Anssi Laukkanen</i></p>	<p>Phase Field Simulations of Columnar to Equiaxed Transition in Ti-Cu Alloys</p> <p><i>Bala Radhakrishnan*, Tahany El-Wardany, Ranadip Acharya</i></p>	<p>Homogeneous nucleation driven by out-of-equilibrium solution processing</p> <p><i>René de Bruijn*, Paul van der Schoot, Jasper Michels</i></p>	

Monday Afternoon, October 3 / TECHNICAL PROGRAM

1:45 PM	2:15 PM	2:35 PM	2:55 PM	3:15 PM
5th Floor Maryland Ballroom E	Symposium 24	Stochastic Methods in Materials Simulation, Chair(s): Tom Swinburne		
<p>Keynote presentation: OptiBoost: An Adaptive Method for Hyperdynamics Simulation</p> <p><i>Kristen Fichthorn*</i></p>	<p>Diffusive Molecular Dynamics for Long-Term Atomistic Simulations</p> <p><i>Xingsheng Sun*</i></p>	<p>Learning Effective SDEs from Brownian Dynamics Simulations of Colloidal Particles</p> <p><i>Nikolaos Evangelou*, Felix Dietrich, Juan M. Bello-Rivas, Alex Yeh, Rachel Stein, Michael A. Bevan, Ioannis G. Kevrekidis</i></p>	<p>Exploring the Phase Behaviour of Hard-Sphere Dimers with Nested Sampling</p> <p><i>Omar-Farouk Adesida*, Livia Bartok-Partay, David Quigley</i></p>	

Monday Evening, October 3 / TECHNICAL PROGRAM

4:00 PM	4:30 PM	4:50 PM	5:10 PM
5th Floor Guilford Room Keynote presentation: Cooperative melting in a double-stranded rod model of DNA <i>Prashant Purohit*</i>	Symposium 1 Coarse-Grained Modeling of Phase Transitions in Biomolecular Systems <i>Ruoyao Zhang*, Mikko Haataja, Sharareh Jalali, Cristiano Dias</i>	Advances in Methods for Bridging Spatiotemporal Scales in Soft Matter, Polymer and Network Materials, Chair(s): Frederick Phelan Jr. Coarse-Grained Molecular Modeling of Microporous Nanocomposite Emulsion Thermosets <i>Yiqun Xu*, Jonathan Singer, Ryan Sills</i>	Stochastic Kinetic Model Description of Dissipation and Recovery of Collagen Fibrils Under Cyclic Loading <i>Amir Suhail*, Anuradha Banerjee, Rajesh Ravindran</i>
5th Floor Maryland Ballroom F Keynote presentation: Structure-Search Based Machine-Learning Potentials from an Automated Workflow <i>Noam Bernstein*</i>	Symposium 2 Machine Learned Interatomic Potential Development of W-ZrC for Fusion Divertor Microstructure and Thermomechanical Properties <i>Ember Sikorski*, Mary Alice Cusentino, Megan McCarthy, Julien Tranchida, Mitchell Wood, Aidan Thompson</i>	Bridging Scales in the Microstructure Modeling of Nuclear Materials, Chair(s): Benjamin Beeler Analytic bond-order potential study of the influence of Re and Os on dislocations in W <i>Aparna P. A. Subramanyam*, Ralf Drautz, Thomas Hammerschmidt</i>	Improving Empirical Interatomic Potentials for Predicting Thermophysical Properties by Using an Irreducible Derivatives Approach: the Case of Thorium Dioxide <i>Shuxiang Zhou*, Chao Jiang, Enda Xiao, Michael Cooper, Miaomiao Jin, Chris Marianetti, David Hurley, Marat Khafizov</i>
5th Floor Baltimore Ballroom B Keynote presentation: Large-Scale Molecular Dynamics Simulations on Chemical and Mechanical Wear Processes of Solid Lubricants <i>Momiji Kubo*</i>	Symposium 4 From molecular to multi-asperity contacts: the role of roughness in the transient friction response <i>Lucas Frérot*, Alexia Crespo, Jaafar El-Awady, Mark Robbins, Juliette Cayer-Barrioz, Denis Mazuyer</i>	Contact, Friction, Adhesion: Mechanics of Interfaces Across Scales, Chair(s): Lars Pastewka Adhesive Hysteresis in Soft Matter Contacts <i>Jan Steven Van Dokkum*, Francesc Pérez-Ràfols, Lucia Nicola</i>	
6th Floor Kent Room Keynote presentation: MaterialsDigital - Workflows and Machine Learning Applications for Process Control and Materials Characterization <i>Peter Gumbsch*</i>	Symposium 9 Explore the Energy Landscape of Metastable Titanium Alloys <i>Ganlin Chen*, Liang Qi</i>	Integrated Multiscale/Multiphysics Modeling of Structural Materials, Chair(s): Liang Qi Modeling Al-6061 Microstructural Evolution during Integrally Stiffened Cylinder Formation <i>Elizabeth Urig*, Leonid Zhigilei, Karen Taminger</i>	

Monday Evening, October 3 / TECHNICAL PROGRAM

4:00 PM	4:30 PM	4:50 PM	5:10 PM
5th Floor Maryland Ballroom D Keynote presentation: Effect of Elastic Strain on the Structure and Migration of Self-Interstitials in Copper <i>Baiyu Zhang, Christopher Wheatley, Peng Chen, Xiaofeng Qian, Michael Demkowicz*</i>	Symposium 12 Mechanics of Micropillar Confined Thin Film Plasticity <i>Abhishek Arora*, Rajat Arora, Amit Acharya</i>	Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem, Chair(s): Nasr Ghoniem Grain Boundary Complexions in Rock-Salt Materials <i>Pierre Hirel, Philippe Carrez*, Patrick Cordier</i>	Investigating Defect-Controlled Plastic Deformation Mechanisms of Nano-Porous Metals Using Defect Dynamics Element Method <i>Phu Cuong Nguyen*, Ill Ryu</i>
5th Floor Fells Point Room Keynote presentation: In-situ x-ray and neutron diffraction-based calibration of a physics-based constitutive model of the shape memory effect <i>Sean Agnew*, Daniel Savage, Miroslav Zecevic, Ricardo Lebensohn, Carlos Tome, Donald Brown</i>	Symposium 13 Emergence of Viscosity and Dissipation via Stochastic Bonds <i>Travis Leadbetter*, Ali Seiphooori, Celia Reina, Prashant Purohit</i>	Mechanics and Physics of Material Failure, Chair(s): Hojun Lim Investigation of the inelastic behaviour of reinforced concrete walls - impactors against impact loads during an earthquake <i>Vasiliki Tsotoulidi*, Konstantinos V. Spiliopoulos</i>	
6th Floor Gibson Room Keynote presentation: Data-Driven Models for Nanoscale Plasticity and Thermodynamics <i>Thomas Swinburne*</i>	Symposium 14 Insights into the impact of the wet-synthesis conditions on the structure and composition of metal nano-aerogels from ab initio calculations and experiments <i>Mira Todorova*, Su-Hyun Yoo, Poulami Chakraborty, Tilmann Hickel, Se-Ho Kim, Baptiste Gault, Joerg Neugebauer</i>	Metals at the Nanoscale and Metals-Based Nanoparticles: Environmental, Mechanical and Kinetic Properties, Chair(s): Pyrough : a new tool to model rough samples in atomistic and finite element simulations <i>Hugo Iteney*, Javier Gonzalez, Christophe Le Boulot, Thomas Cornelius, Olivier Thomas, Jonathan Amodeo</i>	
5th Floor Pride of Baltimore Room Keynote presentation: Controllable Soft Elasticity via Domain Formation in Magnetoactive Laminates <i>Pedro Ponte Castaneda*, Joshua Furer</i>	Symposium 15 Multiscale Modeling of Nanoarchitected Materials Under Large Deformations <i>Joshua Crone*, Jaroslav Knap, Richard Becker</i>	Modeling and Design of Architected Materials, Chair(s): Andrew Gross Nonlinear mechanics of lightweight architected materials: collapse, instabilities, shocks, and fracture <i>Stavros Gaitanaros*</i>	A Reduction-based Method for Modelling Lattice Materials <i>Yash Agrawal*, Ananthasuresh G. K., James Guest</i>

Monday Evening, October 3 / TECHNICAL PROGRAM

4:00 PM	4:30 PM	4:50 PM	5:10 PM
5th Floor Federal Hill Room Keynote presentation: Structuro-Elastoplastic (StEP) Model of Plastic Deformation in Disordered Solids <i>Douglas Durian*, Hongyi Xiao, Ge Zhang, Entao Yang, Robert Ivancic, Sean Ridout, Robert Riggelman, Andrea Liu</i>	Symposium 21 Multi-Body Finite Element Simulations of Amorphous Packings of Hydrogel Particles <i>Ahmed Elgailani, Craig E Maloney*</i>	Multiscale Modeling of Glasses and Structurally Disordered Materials, Chair(s): M. Lisa Manning An Equation-free Model of Plasticity in a Metallic Glass Derived from Atomistic Simulation Data <i>Michael L. Falk*, Bin Xu</i>	
5th Floor Baltimore Ballroom A Keynote presentation: Multiscale Modeling of Dendritic Growth with Fluid Flow <i>Damien Tournet*, Thomas Isensee</i>	Symposium 22 Facilitating Phase-field simulations of alloys with CALPHAD thermodynamic driving forces <i>Jean-Luc Fattebert*, Stephen DeWitt, John Turner</i>	Multiscale Solidification Modeling, Chair(s): Joel Berry Sharp phase-field modeling of isotropic solidification with a super efficient spatial resolution <i>Michael Fleck*, Felix Schleifer</i>	
5th Floor Maryland Ballroom E Keynote presentation: Efficient mass transport calculations using a variational principle <i>Dallas Trinkle*</i>	Symposium 24 Data assimilation for microstructure evolution in kinetic Monte Carlo <i>Anh Tran*, Theron Rodgers</i>	Stochastic Methods in Materials Simulation, Chair(s): Mihai-Cosmin Marinica Pipe diffusion mechanism in magnesium oxide <i>Marie Landeiro dos Reis, Philippe Carrez, Yvelin Giret, Patrick Cordier*</i>	Diffusion in a rough potential energy surface <i>Qianran Yu, Fadi Abdeljabad, Murray Daw, Enrique Martinez*</i>

Tuesday Morning, October 4 / TECHNICAL PROGRAM
PLENARY LECTURE / 8:30 – 9:30 AM
Prof. Norman A. Fleck
“The Mechanics of Multi-OPhase Lattices”
Chair: Peter Chung

Maryland Ballroom AB&C

10:00 AM	10:30 AM	10:50 AM	11:10AM	11:30 AM
5th Floor Guilford Room Keynote presentation: Adaptive Resolution as a Multi-Scale, Non-Equilibrium Molecular Dynamics Simulations Tool <i>Robin Cortes Huerto*, Luis A. Baptista, Mauricio Sevilla, Kurt Kremer</i>	Symposium 1 Optimization and Application of Mass exchange scheme in multi-scale simulation <i>Minsub Han*</i>	Advances in Methods for Bridging Spatiotemporal Scales in Soft Matter, Polymer and Network Materials, Chair(s): Omar Valsson		
		Hybrid Molecular Dynamics/Lattice Boltzmann <i>Colin Denniston*</i>	Dissipative Particle Dynamics Simulation of Ultrasound Propagation through Liquid Water <i>Petra Papež, Matej Praprotnik*</i>	The Local Structure of Water from Combining Diffraction and X-Ray Spectroscopy <i>Lars G.M. Pettersson*</i>
5th Floor Maryland Ballroom F Keynote presentation: Effects of Short-Range Ordering on Strength, Ductility, and Fracture Toughness of High Entropy Alloys <i>Yong-Wei Zhang, Shuai Chen, Ping Liu, Zhi-Gen Yu, Zachary Aitken*, Qing-Xiang Pei</i>	Symposium 2 A mesoscale model of tritium release in polycrystalline LiAlO ₂ with strong diffusivity inhomogeneity under irradiation <i>Shenyang Hu*, Yulan Li, Zirui Mao, Andrew Casella, David Senor</i>	Bridging Scales in the Microstructure Modeling of Nuclear Materials, Chair(s): Ludovic Thuinet		
		Phase-field Modeling of Radiation Induced Segregation for Multicomponent Alloys: Kinetic Monte Carlo and CALPHAD-Informed Simulations <i>Sourabh Bhagwan Kadambi*, Daniel Schwen, Yongfeng Zhang, Lingfeng He</i>	Phase Field approach of the formation of an Interaction Compound in material testing reactors fuels <i>Gatien Rolland*, Lucile Dezerard, Benoît Appolaire, Stéphane Valance</i>	Phase field modeling of microstructural evolution of alloys during irradiation <i>Pascal Bellon*, Gabriel Bouobda Moladje, qun Li, robert Averback</i>
5th Floor Baltimore Ballroom A Keynote presentation: (Physics-Informed) Machine Learning for Atomistic Materials Science <i>Alexandra Goryaeva, Clovis Lapointe, Jacopo Baima, Arnaud Allera, Thomas Swinburne, Mihai-Cosmin Marinica*</i>	Symposium 5 A Machine-Learned Spin-Lattice Interatomic Potential for Dynamic Simulations of Defective Magnetic Iron <i>Jacob Chapman*, Pui-Wai Ma</i>	Data-Driven and Physics-Informed Multiscale Materials Modelling, Chair(s): Tilmann Hickel		
		Predicting melting temperatures from bulk properties with pyiron <i>Jan Janssen*, Tilmann Hickel, Danny Perez, Joerg Neugebauer</i>	Approximating the Impact of Nuclear Quantum Effects on Thermodynamic Properties of Crystalline Solids by Temperature Remapping <i>Raynol Dsouza*, Liam Huber, Blazej Grabowski, Jörg Neugebauer</i>	Effect of Microstructural Inclusions on the Bulk Flexoelectric Response of Aluminized THV Composites <i>Ju Hwan (Jay) Shin, Mikel Zaitzeff, Lori Groven, Min Zhou*</i>

Tuesday Morning, October 4 / TECHNICAL PROGRAM

10:00 AM	10:30 AM	10:50 AM	11:10AM	11:30 AM
5th Floor Homeland Room	Symposium 6	Defects and Microstructure Complexity in Materials: Experiments and Multiscale Modeling, Chair(s): Todd Hufnagel		
<p>Keynote presentation: Microstructural complexity and multiscale residual stresses resulting from laser powder bed fusion additive manufacturing</p> <p><i>Lyle Levine*</i></p>	<p>Towards robust characterization of structural defects at the atomic scale: from high-temperature simulations to Atom Probe Tomography</p> <p><i>Arnaud Allera*, Alexandra Goryaeva, Isabelle Mouton, Camille Flament, Jean-Bernard Maillet, Mihai-Cosmin Marinica</i></p>	<p>Stress induced subgrain formation in Sn thin films</p> <p><i>Marisol Koslowski*, Xiaorong Cai, Congying Wang, Carol Handwerker, John Blendell</i></p>	<p>Transfer and incorporation effects of dislocation to grain boundary of bicrystal using crystal plasticity FEM</p> <p><i>Toshiro Amaishi*, Nobuhisa Ochi, Tei Hirashima, Yoji Shibutani</i></p>	<p>Impact of Technological and Computational Advances on X-Ray Materials Physics Investigations*</p> <p><i>Bennett Larson*</i></p>
5th Floor Baltimore Ballroom B	Symposium 7	Dislocation, Twinning, Phase Transformation, Phonon, Diffusion, and Their Interactions in Materials Manufacturing, Processing, and Testing, Chair(s): Penghui Cao		
<p>Keynote Presentation: Slip Transmission and Voiding during Slip Band Intersections in Fe70Ni10Cr20 Stainless Steel</p> <p><i>Xiaowang Zhou, Richard Skelton, Ryan B. Sills, Christopher San Marchi</i></p>	<p>A Study about Shock-Induced Spallation in Mono- and Nanocrystalline High-Entropy Alloys</p> <p><i>Daniel Thuermer*, Nina Merkert (née Gunkelmann), Shiteng Zhao, Orlando Deluigi, Camelia Stan, Iyad Alhafez, Herbert Urbassek, Marc Meyers, Eduardo Bringa</i></p>	<p>Interactions between Dislocation and Twin Boundary in Ni-based Concentrated Alloys</p> <p><i>Haixuan Xu*, Sho Hayakawa</i></p>		
6th Floor Kent Room	Symposium 9	Integrated Multiscale/Multiphysics Modeling of Structural Materials, Chair(s): Katsuyo Thornton		
<p>Keynote presentation: Integrated materials design for extreme environments</p> <p><i>K. T. Ramesh*, Lori Graham-Brady</i></p>	<p>Quantitative Electrochemical Phase-field Modeling for Corrosion of Engine Materials at High Temperature</p> <p><i>Xueyang Wu*, Michael Tonks, Wen Jiang, Iman Abdallah</i></p>	<p>Investigation of the Effect of Microstructure on Micro-galvanic Corrosion in Magnesium Alloys Using Continuum-scale Phase-field Modeling</p> <p><i>Yanjun Lyu*, Vishwas Goel, David Montiel Taboada, Katsuyo Thornton</i></p>	<p>Sensitivity Study of Multiscale and Phenomenological Elasto-Viscoplastic Grade 91 Material Models for Component-Scale Response</p> <p><i>Lynn Munday*, Benjamin Spencer, Laurent Capolungo, M. Arul Kumar, Christopher Matthews, Aaron Tallman, Aritra Chakraborty, Mark Messner</i></p>	
5th Floor Maryland Ballroom E	Symposium 10	Interface-Driven Phenomena in Materials: Thermodynamics, Kinetics, and Chemistry, Chair(s): Fadi Abdeljawad		
<p>Keynote presentation: Grain Boundary Dislocation Interaction Using Atomistic Modeling</p> <p><i>Saryu Fensin*, Sumit Suresh, Khanh Dang, Nithin Mathews, Avanish Mishra, Abigail Hunter</i></p>	<p>Grain Boundary Stress Field Evolution due to Dislocation-Grain Boundary Interactions and Influence on Subsequent Slip Transmission</p> <p><i>Darshan Bamney, Laurent Capolungo, Douglas Spearot*</i></p>	<p>Shear Coupled Microstructure Evolution with Phase Field Emergent Disconnections</p> <p><i>Brandon Runnels*</i></p>	<p>Interface dislocations and grain boundary disconnections using Smith normal bicrystallography</p> <p><i>Nikhil Chandra Admal*, Enrique Martínez, Giacomo Po</i></p>	<p>Polycrystal plasticity-driven static recrystallization model in iron</p> <p><i>Cameron McElfresh*, Jaime Marian</i></p>

Tuesday Morning, October 4 / TECHNICAL PROGRAM

10:00 AM	10:30 AM	10:50 AM	11:10AM	11:30 AM
5th Floor Maryland Ballroom D Keynote presentation: Non-Equilibrium Effects on Irradiation Defects in Metals Steve Fitzgerald*	Symposium 12 A 3D dislocation dynamics model of thermal and irradiation creep Giacomo Po*, Yue Huang, Yang Li, Nasr Ghoniem, Benjamin Ramirez, Christopher Baker, Thomas Black, James Hollenbeck	Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem, Chair(s): Emmanuel Clouet A Coupled Vacancy Diffusion-Dislocation Dynamics Model for the Climb-Glide Motion of Jogged Screw Dislocations Yang Li*, Nasr Ghoniem, Giacomo Po	New insights into localized plasticity: Nanoimprint formation and plastic instabilities in pure metals and alloys Jan Ocenášek, Javier Varillas, Jorge Alcalá*	Experimental-numerical analysis of quasi-2D steel microstructures Job Wijnen*, Tijmen Vermeij, Ron Peerlings, Johan Hoefnagels, Marc Geers
5th Floor Fells Point Room Keynote presentation: Atomistic Simulations, Mesoscale Modelling and Micromechanical Testing of Crack – Microstructure Interactions Erik Bitzek*, Polina Baranova, Benedikt Eggle-Sievers, Shivraj Karewar, Stefan Gabel, Benoit Merle, Ralf Wehler, Steffen Neumeier, Mathias Göken, Elena Jover Carrasco, Marc Fivel	Symposium 13 Understanding Void Growth at Grain and Phase Boundaries Paul Christodoulou*, Miroslav Zezevic, Ricardo Lebensohn, Irene Beyerlein	Mechanics and Physics of Material Failure, Chair(s): Curt Bronkhorst Moving window concurrent atomistic continuum methods for shock propagation in crystalline materials Alexander Davis, Vinamra Agrawal*	Understanding Damage Nucleation and Evolution in BCC Microstructures during Spall Failure at the Atomic Scales Marco Echeverria, Avinash Dongare*	Micromechanics of Void Nucleation Revealed by Molecular Dynamics Simulations of Particle Delamination in Aluminum Qian Qian Zhao*, Ryan Sills
6th Floor Gibson Room Keynote presentation: Synthesis and Properties of Defect Scarce Nano-Objects by Physical Vapor Deposition Gunther Richter*, Eylül Suadiye, Olga Iaroslavtseva	Symposium 14 Deformation of thin nanocrystalline films: molecular dynamics simulation of in-situ TEM experiment Lucia Bajtošová*, Barbora Krivská, Rostislav Králík, Jozef Veselý, Jan Hanuš, Petr Harcuba, Jan Fikar, Ankit Yadav, Miroslav Cieslar	Metals at the Nanoscale and Metals-Based Nanoparticles: Environmental, Mechanical and Kinetic Properties, Chair(s): Thin-film (FTO/BaTiO ₃ /AgNPs) for Enhanced Piezo-photocatalytic Degradation of Methylene blue and Ciprofloxacin in Wastewater Daniel Masekela*, Nonhlangabezo Mabuba, Nomso Hintsho-Mbita	Mechanical and Electronic properties of pure Metallic and Bimetallic nanoparticle under deformation Matteo Erbi**	

Tuesday Morning, October 4 / TECHNICAL PROGRAM

10:00 AM	10:30 AM	10:50 AM	11:10AM	11:30 AM
5th Floor Pride of Baltimore Room	Symposium 15	Modeling and Design of Architected Materials, Chair(s): Pai Wang		
<p>Keynote presentation: Topology optimization of material architectures realized by extrusion-based 3D printing</p> <p><i>Hajin Kim, Jackson Jewett, Josephine Carstensen*</i></p>	<p>Large-scale modeling and fast simulations on assembly of 2D materials based architectural structures</p> <p><i>Baoxing Xu, Qingchang Liu*</i></p>	<p>Extreme resilience and dissipation in the interpenetrating, heterogeneous soft crystals</p> <p><i>Gisoo Lee*, Jaehee Lee, Hansohl Cho</i></p>		
5th Floor Federal Hill Room	Symposium 21	Multiscale Modeling of Glasses and Structurally Disordered Materials, Chair(s): Francesco Zamponi		
<p>Keynote presentation: Stress Localization and Relaxation in Jammed Soft Solids Under Shear: From Transient Shear Banding to Flow Cessation</p> <p><i>Emanuela Del Gado*</i></p>	<p>Rigidity Percolation in Shear Thickening Suspensions</p> <p><i>Abhay Goyal, Nicos Martys*, Emanuela Del Gado</i></p>	<p>The Phase Diagram of Active Deformable Particles</p> <p><i>Francesco Arceri*, Corey O'Hern, Mark Shattuck, Yuxuan Cheng, Dong Wang, Jack Treado</i></p>	<p>Large-Scale Frictionless Jamming with Power-Law Particle Size Distributions</p> <p><i>Joseph Monti*, Joel Clemmer, Ishan Srivastava, Leonardo Silbert, Gary Grest, Jeremy Lechman</i></p>	<p>Unexpected Ductility in Semiflexible Polymer Glasses with $N_e = C_{inf}$</p> <p><i>Robert Hoy*, Joseph Dietz, Kai Nan</i></p>

Tuesday Afternoon, October 4 / TECHNICAL PROGRAM
SEMI-PLENARY LECTURES / 1:00 – 1:45 PM

Prof. Giulia Galli

“Complex Materials from First Principles: From Sustainable Energy Sources to Quantum Information Science”

Chair: Nasr Ghoniem

Maryland Ballroom D

Prof. David L. McDowell

“Model Form and Parameter Uncertainty in Multiscale Mesoscopic Dislocation Plasticity”

Chair: Lyle Levine

Maryland Ballroom D

1:45 PM	2:15 PM	2:35 PM	2:55 PM	3:15 PM
5th Floor Guilford Room	Symposium 1	Advances in Methods for Bridging Spatiotemporal Scales in Soft Matter, Polymer and Network Materials, Chair(s): Sinan Keten		
Keynote presentation: How Brownian Forces Alter Strain Routing in Fibrous Materials <i>Preethi Chandran*</i>	Composite Stochastic Network Materials <i>Catalin Picu*</i>	Size-dependent fracture in elastomers: experiments and phase-field modeling <i>Jaehee Lee*, Seunghyeon Lee, Jeongwoon Lee, Hansohl Cho</i>	Origin of anomalous collagen fiber realignment in the facet capsular ligament via multiscale FEM <i>Jacob Merson*, Catalin Picu</i>	Energy Release Rate for Cracks in Hydrogels Undergoing Finite Deformations <i>Konstantinos Garyfallogiannis*, Prashant Purohit, John Bassani</i>
5th Floor Maryland Ballroom F	Symposium 2	Bridging Scales in the Microstructure Modeling of Nuclear Materials, Chair(s): Sophie Blondel		
Keynote presentation: Molecular Dynamics Modeling of Hydrogen and Nitrogen Implantation in Tungsten Using Machine Learned Interatomic Potentials <i>Mary Alice Cusentino*, Megan McCarthy, Ember Sikorski, Mitchell Wood, Aidan Thompson</i>	A temporal multiscale framework to simulate the long-term diffusion of radiation damage induced defects <i>Mauricio Ponga*, Mohamed Hendy</i>	Atomic-scale simulation of Xe-filled vacancies in UO ₂ nuclear fuel <i>Théo Beigbeder*, Julien Tranchida, Laurence Noirot, Emeric Bourasseau</i>	Long Time-Scale Molecular Dynamics Modeling of He Bubble Growth at W Grain Boundaries <i>Peter Hatton, Danny Perez, Blas Uberuaga</i>	Molecular Dynamics Simulation of Deformation in Nickel Containing Helium Bubbles <i>Tung Yan Liu*, Michael Demkowicz</i>
5th Floor Baltimore Ballroom A	Symposium 5	Data-Driven and Physics-Informed Multiscale Materials Modelling, Chair(s): Tilmann Hickel		
Keynote presentation: Characterizing Evolving Discrete Dislocation Configurations with Alignment Tensors and Correlations <i>Thomas Hochrainer*, Benedikt Weger, Bernhard Heining, Satyapriya Gupta</i>	Predicting dislocation-grain boundary interactions with high-throughput atomistic simulations <i>Sumit Athikavil Suresh*, Khanh Dang, Avinish Mishra, Nithin Mathew, Edward Kober, Reeru Pokharel, Abigail Hunter, Saryu Fensin</i>	Data-driven Exploration of Dislocation Networks using Reduced Data Sets <i>Katrin Schulz*, Balduin Katzer, Kolja Zoller</i>	Predicting the failure of two-dimensional silica glasses <i>Francesco Font-Klos, Marco Zanchi, Stefan Hiemer*, Silvia Bonfanti, Roberto Guerra, Michael Zaiser, Stefano Zapperi</i>	Uncertainty-Quantified Parametrically-Upscaled Continuum Damage Mechanics (UQ-PUCDM) Model for unidirectional composites with nonuniform microstructural distributions <i>Yanrong Xiao*, Xiaofan Zhang, Somnath Ghosh</i>

Tuesday Afternoon, October 4 / TECHNICAL PROGRAM

1:45 PM	2:15 PM	2:35 PM	2:55 PM	3:15 PM
5th Floor Homeland Room	Symposium 6	Defects and Microstructure Complexity in Materials: Experiments and Multiscale Modeling, Chair(s): Lyle Levine		
<p>Keynote presentation: The Influence of Microstructure on Martensite Formation During Deformation of an Austenitic Steel</p> <p><i>Todd Hufnagel*, Ye Tian, Xiaohui Tu</i></p>	<p>Characterizing deformation mechanisms in irradiated metal thin films using in situ TEM straining</p> <p><i>Sandra Stangebye*, Kunqing Ding, Yin Zhang, Ting Zhu, Olivier Pierron, Josh Kacher</i></p>	<p>Phase Field Modeling Study of Zirconium Hydride Morphology in a Polycrystalline Structure</p> <p><i>Pierre-Clement Simon*, Arthur Motta, Michael Tonks</i></p>	<p>Investigation of Adiabatic Shear Banding in FCC Single and Poly-crystals by using a Micromorphic Crystal Plasticity model</p> <p><i>Vikram Phalke, Hyung-Jun Chang*, Arjen Roos, Samuel Forest</i></p>	<p>A Mesoscopic RVE for Parts Manufactured through Fused Deposition Modeling and Reinforced with Short Fibers</p> <p><i>Khadija Ouajani*, Nicholas Smith</i></p>
5th Floor Baltimore Ballroom B	Symposium 7	Dislocation, Twinning, Phase Transformation, Phonon, Diffusion, and Their Interactions in Materials Manufacturing, Processing, and Testing, Chair(s): Antoine Ruffini		
<p>Keynote presentation: Atomistic Mechanisms of Defects Diffusion and Atomic Transport in Concentrated Alloys</p> <p><i>Yuri Osetsky*, Yanwen Zhang</i></p>	<p>Cu Surface Diffusion Bias under Electric Field Gradient - Accelerated Molecular Dynamics, Finite Elements Method, and Density Functional Theory</p> <p><i>Jyri Kimari*, Ye Wang, Andreas Kyritsakis, Veronika Zadin, Flyura Djurabekova</i></p>	<p>Characterize the Stress Complexity Induced by a Slip-Interface Interaction and Its Role in the Subsequent Structure Changes through Adaptive Concurrent Atomistic-Continuum Simulations</p> <p><i>Liming Xiong*</i></p>	<p>On the interaction between gliding dislocations and a pore in a single crystal superalloy placed under HIP conditions</p> <p><i>Antoine Ruffini*, Yann Le Bouar, Alphonse Finel</i></p>	<p>The Role of Short-Range Order on Diffusion and Deformation Mechanisms in Multi-Principal Element Alloys</p> <p><i>Penghui Cao*</i></p>
5th Floor Maryland Ballroom E	Symposium 10	Interface-Driven Phenomena in Materials: Thermodynamics, Kinetics, and Chemistry, Chair(s): Fadi Abdeljawad		
<p>Keynote presentation: Trapping of Hydrogen at Grain Boundaries in Ferritic Steels – the Role of Grain Boundary Structure and Composition</p> <p><i>Alexander Hartmaier*, Abril Azócar Guzmán, Rebecca Janisch</i></p>	<p>Predicting Segregation Energy at Disordered Atomic Interfaces: Increasing Interfacial Stability</p> <p><i>Jacob Tavenner, Garritt Tucker*</i></p>	<p>Iron grain boundary wetting by low melting point liquid metals</p> <p><i>Thierry Auger*, Duane Johnson, LinLin Wang</i></p>	<p>A Stochastic Framework for Efficiently Evolving Grain Statistics</p> <p><i>Jaekwang Kim*, Nikhil Admal</i></p>	<p>Multi-Scale Simulation of Microstructure Evolutions Using Phase-Field Method and Molecular Dynamics Method with Machine Learning Interatomic Potential</p> <p><i>Kyoyu Kondo*, Akinori Yamanaka, Akimitsu Ishii, Akiyasu Yamamoto</i></p>
5th Floor Maryland Ballroom D	Symposium 12	Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem, Chair(s): Steve Fitzgerald		
<p>Keynote presentation: Ab Initio Modeling of Dislocation Plasticity in BCC Metals</p> <p><i>David Rodney*, Baptiste Bienvenu, Lucile Dezerald, Emmanuel Clouet, François Willaime</i></p>	<p>Interplay between Dislocations and Correlated Stress Environments in Random Alloys</p> <p><i>Ali Rida*, Enrique Martinez, David Rodney, Pierre-Antoine Geslin</i></p>	<p>Statistical Properties of Internal Stress Fields in Linear Elastic Solids</p> <p><i>Yejun Gu*, Zhi Li, Xialong Ma, Wenxin Zhou, Jaafar El-Awady, Huajian Gao</i></p>	<p>Analysis of different noise sources on dislocation mobility</p> <p><i>Hyunsoo Lee*, Giacomo Po, David Rodney, Pierre-Antoine Geslin, Enrique Martinez</i></p>	<p>Investigation of Mechanical Properties at Ultra Low Scale Using Finite Temperature Ab Initio Molecular Dynamics</p> <p><i>Laurent Pizzagalli*</i></p>

Tuesday Afternoon, October 4 / TECHNICAL PROGRAM

1:45 PM	2:15 PM	2:35 PM	2:55 PM	3:15 PM
5th Floor Fells Point Room				
Symposium 13				
Mechanics and Physics of Material Failure, Chair(s): Hojun Lim and Coleman Alleman				
<p>Keynote presentation: Multiscale Model for Two-Way Coupled Hydrogen Transport and Point-Line Defect Interaction Processes in Austenitic Stainless Steels</p> <p><i>Theodore Zirkle, Ting Zhu, David McDowell*</i></p>	<p>Investigating the microstructural origins of hydrogen effects on deformation and fracture</p> <p><i>Coleman Alleman*, Christopher San Marchi</i></p>	<p>Intergranular ductile failure of materials with plastically heterogeneous grains</p> <p><i>Edwin Chiu*, Ankit Srivastava</i></p>	<p>Crystal plasticity and micro-CT characterization of voids in plastic deformation of Al6061</p> <p><i>Hojun Lim*, Philip Noell, Raiyan Seede, John Emery, Kyle Johnson</i></p>	<p>Environmental Fracture of Alpha-brass in a Multi-scale QM/MM Approach</p> <p><i>Antoine Clement*, Thierry Auger</i></p>
5th Floor Pride of Baltimore Room				
Symposium 16				
Modeling and Experimental Measurements for Metal Additive Manufacturing, Chair(s): Lyle Levine				
<p>Keynote presentation: Microstructure prediction for Selective Laser Melting using cellular automata: sensitivity to process model data and solidification process uncertainty</p> <p><i>Matt Rolchigo*, John Coleman, Sam Reeve, Gerry Knapp, Jim Belak</i></p>	<p>Accelerating phase-field simulation of microstructure evolution in additive manufacturing using physics-embedded graph networks</p> <p><i>Zhengtao Gan*</i></p>	<p>Connecting additive manufacturing process-aware built microstructures to part scale properties using a micromechanical workflow</p> <p><i>Robert Carson*, Jim Belak, Matthew Rolchigo, Leonidas Zisis, Michael Sangid</i></p>	<p>Compositional and Microstructural Effects on the Solidification Mode of Laser Melted Single Tracks of 316L Stainless Steel</p> <p><i>Anna Rawlings*, Andrew Birnbaum, John Steuben, Athanasios Iliopoulos, John Michopoulos</i></p>	
6th Floor Kent Room				
Symposium 18				
Multiscale Materials Modeling Using Ab-Initio Accuracy Methods, Chair(s): Gabor Csanyi				
<p>Keynote presentation: Embedding Theories for Ab Initio Simulations on Hybrid Classical-Quantum Architectures</p> <p><i>Giulia Galli*</i></p>	<p>A Data Driven Approach to Improved Exchange-Correlation Functionals in DFT</p> <p><i>Bikash Kanungo, Vikram Gavini*</i></p>	<p>Stochastic algorithms for electrons structure calculations</p> <p><i>Taehee Ko*, Xiantao Li</i></p>	<p>SPARC: Real space Density Functional Theory for large length and time scales</p> <p><i>Phanish Suryanarayana*</i></p>	
5th Floor Federal Hill Room				
Symposium 21				
Multiscale Modeling of Glasses and Structurally Disordered Materials, Chair(s): Craig Maloney				
<p>Keynote presentation: Using Non-Linear Modes to Predict and Understand Plastic Flow in Disordered Solids</p> <p><i>David Richard*</i></p>	<p>Modeling the dynamics of machine-learned Softness in supercooled liquids</p> <p><i>Sean Ridout*, Andrea Liu</i></p>	<p>Stress-stress correlations in soft amorphous solids</p> <p><i>Vinutha H A*, Xiaoming Mao, Bulbul Chakraborty, Emanuela Del Gado</i></p>	<p>Manifold Learning to Map Amorphous Microstructural Features to Local Yield Stress</p> <p><i>Rahul Meena*, Thomas J. Hardin, Spencer Fajardo, Michael Chandross, Yannis Kevrekidis, Dimitris Giovanis, Michael Falk, Michael D. Shields</i></p>	<p>Mechanism of deformation in metallic glasses: Is the concept of defects useful?</p> <p><i>Charles Lieou*, Takeshi Egami</i></p>

Tuesday Evening, October 4 / TECHNICAL PROGRAM

4:00 PM	4:30 PM	4:50 PM	5:10 PM
5th Floor Guilford Room Keynote presentation: Rare Event Methods: Chemical Reactions in Enzymes. Multidimensional Coupling, Catalytic Mechanism <i>Steven D. Schwartz*</i>	Symposium 1 Driven Dynamics of Long-Time Bond-Breaking Events <i>Yongsheng Leng*, Yuan Xiang, Guanran Zhang</i>	Advances in Methods for Bridging Spatiotemporal Scales in Soft Matter, Polymer and Network Materials, Chair(s): Matej Praprotnik New Developments of Variationally Enhanced Sampling <i>Omar Valsson*</i>	Accelerating Molecular Simulations with Metadynamics to Predict Interactions between Perfluoroalkyl Molecules and Filter Materials <i>K. Michael Salerno*, James Johnson, Danielle Schlesinger, Nam Le, Jesse Ko, Zhiyong Xia</i>
5th Floor Maryland Ballroom F Keynote presentation: Breakaway Growth Modelling of Zirconium: Importance of <a> Loops Layers <i>Clément Sakaël, Christophe Domain*, Antoine Ambard, Christopher Race, Ludovic Thuinet, Alexandre Legris</i>	Symposium 2 Tackling diffusion properties in complex concentrated alloys machine learning based via kinetic Monte Carlo <i>Anus Manzoor*, Yongfeng Zhang</i>	Bridging Scales in the Microstructure Modeling of Nuclear Materials, Chair(s): Jaime Marian Mass transport computations in alloys through a law of total diffusion <i>Manuel Athènes*, Jérôme Creuze, Gilles Adjanor</i>	Surface and Size Effects on the behaviors of point defects in irradiated crystalline solids <i>Karim Ahmed*</i>
5th Floor Baltimore Ballroom A Keynote presentation: Bridging the Scales with Data-Oriented Constitutive Modeling <i>Alexander Hartmaier*, Ronak Shoghi</i>	Symposium 5 Data-driven surrogate modeling of physics-based creep mechanics <i>Andre Ruybalid*, Christopher Matthews, Laurent Capolungo, Aaron Tallman</i>	Data-Driven and Physics-Informed Multiscale Materials Modelling, Chair(s): Katrin Schulz Prediction of Stress Field in Fiber-Reinforced Composites Using 3-D U-Net Under Cyclic Loading Condition <i>Indrashish Saha*, Ashwini Gupta, Lori Graham-Brady</i>	Neural Network Models of Phase Field Simulations <i>Haiying Yang*, Michael Demkowicz</i>
5th Floor Homeland Room Keynote presentation: Dislocation Patterning During Plastic Deformation: 3D Movies from Dark Field X-Ray Microscopy <i>Henning Friis Poulsen*, Grethe Winther, Felix Frankus, Sina Borghi, Albert Zelenika, Can Yildirim</i>	Symposium 6 Energetic Closure for Continuum Dislocation Dynamics Based on Discrete Dislocation Data <i>Benedikt Weger*, Thomas Hochrainer</i>	Defects and Microstructure Complexity in Materials: Experiments and Multiscale Modeling, Chair(s): Thomas Hochrainer Dislocation microstructure evolution during cyclic deformation: A continuum dislocation dynamics study <i>Vignesh Vivekanandan*, Peng Lin, Gretha Winther, Anter El-Azab</i>	Finite-Strain Continuum Dislocation Dynamics and Dislocation Patterning in Deformed Crystals <i>Khaled Abdelaziz*, Kyle Starkey, Anter Elazab</i>

Tuesday Evening, October 4 / TECHNICAL PROGRAM

4:00 PM	4:30 PM	4:50 PM	5:10 PM
5th Floor Baltimore Ballroom B Keynote presentation: Plasticity and Plastic Strain-Induced Phase Transformations under High Pressure: Four-Scale Theory, Experiment, and Phenomena <i>Valery Levitas*</i>	Symposium 7 Dislocations in Molecular Crystals: the case of HMX and RDX <i>Catalin Picu, Zhaocheng Zhang*</i>	Dislocation, Twinning, Phase Transformation, Phonon, Diffusion, and Their Interactions in Materials Manufacturing, Processing, and Testing, Chair(s): Liming Xiong Solute-Strengthening in Alloys with Short-Range Order <i>Xin Liu*, William Curtin</i>	Phase-field modeling approach for martensite and bainite microstructure formation <i>Hesham Salama*, Dhanunjaya Kumar Nerella, Oleg Shchyglo, Ingo Steinbach</i>
6th Floor Kent Room Keynote presentation: Machine Learning-Enabled and Uncertainty Quantified Parametrically-Upscaled Constitutive Models for Multiscale Fatigue Modeling <i>Somnath Ghosh*</i>	Symposium 9 Multiscale Modeling of Creep and Transient Conditions in Steels: Effect of Microstructure and Chemistry <i>M. Arul Kumar*, A. . Ruybalid, R. . Lebensohn, L. Capolungo</i>	Integrated Multiscale/Multiphysics Modeling of Structural Materials, Chair(s): Mohammedreza Yaghoobi Leveraging deep learning models to expedite and expand the exploration of material structures for mechanical design <i>Andrew Lew*, Markus Buehler</i>	
5th Floor Maryland Ballroom E Keynote presentation: Nucleation of Grain Boundary Phases in Tungsten <i>Ian Winter, Tomas Ooppelstrup, Robert Rudd, Timofey Frolov*</i>	Symposium 10 How interfaces separate: Line tension models for decohesion at disordered interfaces <i>Antoine Sanner, Lars Pastewka*</i>	Interface-Driven Phenomena in Materials: Thermodynamics, Kinetics, and Chemistry, Chair(s): Saryu Fensin Diffusionless Congruent Grain Boundary Phase Transitions in Pure Copper <i>Tobias Brink*, Lena Frommeyer, Rodrigo Freitas, Timofey Frolov, Christian H. Liebscher, Gerhard Dehm</i>	Incompatibility Between Neighboring Grains Determines the Local Structure of Amorphous Grain Boundary Complexions <i>Pulkit Garg*, Timothy Rupert</i>
6th Floor Gibson Room Keynote presentation: Mechanisms of Charging and Degradation of Amorphous Oxide Films in Electronic Devices <i>Alexander Shluger*, Jack Strand</i>	Symposium 11 Corrosion in Encapsulated Cu-Al Wire-Bonding Interconnects in Microelectronics Packages <i>Kai-chieh Chiang*, Marisol Koslowski</i>	Materials for Microelectronics: Manufacturing Process, Implantation and Reliability, from Atomic Scale to Industrial Design, Chair(s): Markus Sudmanns A Multilevel Modeling Study of the Nickel Silicidation Process <i>César Jara*, Julien Lam, Antoine Jay, Anne Hémerlyck</i>	

Tuesday Evening, October 4 / TECHNICAL PROGRAM

4:00 PM	4:30 PM	4:50 PM	5:10 PM
5th Floor Maryland Ballroom D Keynote presentation: Anomalous Slip in Body-Centred Cubic Metals <i>Daniel Caillard, Baptiste Bienvenu, Emmanuel Clouet*</i>	Symposium 12 Discrete Dislocation Dynamics Simulations of <a>-type Prismatic Loops in Zirconium <i>Daniel Hortelano Roig*, Rakesh Kumar, Daniel Balint, Edmund Tarleton</i>	Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem, Chair(s): David Rodney Interaction of <a> Prismatic Screw Dislocations with alpha-beta Interfaces in alpha-beta Ti Alloys from Atomistic Simulations <i>Ali Rida*, Satish Rao, Jaafar El-Awady</i>	Multiscale study of Dislocation-Mediated Plasticity in HCP metals starting from First-Principles <i>Davide Fioravanti, Erik van der Giessen, Francesco Maresca*</i>
5th Floor Pride of Baltimore Room Keynote presentation: In-Situ Microstructural Characterization of Additively Manufactured Lattice Structures <i>Donald Brown*, Nathan Johnson, Maria Strantza, Jenny Wang, Ibo Matthews, Jun-Sang Park, Peter Kenesei</i>	Symposium 16 A Numerical Method for Simulation of Multicomponent Metal Additive Manufacturing <i>Zhongsheng Sang*, Arash Samaei, Gregory Wagner</i>	Modeling and Experimental Measurements for Metal Additive Manufacturing, Chair(s): Gregory Wagner Multiphysics Modeling for Prediction of Epitaxial Grain Growth in Multilayer/Multitrack Powder Bed Fusion Process of Ti-6Al-4V <i>Kang-Hyun Lee*, Min Gyu Chung, Yeon Su Lee, Gun Jin Yun</i>	Length scale effects of nanoindentation on additively manufactured stainless steel <i>Kunqing Ding*, Yin Zhang, Ting Zhu, David McDowell</i>
5th Floor Fells Point Room Keynote presentation: Machine Learning for Battery: From Materials Discovery to Deployment and Recycling <i>Chen Ling*</i>	Symposium 20 Simulation-based Optimization of the HOLE Design to Enable Fast Charging Capability in Energy-Dense Li-ion Batteries <i>Vishwas Goel*, Kuan-Hung Chen, Min Ji Namkoong, Chenglin Yang, Jyoti Mazumder, Jeff Sakamoto, Neil P. Dasgupta, Katsuyo Thornton</i>	Multiscale Modeling of Battery Materials, Chair(s): Yue Qi Exploration of novel Li-rich inverse-perovskite-type solid electrolytes for all-solid-state batteries by DFT and machine-learning approaches <i>Randy Jalem*, Yoshitaka Yoshitaka Tateyama, Kazunori Takada, Masanobu Nakayama</i>	Understanding interfacial chemo-mechanics of two-dimensional materials-based heterostructures for energy storage <i>Dibakar Datta*</i>

Wednesday Morning, October 5 / TECHNICAL PROGRAM
PLENARY LECTURE / 8:30 – 9:30 AM
Prof. James Sethian
“Advances in Advancing Interfaces: The Mathematics of Manufacturing of Industrial Foams, Fluidic Devices, and Automobile Painting”
Chair: Maria Emelianenko

10:00 AM	10:30 AM	10:50 AM	11:10AM	11:30 AM
5th Floor Maryland Ballroom F Keynote presentation: Modeling Fission Gas Release in 3D UO ₂ Polycrystals Using a Coupled Phase Field/Cluster Dynamics Model <i>Michael Tonks*, Sourav Chatterjee, Ali Muntaha, Sophie Blondel, Brian Wirth, David Bernholdt, David Andersson</i>	Symposium 2 Systematic continuum-scale simulations in tungsten to refine the temperature dependence of helium bubble bursting <i>Sophie Blondel*, Dwaipayan Dasgupta, Karl D. Hammond, Dimitrios Maroudas, Yogendra S. Panchal, Wahyu Setyawan, Brian D. Wirth</i>	Bridging Scales in the Microstructure Modeling of Nuclear Materials, Chair(s): Michael Cooper Multiscale Modeling for High-burnup Structure Formation in UO ₂ <i>Sudipta Biswas, Larry Aagesen*, Andrea Jokisaari, Wen Jiang, Sophie Blondel, Fande Kong</i>		
			Phase-Field Modeling of Fission Gas Behavior in Polycrystalline Uranium Oxides with Complex Microstructures <i>Luca Messina*, Marc Josien, Larry K Aagesen</i>	Multi-scale simulation of high burnup UO ₂ nuclear fuel during loss-of-coolant accident conditions <i>Larry Aagesen*, Sudipta Biswas, Wen Jiang, Michael Cooper, David Andersson, Kyle Gamble</i>
6th Floor Gibson Room Keynote presentation: Laser Interactions with Silica Glasses <i>Anne Tanguy*, Nikita Shcheblanov, Razvan Stoian</i>	Symposium 3 Selective Phonon Stimulation via Infrared Radiation to Tune Thermal Transport <i>Gaurav Kumar, Peter Chung*</i>	Computer Modeling of Laser and Ion Beam Interactions with Materials, Chair(s): Alfredo A. Correa Multiscale Computational Study of Surface Modification by Nonlinear Laser-Induced Surface Acoustic Waves <i>Yuan Xu*, Maxim Shugaev, Leonid Zhigilei</i>		
			Towards Description of Mechanical Damage of Thin Molybdenum Film upon Pulsed Laser Irradiation <i>Kryštof Hlinomaz*, Alexander S. Fedotov, Igor Timoshchenko, Alexander Kozlovski, Yoann Levy, Thibault J.-Y. Derrien, Vladimir P. Zhukov, Oleg G. Romanov, Nadezhda M. Bulgakova</i>	Kinetics of laser-induced melting of thin gold film: How slow can it get? <i>Mikhail Arefev*, Maxim Shugaev, Leonid Zhigilei</i>
5th Floor Baltimore Ballroom A Keynote presentation: Quantity or Quality? Capitalizing on Small but Rich Materials Data Sets <i>Elizabeth Holm*</i>	Symposium 5 Machine Learning-based Constitutive Laws for Multi-Scale Materials Modeling <i>Ning Li*, Huck Beng Chew</i>	Data-Driven and Physics-Informed Multiscale Materials Modelling, Chair(s): Katrin Schulz Integrating Data-Driven Techniques with 3D Constitutive Modeling to Design Textures with Nearly Isotropic Elastic and Plastic Properties in Titanium-Based Materials <i>Behnam Ahmadikia*, Orestis Paraskevas, William Van Hynning, Jonathan Hestroffer, Irene Beyerlein, Christos Thrampoulidis</i>		
			Data-oriented Description of Texture-dependent Anisotropic Material Behavior <i>Jan Schmidt*, Alexander Hartmaier, Abhishek Biswas, Napat Vajragupta</i>	Rapid Mechanical Property Prediction and de Novo Design of Three-Dimensional Spider Webs Through Graph and GraphPerceiver Neural Networks <i>Wei Lu*, Zhenze Yang, Markus Buehler</i>

Wednesday Morning, October 5 / TECHNICAL PROGRAM

10:00 AM	10:30 AM	10:50 AM	11:10AM	11:30 AM
5th Floor Homeland Room	Symposium 6	Defects and Microstructure Complexity in Materials: Experiments and Multiscale Modeling, Chair(s): Alejandro Strachan		
Keynote presentation: Localized Interactions Among Large Populations of Voids in Ductile Metals <i>Richard Becker*</i>	Discrete and Continuum Dislocation Modeling of Micromechanical Experiments Based on Acoustic Emission and High Resolution EBSD Measurements <i>Péter Dusán Ispánovity*, Dávid Ugi, Gábor Péterffy, István Groma, Kristián Máthi, Szilvia Kalácska, Kolja Zoller, Katrin Schulz</i>	Atomistic coupling of electric fields and dislocation-driven material behavior at the extremes <i>Soumendu Bagchi*, Danny Perez</i>	Finite element Level-Set methods to study dynamic recrystallization <i>Daniel Pino Muñoz*, Marc Bernacki, Nathalie Bozzolo</i>	Deformation and failure behavior of thick aluminum plates <i>Jeffrey Lloyd*, Philip McKee, Daniel Casem, Christopher Meredith, Daniel Magagnosc</i>
5th Floor Baltimore Ballroom B	Symposium 7	Dislocation, Twinning, Phase Transformation, Phonon, Diffusion, and Their Interactions in Materials Manufacturing, Processing, and Testing, Chair(s): Avinash Dongare		
Keynote presentation: Models for Extended Continua Based on the Statistical Mechanics of Particles with Structure <i>Bob Svendsen*</i>	On the physical foundation and consistent formulation of transport fluxes in inhomogeneous systems <i>Youping Chen*, Adrian Diaz</i>	Atomistic Modeling of Short-Ranged Order in Disordered Spinel and the Impact on Mass Transport <i>Peter Hatton*, Blas Uberuaga</i>	Modeling Plasticity Contributions from Dislocation Slip, Twinning, and Phase Transformation Behavior in metals at the Mesoscales <i>Avinash Dongare*, Avinash Mishra, Marco Echeverria, Ke Ma</i>	
5th Floor Maryland Ballroom E	Symposium 10	Interface-Driven Phenomena in Materials: Thermodynamics, Kinetics, and Chemistry, Chair(s): Damien Tournet		
Keynote presentation: Defect Phase Diagrams: Concepts, Computational Approaches and Materials Design Strategies <i>Liam Huber, David Holec, Dominik Gehringer, Tilmann Hickel, Joerg Neugebauer*</i>	Modeling and simulation of solute drag by moving grain boundaries <i>Yuri Mishin*</i>	Atomistic Simulation Study of Grain-boundary Solute Clustering and Associated Strain Localization Mechanisms in Polycrystals <i>Frederic Sansoz*, Tara Nenninger, Eve-Audrey Picard</i>	Learning Grain Boundary Solute Segregation in Polycrystals from First Principles <i>Malik Wagih*, Christopher Schuh</i>	Hydrogen sorption and water dissociative adsorption properties in CrMnFeCoNi alloy from density functional theory calculations <i>Yichen Qian*, ShinYoung kang, Artur Tamm, David Cereceda</i>
5th Floor Maryland Ballroom D	Symposium 12	Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem, Chair(s): Karsten Albe		
Keynote presentation: Natural Fluctuations in Slip-Dominated Mechanics: Stochastic Crystal Plasticity Simulations <i>Jaime Marian*, Qianran Yu, Javier Segurado, Enrique Martinez</i>	Shear-coupled Grain Boundary Migration and Sliding in Alloy Systems <i>Spencer Thomas*, Jason Trelewicz</i>	Modeling grain boundary mediated plasticity with massively parallel atomistic simulations <i>Timofey Frolov, Tomas Oppelstrup*, Nicolas Bertin, Alexander Chernov</i>	Analytical Homogenization Model for the Overall Response of Porous Polycrystals: Effects of Crystallographic Texture and Pores <i>Shuvrangs Das*, Pedro Ponte Castañeda</i>	Mesoscale theory and numerical simulations of microstructure evolution and mechanical response in the presence of defects <i>Maria Emelianenko*</i>

Wednesday Morning, October 5 / TECHNICAL PROGRAM

10:00 AM	10:30 AM	10:50 AM	11:10AM	11:30 AM
5th Floor Pride of Baltimore Room Keynote presentation: Thermal Modeling of Laser Powder Bed Fusion Additive Manufacturing of Refractory Materials <i>Li Ma*, Gianna Valentino, Morgana Trexler, Mitra Taheri</i>	Symposium 16 Enriched Analytical Solutions for Thermoelasticity Applied to Single Track Laser Powder Bed Fusion <i>Nicole Apetre*, John Michopoulos, John Steuben, Athanasios Iliopoulos, Andrew Birnbaum</i>	Modeling and Experimental Measurements for Metal Additive Manufacturing, Chair(s): John Michopoulos Unifying discrete and continuum approaches for multiscale modeling of sintering processes <i>John Steuben*, John Michopoulos, Athanasios Iliopoulos, Andrew Birnbaum, Steven Rodriguez, Benjamin Graber</i>		
			Metal Powder Additive Manufacturing Process to Performance Linkages via Multiscale Multiphysics Integrated Computational Material Engineering <i>John Michopoulos*, Athanasios Iliopoulos, John Steuben, Andrew Birnbaum, Anna Rawlings, Nicole Apetre, Benjamin Graber, Steven Rodriguez, Robert Saunders, Jeong Hoon Song, Yao Fu, Ajit Achuthan</i>	
6th Floor Kent Room Keynote presentation: DFT-Based Study of the Mobility of Carbon-Decorated Screw Dislocations in BCC Iron <i>Lisa Ventelon, Emmanuel Clouet, David Rodney, Daniel Caillard, Francois Willaime*</i>	Symposium 18 First-principles pyramidal dislocation and dislocation-solute energetics for ductility prediction in magnesium using DFT-FE --- a massively parallel real-space density functional theory code using adaptive finite-element discretization <i>Sambit Das*, Vikram Gavini</i>	Multiscale Materials Modeling Using Ab-Initio Accuracy Methods, Chair(s): Krishna Garikipati Isolated Dislocation Core Energy from First Principles Energy Density Method <i>Dallas Trinkle*, Yang Dan</i>		
			Predicting Crack Tip Mechanism of Iron via Quantum-accurate GAP <i>Lei Zhang, Gábor Csányi, Erik van der Giessen, Francesco Maresca*</i>	
5th Floor Fells Point Room Understanding Mechanical Deformation of Li-Ion Battery Electrodes; Insights from Multiscale Modelling and Experiment <i>Elham Sahraei* Huzefa Saifee, Youngwon Hahn, Victor Oancea, Jamie Foster</i>	Symposium 20 Accelerate Cell-Level Battery Simulations with Analytical Models <i>Ming Tang*</i>	Multiscale Modeling of Battery Materials, Chair(s): Victor OANCEA Modeling the anisotropic behavior and aging of highly orthotropic polymer separators in lithium-ion batteries <i>Georges Ayoub*, Mustapha Makki, Cheol Lee</i>		
			Designing Temperature Dependent Free Energy Functionals for Multi-Scale Modelling of Cathode Materials <i>Souzan Hammadi*, Jolla Kullgren, Daniel Brandell, Peter Broqvist</i>	

Wednesday Morning, October 5 / TECHNICAL PROGRAM

10:00 AM	10:30 AM	10:50 AM	11:10AM	11:30 AM
5th Floor Federal Hill Room	Symposium 21	Multiscale Modeling of Glasses and Structurally Disordered Materials, Chair(s): Yue Fan		
<p>Keynote presentation: Sound Attenuation in Low Temperature Amorphous Solids is Primarily Determined by Non-Affine Displacements</p> <p><i>Grzegorz Szamel*, Elijah Flenner</i></p>	<p>Thermal Management at the Nanoscale with Amorphous Materials</p> <p><i>Anne Tanguy*</i></p>	<p>Low frequency vibrational modes of realistic model of glasses</p> <p><i>Silvia Bonfanti*, Rene Alvarez-Donado, Roberto Guerra, Stefano Zapperi, Pawel Sobkowicz, Mikko Alava</i></p>	<p>Structure-Properties Relations and Scaling Laws for the Energy Absorption of Glassy Polymer Films Under Nanoballistic Impact</p> <p><i>Andrea Giuntoli*, Yuwen Zhu, Nitin Hansoge, Zhongqin Lin, Sinan Keten</i></p>	<p>Nonaffine Elastic Signatures of the Polyamorphic Transition in Amorphous Silicon</p> <p><i>Jan Griebner*, Lars Pastewka</i></p>
5th Floor Guilford Room	Symposium 23	Scale Bridging in Materials Science, Chair(s): Ryan Sills		
<p>Keynote presentation: Cross-scale matching: Dislocation Dynamics vs Molecular Dynamics</p> <p><i>Vasily Bulatov*</i></p>	<p>A Multi-scale Approach to the Development of Microstructure-aware Constitutive Models for Magnesium Alloys</p> <p><i>David Wason*, Dan Eakins, Simone Falco, Nik Petrinic</i></p>	<p>Incorporating Uncertainty Through Neural Network Ensembles to Predict Mechanical Deformation of Solids Using a Coupled Finite Element – Neural Network Approach</p> <p><i>Guy Bergel, Hojun Lim, David Montes de Oca Zapain*</i></p>	<p>Defect dynamics element models for defect-controlled plasticity in nanostructures</p> <p><i>ILL RYU*</i></p>	

Wednesday Afternoon, October 5 / TECHNICAL PROGRAM
SEMI-PLENARY LECTURES / 1:00 – 1:45 PM

Prof. Bruce E. Engelman

“Physics- and AI-based ICME methodologies relying on multi-scale digital twin of heterogeneous materials”

Chair: Somnath Ghosh

Maryland Ballroom AB&C

Prof. Markus J. Buehler

“Multiscale Mechanics of Bioinspired Material Intelligence”

Chair: Vicky Nguyen

Maryland Ballroom D

1:45 PM	2:15 PM	2:35 PM	2:55 PM	3:15 PM
5th Floor Maryland Ballroom F Keynote presentation: A Phase-Field Model for Dislocation Climb Under Irradiation: Formalism and Applications to Radiation Induced Segregation in Fe-Cr Alloys <i>Ludovic Thuinet*, Gabriel Bouobda Moladje, Charlotte Becquart, Alexandre Legris</i>	Symposium 2 Dislocation Loop Bias in BCC Iron <i>Ziang Yu*, Haixuan Xu</i>	Bridging Scales in the Microstructure Modeling of Nuclear Materials, Chair(s): Pascal Bellon		
		The volume of dislocation networks created by irradiation <i>Max Boleininger*, Sergei Dudarev, Daniel Mason, Enrique Martinez</i>	Multi-scale modeling of irradiation-induced strengthening in UO2 <i>Marion Borde*, Adrien Pivano, Bruno Michel, Laurent Dupuy, David Rodney, Jonathan Amodeo</i>	An Eigenstrain-body force Multi-scale Model for Stress, Strain and Swelling of Nuclear Reactor Components Under Irradiation <i>Luca Reali*, Max Boleininger, Mark Gilbert, Sergei Dudarev</i>
6th Floor Gibson Room Keynote presentation: A Kinetic Model for Simulations of Laser-Induced Plasma Plume Expansion Induced by Irradiation of Metal Targets with Bursts of Short and Ultrashort Laser Pulses <i>Alexey Volkov*, Michael Stokes, Nathan Humphey, Omid Ranjbar, Zhibin Lin</i>	Symposium 3 Computational Modeling of Laser Ablation of Aluminum with Plume Shielding Effect <i>Max Hanich, Alex Povitsky*</i>	Computer Modeling of Laser and Ion Beam Interactions with Materials, Chair(s): Miao He		
		Combining Electromagnetic Wave Calculations and Atomistic Simulations of Laser-Material Interaction <i>Chaobo Chen*, Leonid Zhigilei</i>	The importance of laser-generated bubble expansion, plasma and cavitation erosion mechanisms for pulsed laser interactions and nanoparticle formation in liquid <i>Svetlana Selezneva*, Tatiana Itina</i>	Effect of Material Properties on Surface Morphology Generation in Short Pulse Laser Processing of Mo Targets <i>Antonios Stylianos Valavanis, Leonid Zhigilei</i>

Wednesday Afternoon, October 5 / TECHNICAL PROGRAM

1:45 PM	2:15 PM	2:35 PM	2:55 PM	3:15 PM
5th Floor Baltimore Ballroom A Keynote presentation: An automated framework for structure determination of nanoscale materials using experimental data and theory <i>Venkata Surya Chaitanya Kolluru*, Davis Unruh, Eric Schwenker, Maria Chan</i>	Symposium 5 Automated Classification of Big X-ray Diffraction Data Using Deep Learning <i>Jerardo Salgado*, Zhaotong Du, Ali Shargh, Samuel Lerman, Chenliang Xu, Niaz Abdolrahim</i>	Data-Driven and Physics-Informed Multiscale Materials Modelling, Chair(s): Elizabeth Holm Deep-Dream Generation of Material Defect Micro-Structures from X-ray Diffraction Characterization <i>Dylan Madisetti*, Jaafar El-AAwady, Christopher Stiles</i>	AutoML-accelerated EELS as an advanced structure characterization tool <i>Haili Jia*, Yiming Chen, Maria Chan</i>	
5th Floor Homeland Room Keynote presentation: Uncovering the Role of Nanoscale Precipitates on Martensitic Transformation and Superelasticity <i>Alejandro Strachan*</i>	Symposium 6 Origin of variable propensity for anomalous slip in body-centered cubic metals <i>Roman Gröger*, Vaclav Vitek</i>	Defects and Microstructure Complexity in Materials: Experiments and Multiscale Modeling, Chair(s): Richard Becker Quantifying Phase Transformations in AM Ti-6Al-4V using Phase Field Modeling and High-Energy X-ray Diffraction Measurements <i>Bonnie Whitney*, Anthony Spangenberg, Donald Brown, Travis Carver, Dan Savage, Diana Lados</i>	The Effect of Crystal Orientation on Electromigration in Cu-Sn Solders <i>Andrew Pham*, Marisol Koslowski</i>	
5th Floor Baltimore Ballroom B Keynote presentation: Modeling Local Stress Tensors and Multiscale Stress-Strain Curves up to Failure Using IFF-R <i>Hendrik Heinz*</i>	Symposium 7 Dislocation Pile-ups and Grain Boundary Interactions Studied using In situ Cross-Correlation EBSD in High Purity Nickel <i>Yang Su*, Josh Kacher</i>	Dislocation, Twinning, Phase Transformation, Phonon, Diffusion, and Their Interactions in Materials Manufacturing, Processing, and Testing, Chair(s): Xiaowang Zhou An Adaptive Concurrent Atomistic Continuum Approach for Predicting How Plasticity Flows in Heterogeneous Materials from Nanometer to Micrometer Level <i>Thanh Phan*, Liming Xiong, Yipeng Peng</i>	Phase Field Dislocation Dynamics Modeling of Dislocation-Interface Interactions <i>Xiaoyao Peng*, Avani Mishra, Nithin Mathew, Edward Kober, Darby Jon Luscher, Irene Beyerlein, Abigail Hunter</i>	
5th Floor Maryland Ballroom E Keynote presentation: Topology-Generating Interfacial Pattern Formation During Dealloying <i>Mingwang Zhong, Longhai Lai, Alain Karma*</i>	Symposium 10 A phase-field model for pressure and density variation: consequences for interfaces <i>Nana Ofori-Opoku*, Michael Welland</i>	Interface-Driven Phenomena in Materials: Thermodynamics, Kinetics, and Chemistry, Chair(s): Yasushi Shibuta The role of grain boundaries in the morphological instabilities of polycrystalline nanorods <i>Omar Hussein*, Keith Coffman, Khalid Hattar, Eric Lang, Shen Dillon, Fadi Abdeljawad</i>	Grain boundary dynamics revealed by markov state models trained by graph dynamical networks <i>Siavash Soltani, Joerg Rottler, Chad Sinclair*</i>	A Machine Learning Investigation of Growth Advantages in Microstructural Evolution for Abnormal Grain Growth <i>Meizhong Lyu*, Elizabeth Holm, Ryan Cohn</i>

Wednesday Afternoon, October 5 / TECHNICAL PROGRAM

1:45 PM	2:15 PM	2:35 PM	2:55 PM	3:15 PM
5th Floor Maryland Ballroom D Keynote presentation: Repulsion Leads to Coupled Dislocation Motion in Tungsten and Other BCC Metals <i>Peter Gumbsch, Klushuk Srivastava, Daniel Caillard, Daniel Weygand*</i>	Symposium 12 Cross-scale matching of crystal plasticity: from large-scale MD simulations to discrete dislocation dynamics <i>Nicolas Bertin*, Wei Cai, Sylvie Aubry, Vasily Bulatov</i>	Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem, Chair(s): Jaime Marian A phase field crystal theory of the kinematics of dislocation lines <i>Vidar Skogvoll*, Marco Salvalaglio, Luiza Angheluta, Jorge Viñals</i>		
		Representative volume effects on the predicted dislocation microstructure evolution under high thermal and mechanical loading conditions <i>Markus Sudmanns*, Athanasios Iliopoulos, Andrew Birnbaum, John Micholoulos, Jaafar El-Awady</i>		On Dislocation Cross-Slip Modeling in FCC Metals by Means of Evolving Curves <i>Miroslav Kolar*, Petr Paus, Michal Benes</i>
5th Floor Pride of Baltimore Room Keynote presentation: A framework for computational materials design for metal additive manufacturing <i>Evgeniya Kabliman*, Sebastian Tonatiuh Carrion Ständer</i>	Symposium 16 Role of Micro Residual Stress on the Deformation of Additively Manufactured Steel <i>Abdullah Al Mamun*</i>	Modeling and Experimental Measurements for Metal Additive Manufacturing, Chair(s): Donald Brown Computational Homogenization of Thermoelectric Properties of Powders for the Multi-scale Modeling and Simulation of Additive Manufacturing Processes <i>Athanasios Iliopoulos*, John Steuben, John Michopoulos, Benjamin Graber, Andrew Birnbaum</i>		
6th Floor Kent Room Keynote presentation: Guided Design of Alloys <i>Nikolai Zarkevich*, Timothy Smith, John Lawson</i>	Symposium 18 Screening High Entropy Alloys for Catalysis Applications using Alchemical Perturbation Density Functional Theory <i>Mohamed Hendy*, Okan Orhan, Homin Shin, Ali Malek, Mauricio Ponga</i>	Multiscale Materials Modeling Using Ab-Initio Accuracy Methods, Chair(s): Francois Williams A Predictive Atomistic Model for Hydrogen Adsorption on Metal Surfaces <i>Yves Ferro*, Robert Kolasinski, Etienne Hodille, Zachary Piazza, Ajmalghan Muthali</i>		
5th Floor Fells Point Room Keynote presentation: Understanding Formation, Morphology and Function of the Solid Electrolyte Interphase (SEI) <i>Arnulf Latz*, Lars von Kolzenberg, Lukas Köbbing, Birger Horstmann</i>	Symposium 20 Unlocking multiphysics design guidelines on Si/C composite nanostructures for high-energy-density and robust lithium-ion batteries <i>Jun Xu*, Xiang Gao</i>	Multiscale Modeling of Battery Materials, Chair(s): Chen Ling Ab-Initio Based Thermodynamic Models of the Li-Si System <i>Charbel Jose El Khoury*, Maylise Nastar, Fabien Bruneval</i>		
		Microstructure-level simulation of electrochemical dynamics in hybrid electrodes <i>Affan Malik, Danqi Qu, Hui-Chia Yu*</i>		Atomically-Informed Phase-Field Model of Concurrent Solid Electrolyte Interphase Formation and Li-Metal Deposition or Stripping <i>Yanzhou Ji, Qisheng Wu, Seyed Amin Nabavizadeh, Yue Qi, Long-Qing Chen*</i>

Wednesday Afternoon, October 5 / TECHNICAL PROGRAM

1:45 PM	2:15 PM	2:35 PM	2:55 PM	3:15 PM
5th Floor Federal Hill Room	Symposium 21	Multiscale Modeling of Glasses and Structurally Disordered Materials, Chair(s): Anne Tanguy		
Keynote presentation: Emerging Fractal Potential Energy Landscape as the Origin of Activation Volume in Metallic Glasses <i>Yue Fan*</i>	Effect of the Microstructure on the Dynamical Relaxations in Glasses and Glass Composites Investigated by Atomistic Simulations <i>Claudio Fusco*, Guojian Lyu, Jichao Qiao, Yao Yao, Yun-Jiang Wang, Julien Morthomas, David Rodney</i>	Low-energy excitations in metallic glass models <i>Felix-Cosmin Mocanu, Ludovic Berthier, Simone Ciarella, Dmytro Khomenko, David Reichman, Camille Scalliet, Francesco Zamponi*</i>	Exploring glassy dynamics with Markov state models from graph dynamical neural networks <i>Siavash Soltani, Chad Sinclair, Joerg Rottler*</i>	Lattice instabilities and amorphous shear band formation in intermetallic alloys <i>Prakarsh Pandey*, Shiva Rudraraju</i>
5th Floor Guilford Room	Symposium 23	Scale Bridging in Materials Science, Chair(s): Thomas Hochrainer		
Efficient FFT-based mechanical solvers for abrupt interfaces <i>Alphonse Finef*</i>	Dynamic Length Scale and Weakest Link Behavior in Crystal Plasticity <i>Dénes Berta*, Gábor Péterffy, Péter Dusán Ispánovity</i>	Coarse-graining and scale-bridging stochastic phenomena with Gaussian process regression <i>Yating Fang, Ahmed Aziz Ezzat, Ryan Sills*</i>	Scale Separation or Lack Thereof in 3D Woven Composite Structures <i>Nicolas Feld*</i>	

Wednesday Evening, October 5 / TECHNICAL PROGRAM

4:00 PM	4:30 PM	4:50 PM	5:10 PM
5th Floor Maryland Ballroom F Keynote presentation: On the Onset of 'Fuzz' Formation in Plasma-Facing Materials: A Hierarchical Multiscale Modeling Approach <i>Dwaipayan Dasgupta*, Sophie Blondel, Asanka Weerasinghe, Chao-Shou Chen, Dimitrios Maroudas, Brian Wirth</i>	Symposium 2 Physics-based model of irradiation creep for ferritic materials under DEMO first-wall operation conditions <i>Qianran Yu*, Sabyasachi Chatterjee, Giacomo Po, Jaime Marian</i>	Bridging Scales in the Microstructure Modeling of Nuclear Materials, Chair(s): Larry Aagesen Dislocation Processes in Uranium Dioxide Single Crystal: on the Role of Composite Slip <i>Ronan Madec*, Luc Portelette, Jonathan Amodeo, Bruno Michel</i>	Analytical Prediction of the Mechanical Behavior of Cast Duplex Stainless Steels Using the Kocks-Mecking Framework and the Taylor Homogenization Rule <i>Ghiath Monnet*</i>
6th Floor Gibson Room Keynote presentation: Semi-classical Modeling of Hot Electron Spatio-Temporal Dynamics in Ultrashort Laser-Excited Plasmonic Nanostructures <i>Anton Rudenko*, Jerome Moloney</i>	Symposium 3 Ultrafast excitation of electrons in crystals: insights from non-equilibrium band structure calculations <i>Thibault Derrien*</i>	Computer Modeling of Laser and Ion Beam Interactions with Materials, Chair(s): Herbert Urbassek First Principles Modelling of the electronic energy loss and excitation in ion-matter and laser-matter interactions. <i>Alfredo A. Correa*, Artur Tamm</i>	Pure spin photocurrent in non-centrosymmetric crystals: bulk spin photovoltaic effect <i>Haowei Xu*</i>
5th Floor Baltimore Ballroom A Keynote presentation: Development of the System for Evaluation of Dislocation Behavior During Deformation of Metals Using Machine Learning <i>Mayu Muramatsu*, Kai Sasaki, Kenta Hirayama, Katsuhiko Endo, Mitsuhiro Murayama</i>	Symposium 5 Data-Driven Thermal Transfer Modeling for Enabling Advanced Experiments <i>Guanglong Huang*, Daniel O'Nolan, Jonathan Denney, Yusu Wang, Mojue Zhang, David Montiel, Praveen Soundararajan, Gabrielle Kamm, Antonin Grenier, Chia-Hao Liu, Paul Todd, Allison Wustrow, Gia Tran, James Neilson, Simon Billinge, Adam Corrao, Peter Chupas, Peter Khalifah, Karena Chapman, Katsuyo Thornton</i>	Data-Driven and Physics-Informed Multiscale Materials Modelling, Chair(s): Alexander Hartmaier Genetic programming for interpretable, data-driven continuum damage models <i>Michael Buche*, Anthony M. Su, John Emery, Jacob Hochhalter, Geoffrey Bomarito, Coleman Alleman</i>	Application of Machine Learning to Predict Shock Compression Response in Notional Unreacted Solids <i>Sangeeth Balakrishnan*, Francis G. VanGessel, Brian C. Barnes, Zois Boukouvalas, Mark D. Fuge, William Wilson, Ruth Doherty, Peter W. Chung</i>
5th Floor Homeland Room Keynote presentation: The Next Decade of the MGI <i>James Warren*</i>	Symposium 6 In-depth high entropy alloys defect characterization in transmission electron micrographs with deep learning approach <i>Thomas Bilyk*, Estelle Meslin, Mihai-Cosmin Marinica, Alexandra Gorayaeva</i>	Defects and Microstructure Complexity in Materials: Experiments and Multiscale Modeling, Chair(s): James Warren Predicting dislocation kink energies and ductile-brittle transition in body-centred cubic metals and high-entropy alloys <i>Christian Brandl*, Korbinian Deck</i>	

Wednesday Evening, October 5 / TECHNICAL PROGRAM

4:00 PM	4:30 PM	4:50 PM	5:10 PM
5th Floor Baltimore Ballroom B	Symposium 7	Dislocation, Twinning, Phase Transformation, Phonon, Diffusion, and Their Interactions in Materials Manufacturing, Processing, and Testing, Chair(s): Rasool Ahmad	
Keynote presentation: Interfacial Transitions and Phonon Interactions <i>Jeffrey Rickman*</i>	Selective phonon stimulation in molecular crystals <i>Zhiyu Liu*, Gaurav Kumar, Peter Chung</i>	Heat Diffusivity Studies in Pure Metals with Molecular Dynamics Combined with an Electron-Phonon Coupling for Irradiated Metals <i>Maxime Malingre*, Laurent Proville</i>	Free energy computation of crystalline defects using normalizing flow <i>Rasool Ahmad*, Wei Cai</i>
5th Floor Maryland Ballroom E	Symposium 10	Interface-Driven Phenomena in Materials: Thermodynamics, Kinetics, and Chemistry, Chair(s): Mitra Taheri	
Disconnection modes and coupling factors of asymmetric tilt grain boundaries using Smith normal bicrystallography <i>Himanshu Joshi*, Nikhil Chandra Admal, Brandon Runnels, Ian Chesser</i>	Stable Grain Boundary Complexions in Forsterite : Properties and Implications <i>Jean Furstoss*, Pierre Hirel, Philippe Carrez, Patrick Cordier</i>	Crack-Tip Grain Boundary Complexion Transition Drives Fracture in Aluminum <i>David Gordon*, Keith Horne, Ryan Sills</i>	
5th Floor Maryland Ballroom D	Symposium 12	Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem, Chair(s): Daniel Weygand	
Keynote presentation: Jerky Dislocation Motion in Multi-Principle Element Alloys: From Atomic Peierls Stress to Dislocation Mobility <i>Daniel Utt, Subin Lee, Yaolong Xing, Hyejin Jeong, Alexander Stukowski, Sang Ho Oh, Gerhard Dehm, Karsten Albe*</i>	The Hierarchical Energy Landscape of Dislocation Motion in Refractory High-Entropy Alloys <i>Penghui Cao, Xinyi Wang*</i>	Quantifying the Effect of Hydrogen on Additively Manufactured Multi-Principal Element Alloys Through Discrete Dislocation Dynamics Simulations <i>Jing Luo*, Jaafar El-Awady, Yejun Gu</i>	Atomistic Simulations of Dislocation Glide and Pinning in Fe-C Steels <i>Arnaud Allera*, Fabienne Ribeiro, Michel Perez, Alexandra Goryaeva, Mihai-Cosmin Marinica, Baptiste Bienvenu, Emmanuel Clouet, Lisa Ventelon, David Rodney</i>
6th Floor Kent Room	Symposium 18	Multiscale Materials Modeling Using Ab-Initio Accuracy Methods, Chair(s): Daniel Massatt	
Keynote presentation: A Free Energy-Based Framework for Scale Bridging in Crystalline Solids Using Machine Learning <i>Krishna Garikipati*, Gregory Teichert, Sambit Das, Mostafa Faghghi Shojaei, Jamie Holber, Vikram Gavini</i>	Kinetic Monte Carlo Simulations of Solute Clustering in Multicomponent Al Alloys <i>Zhucong Xi*, Louis Hector, Amit Misra, Liang Qi</i>	First-Principles Calculations and Correlation Analysis of Dilute Ni-based Alloy Ideal Shear Strength <i>John D. Shimanek*, Shun-Li Shang, Allison M. Beese, Zi-Kui Liu</i>	

Wednesday Evening, October 5 / TECHNICAL PROGRAM

4:00 PM	4:30 PM	4:50 PM	5:10 PM
5th Floor Fells Point Room Keynote presentation: Atomically-Informed Phase-Field Model of Concurrent Solid Electrolyte Interphase Formation and Li-Metal Deposition or Stripping <i>Yanzhou Ji, Qisheng Wu, Seyed Amin Nabavizadeh, Yue Qi, Long-Qing Chen*</i>	Symposium 20 Mechanistic Insights into Phase Transformation of Iron Oxyfluoride (FeOF) Cathode During Litation <i>Qisheng Wu*, Yue Qi</i>	Multiscale Modeling of Battery Materials, Chair(s): Yifei Mo Multiscale Lithium Nucleation and Growth Characterization (Invited) <i>Gorakh Pawar*, Boryann Liaw</i>	
			Interfacial Atomistic Mechanisms of Lithium Metal Stripping and Plating in Solid-State Batteries <i>Menghao Yang, Yifei Mo*</i>
5th Floor Guilford Room Keynote presentation: Plasticity Without Phenomenology: A First Step <i>Sabyasachi Chatterjee, Giacomo Po, Xiaohan Zhang, Amit Acharya*, Nasr Ghoniem</i>	Symposium 23 Investigating the behavior of BCC tantalum single crystals during Taylor impact testing using a coupled dislocation dynamics and finite element model <i>Nicole Aragon*, Hojun Lim, Ill Ryu</i>	Scale Bridging in Materials Science, Chair(s): Payam Poorsolhjouy Parametric Study of Dislocations in High Entropy Alloys via a Peierls-Nabarro/Phase-Field Model <i>Terrence Moran*, William Curtin</i>	
5th Floor Federal Hill Room Keynote presentation: Active Learning of SNAP Potentials using Bayesian Uncertainty Estimation <i>Logan Williams*, Khachik Sargsyan, Katherine Johnston, Habib N. Najm</i>	Symposium 25 Uncertainty Quantification for Model Uncertainties in MD Simulations and MD-Informed Multiscale Predictions <i>Hao Zhang*, Johann Guilleminot</i>	Uncertainty Quantification, Sensitivity Analysis, and Machine Learning in Materials Modeling, Chair(s): Lori Graham-Brady Uncertainty Quantification in Atomistic Simulations using Interatomic Potentials <i>Iain Best*, James Kermode</i>	
			A micro-macro Markov chain Monte Carlo method for molecular dynamics and proteomics <i>Hannes Vandecasteele*, Giovanni Samaey</i>
5th Floor Pride of Baltimore Room Keynote presentation: Directly coupling point defect transport and dislocation dynamics models to simulate recovery <i>Aaron Kohnert*, Laurent Capolungo</i>	Symposium 27 The interpretation of Discrete Dislocation Dynamics simulation data: Verification and Validation with application to size/scale and free surfaces <i>Tariq Khraishi*, Luo Li</i>	The Physics of Metal Plasticity: A Memorial Symposium in Honor of Professor Hussein Zbib, Chair(s): Ioannis Mastorakos Plasticity of inhomogeneous alloys using a coupled data-driven multiscale discrete dislocation dynamics framework <i>Yash Pachaury*, Anter El-Azab</i>	
			Continuum Dislocation Dynamics-Based Full Field Crystal Plasticity Modeling for Characterizing Dislocation Distribution and Boundary Transmission in Polycrystalline Materials <i>Navid Kermanshahimofared, Georges Ayoub, Ioannis Mastorakos*</i>

Thursday Morning, October 6 / TECHNICAL PROGRAM

PLENARY LECTURE / 8:30 – 9:30 AM

Dr. Julie Christodoulou

“A Point of Reflection: Understanding our Progress and Challenges”

Chair: Irene Beyerlein

Maryland Ballroom AB&C

SPECIAL PRESENTATION / 9:30 – 9:45 AM

Prof. Javier Llorca

“MSMSE Forum and Poster Awards Announcement”

Maryland Ballroom AB&C

10:00 AM	10:30 AM	10:50 AM	11:10 AM	11:30 AM
6th Floor Gibson Room	Symposium 3	Computer Modeling of Laser and Ion Beam Interactions with Materials, Chair(s): Leonid Zhigilei		
<p>Keynote presentation: Irradiation effects in space – ices and dust grains</p> <p><i>Herbert Urbassek*</i></p>	<p>Multiscale Computations on Sputtering of Graphitic Structures for Space Propulsion Applications</p> <p><i>Huy Tran*, Huck Beng Chew</i></p>	<p>Multiscale Simulation of laser-textured surface wettability: toward understanding the role of surface oxidation and molecular adsorption</p> <p><i>Ilemona Omeje*, Patrick Ganster, Tatiana Itina</i></p>	<p>In-situ Tuning of Microstructure Through Synchronized Powder Bed Laser Additive Manufacturing (S-LAM)</p> <p><i>Majid Dousti*, Hamed Attariani</i></p>	<p>Modeling Microstructural Evolution during Laser Processing of Metallic Powders using a Hybrid Mesoscale-Continuum approach</p> <p><i>Ching Chen*, Sergey Galitskiy, Dmitry S. Ivanov, Ranadip Acharya, Vijay Jagdale, Avinash Dongare</i></p>
5th Floor Baltimore Ballroom A	Symposium 5	Data-Driven and Physics-Informed Multiscale Materials Modelling, Chair(s): Mayu Muramatsu		
<p>Keynote presentation: Transferable, Machine Learning-Driven Fast Prediction and Screen of Thermal Transport in Mechanically Stretched Graphene Flakes</p> <p><i>Qingchang Liu*, Baoxing Xu</i></p>	<p>Design of finite temperature stability of complex metallic phases enabled by innovative digital concepts</p> <p><i>Tilman Hickel*, Halil Sözen, Lekshmi Sreekala, Jan Janssen, Sarath Menon, Jörg Neugebauer</i></p>	<p>Variational Onsager Neural Networks (VONNs): A Thermodynamics-based Variational Learning Strategy for Non-equilibrium Material Modeling</p> <p><i>Shenglin Huang*, Zequn He, Bryan Chem, Celia Reina</i></p>	<p>Shannon Entropy Based Multicomponent Materials Design</p> <p><i>Gautam Anand*</i></p>	
5th Floor Homeland Room	Symposium 6	Defects and Microstructure Complexity in Materials: Experiments and Multiscale Modeling, Chair(s): Simon Phillpot		
<p>Keynote presentation: Hierarchically Structure Materials for Sequestration of Radionuclides: Thermodynamics and Atomic-Level Mechanisms</p> <p><i>Simon Phillpot*, Ximeng Wang, Yuan Liu, R. Seaton Ullberg, An T. Ta, Shubham Pandey</i></p>	<p>Atomistically-informed cluster dynamics modelling of defect evolution in irradiated ThO₂</p> <p><i>Sanjoy Mazumder*, Maniesha Singh, Tomohisa Kumagai, Anter El-Azab</i></p>	<p>Modelling the effect of H in the formation, stabilization and evolution of voids in polycrystalline Cu</p> <p><i>Vasileios Fotopoulos*, Alexander Shluger, Ricardo Grau-Crespo</i></p>	<p>On the Variability of Grain Boundary Motion</p> <p><i>Anqi Qiu*, Ian Chesser, Elizabeth Holm</i></p>	<p>Predicting electrical conductivity in Cu/Nb composites: a combined model-experiment study</p> <p><i>Daniel Blaschke*, Cody Miller, Ryan Mier, Carl Osborn, Sean Thomas, Eric Tegtmeier, William Winter, John Carpenter, Abigail Hunter</i></p>

Thursday Morning, October 6 / TECHNICAL PROGRAM

10:00 AM	10:30 AM	10:50 AM	11:10AM	11:30 AM
5th Floor Baltimore Ballroom B Keynote presentation: Effect of Free Surfaces on Dislocation Mobility in the Transonic Regime <i>Ta Duong*, Michael Demkowicz</i>	Symposium 7 On the relationship between twinning dislocation kinetics and twin boundary kinetics in the phonon drag regime <i>Justin Wilkerson*, Nitin Daphalapurkar</i>	Dislocation, Twinning, Phase Transformation, Phonon, Diffusion, and Their Interactions in Materials Manufacturing, Processing, and Testing, Chair(s): Justin Wilkerson		
		Structure-property Linkages in Magnesium Alloys <i>Shailendra Joshi*, Shahmeer Baweja</i>	Twin nucleation and growth mechanism in Ni-based superalloys <i>Valery Borovikov*, Mikhail Mendeleev, Nikolai Zarkevich, Timothy Smith, John Lawson</i>	Molecular Dynamics Simulations of Twin Boundaries in Ni-Ti Shape-Memory Alloys <i>Lorenzo La Rosa*, Francesco Maresca</i>
5th Floor Maryland Ballroom E Keynote presentation: Interpreting Discrete GND Footprints of Atomic-Level Irradiation Defects Near Grain Boundaries <i>Jaime Marian*, Mitra Taheri, David Srolovitz</i>	Symposium 10 Avalanche Mediated Interface Diffusion and Finite Size Effects in Metallic Grain Boundaries <i>Ian Chesser*, Raj Koju, Yuri Mishin</i>	Interface-Driven Phenomena in Materials: Thermodynamics, Kinetics, and Chemistry, Chair(s): Garritt Tucker		
		A Level-Set Numerical Framework for the Modeling of Diffusive Solid - Solid Phase Transformation in Multiphase Polycrystalline Materials <i>Nitish Chandrappa*, Marc Bernacki</i>	Efficient Data Assimilation Method for Phase-Field Simulation of Solid-State Sintering: Tree-Structured Parzen Estimator Approach <i>Akimitsu Ishii*, Michihiko Suda, Akinori Yamanaka</i>	Evaluation of Interpolation Schemes for Elastic Energy Using a Phase-Field Model <i>Wooseob Shin*, Kunok Chang</i>
5th Floor Maryland Ballroom D Keynote presentation: Understanding Strain Hardening of Face-Centered Cubic Metals Using Dislocation Dynamics <i>Wei Cai*, Sh. Akhondzadeh, Ryan B. Sills, Nicolas Bertin</i>	Symposium 12 A Multiscale Investigation of Cyclic Deformation in fcc Single Crystals <i>Sylvain Queyreau*, Benoit Devincze</i>	Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem, Chair(s): Marc Fivel		
		A coupled crystal-plasticity and phase-field model for understanding fracture behaviors of tungsten <i>Yinan Cui*, Zhijie Li</i>	Multiphysics modelling of short crack propagation in ductile materials by coupling phase field and dislocation dynamics <i>Luis Eon, Riccardo Gatti*, Alphonse Finel, Benoit Appolaire</i>	Steady-State Plastic Flow and the Life-Cycle of Dislocation Junctions in FCC Metals <i>Yurui Zhang*, Ryan Sills</i>

Thursday Morning, October 6 / TECHNICAL PROGRAM

10:00 AM	10:30 AM	10:50 AM	11:10AM	11:30 AM
5th Floor Maryland Ballroom F Keynote presentation: Multiscale Modeling and Performance Prediction of Additively Manufactured Polymer and Its Composites <i>Satyajit Mojumder*, Zahabul Islam, Wing Kam Liu</i>	Symposium 17 Rate-Dependent Mixed-Mode Traction Law for Glass Fiber-Epoxy Interphase Developed using Molecular Simulations <i>Sanjib Chowdhury*, John Gillespie Jr.</i>	Multiscale and Multifield Modeling of Composites: from Atomic to Continuum Scale, Chair(s): Matthew Guzewski Stochastic Multiscale Simulation Method for Heterogeneous Catalysts: Concurrent Coupling of Kinetic Monte Carlo and Fluctuating Hydrodynamics <i>Changho Kim*, Andy Nonaka, John Bell, Alejandro Garcia</i>	Imperfect contact laws for micro- and nano-composites taking into account the influence of strain gradient and flexoelectric effects <i>Michele Serpilli*, Raffaella Rizzoni, Reinaldo Rodriguez-Ramos, Frédéric Lebon, Serge Dumont</i>	
6th Floor Kent Room Keynote presentation: First Principles Force Fields <i>Gabor Csanyi*</i>	Symposium 18 Convolutional Moment Tensor Potentials <i>Tobias Olbrich*</i>	Multiscale Materials Modeling Using Ab-Initio Accuracy Methods, Chair(s): Amartya Banerjee Benchmarking of different Machine-Learning Interatomic Potential Approaches for Silica <i>Linus Erhard*, Jochen Rohrer, Karsten Albe, Volker Deringer</i>	Developing a Gaussian Approximation Potential for Simulation of Fracture in Irradiated alpha-Iron <i>Lakshmi Shenoy*, Albert Bartok-Partay, James Kermode</i>	
5th Floor Fells Point Room Keynote presentation: Dynamics and Heterogeneity of Particle Network in Composite Electrodes <i>Kejie Zhao*</i>	Symposium 20 Simulating Sintering of Solid-State Battery Materials with Phase-Field <i>Raphael Schiedung*, Machiko Ode</i>	Multiscale Modeling of Battery Materials, Chair(s): Partha Mukherjee Modeling Lithium-Ion Batteries in EV Applications, a Multi-Scale Problem <i>Elham Sahraei*, Shantanu Shinde</i>	Role of Anisotropy on the Chemo-Mechanical Performance of Polycrystalline NMC Secondary Particle Embedded in a Sulfide-based Solid Electrolyte <i>Avtar Singh, Wei Li, Trevor Martin, Donal Finegan, Juner Zhu*</i>	

Thursday Morning, October 6 / TECHNICAL PROGRAM

10:00 AM	10:30 AM	10:50 AM	11:10AM	11:30 AM
5th Floor Guilford Room	Symposium 23	Scale Bridging in Materials Science, Chair(s): Garritt Tucker		
<p>Keynote presentation: Concurrent multi-scale approach for granular flow problems</p> <p><i>Ken Kamrin*</i></p>	<p>Simulating the pore structure of sustainable cements</p> <p><i>Claire White*</i></p>	<p>An Algorithm for Temporal Scale-Bridging of Chemistry in a Multiscale Model of a Reacting Energetic Material</p> <p><i>Kenneth Leiter*, James Larentzos, Richard Becker, Jaroslaw Knap</i></p>	<p>Bridging Models at Different Scales to Design New Generation Fuel Cells for Electrified Mobility</p> <p><i>Konstantinos Gkagkas*</i></p>	<p>Particle-Based, Mesoscale Reactive Model of High Explosives: Model Development and Application to Shock to Deflagration Transition</p> <p><i>Brian Lee*, Brenden Hamilton, James Larentzos, John Brennan, Alejandro Strachan</i></p>
5th Floor Federal Hill Room	Symposium 25	Uncertainty Quantification, Sensitivity Analysis, and Machine Learning in Materials Modeling, Chair(s): Maryam Shakiba		
<p>Keynote presentation: Robust structure identification using neural networks implemented in OVITO</p> <p><i>Daniel Utt*, Linus C. Erhard, Karsten Albe</i></p>	<p>A Top-Down Characterization of NiTi Single Crystal Inelastic Properties within Confidence Bounds through Bayesian Inference</p> <p><i>Theocharis Baxevanis*, Afzal Md Hossain, Pejman Honarmadi, Raymundo Arroyave</i></p>	<p>Quantitative properties through semantic learning</p> <p><i>Allen Garcia*, Connor O’Ryan, Gaurav Kumar, Zois Boukouvalas, Mark Fuge, Peter Chung</i></p>	<p>Uncertainty Quantification and Machine Learning for Stochastic Hierarchical Multiscale Modeling</p> <p><i>George Soimoiris, Kenneth Leiter, Jaroslaw Knap, Michael Shields</i></p>	<p>Uncertainty quantification of heterogeneous cohesive and smeared crack models</p> <p><i>Golsa Mahdavi*, Amin Hariri-Ardebili</i></p>
5th Floor Pride of Baltimore Room	Symposium 27	The Physics of Metal Plasticity: A Memorial Symposium in Honor of Professor Hussein Zbib, Chair(s): Mu’Tasem Shehadeh		
<p>Keynote presentation: Confined volume enabled unusual plasticity carriers in brittle phase</p> <p><i>Jian Wang*, Amit Misra</i></p>	<p>Origins of the abnormal tensile deformation of additively manufactured Haynes 282</p> <p><i>Indrajit Nandi*, Nabeel Ahmad, Jian Wang, Nima Shamsaei, Shuai Shao</i></p>	<p>Reduced-Order Modeling for Coating Materials in Gas Turbine Engine</p> <p><i>Jiahao Cheng, Xiaohua Hu*, Xin Sun, Drew Lancaster, William Joost</i></p>	<p>Invited Talk: Processing for Designed Heterostructures in AZ31</p> <p><i>Dave Field*, Maryam Jamalian, Mueed Jamal, Gunnar Blaschke</i></p>	<p>Modeling of the Tension-Compression Asymmetry Reduction of ECAPed Mg-3Al-1Zn Through Grain Fragmentation</p> <p><i>Ali Al-Hadi Kobaissy, Georges Ayoub*, Mu’Tasem Shehadeh</i></p>

Thursday Afternoon, October 6 / TECHNICAL PROGRAM

SEMI-PLENARY LECTURES / 1:00 – 1:45 PM

Prof. Elizabeth A. Holm

“Quantity or quality? Capitalizing on small but rich materials data sets”

Chair: Lori Graham-Brady

Maryland Ballroom AB&C

Prof. Shigenobu Ogata

“Atomistic modeling of the impact of hydrogen on metals”

Chair: Michael Falk

Maryland Ballroom D

1:45 PM	2:15 PM	2:35 PM	2:55 PM	3:15 PM
5th Floor Baltimore Ballroom A Keynote presentation: Understanding Dislocation Flow and Avalanches in High Entropy Alloys by Machine Learning-Based Data Mining of In-Situ TEM Experiments <i>Stefan Sandfeld*, Chen Zhang, Marc Legros, Kishan Govind, Hengxu Song, Daniela Oliveros</i>	Symposium 5 Theory-guided Design of High-strength, Ductile, Single-phase BCC High Entropy Alloys <i>You Rao*, Carolina Baruffi, Anthony De Luca, Christian Leinenbach, William Curtin</i>	Data-Driven and Physics-Informed Multiscale Materials Modelling, Chair(s): Thomas Hochrainer Efficient search of novel refractory high entropy alloys with exceptional high-temperature strength <i>Francesco Maresca*, William Curtin</i>		
			Alchemical machine learning for high entropy alloys <i>Nataliya Lopanitsyna*, Guillaume Fraux, Michele Ceriotti</i>	
5th Floor Homeland Room Keynote presentation: Multiobjective Optimization Of The Diffusion Properties Of Nanocavities In Metallic Tungsten <i>Andrée De Backer, Abdelkader Soudi, Etienne A. Hodille, Emmanuel Autissier, Cécile Genevois, Farah Haddad, Antonin Della Noce, Christophe Domain*, Charlotte S. Becquart, Marie-France Barthe</i>	Symposium 6 A homogenization method based on lump sum to representative points of mesoscale structures <i>Duan Zhang*, Paul Barclay</i>	Defects and Microstructure Complexity in Materials: Experiments and Multiscale Modeling, Chair(s): Bennett Larson A new Phase Field Model for Void Nucleation and Growth Under Ion-irradiation <i>Sreekar Annadanam*, Anter El-Azab</i>		
			Surrogate Hot-Spot Model for High-Fidelity Simulation of Shock Loading in Energetic Materials <i>Chongxi Yuan*, Marisol Koslowski</i>	Quantifying Dislocation Structure Evolution through Reconstruction Based on Acoustic Emission <i>Junjie Yang*, Yejun Gu, Daniel Magagnosc, Tamer Zaki, Jaafar El-Awady</i>
5th Floor Baltimore Ballroom B Keynote presentation: Atomic-Size Imperfections Control the Strength of Refractory High Entropy Alloys in the Entire Temperature Range <i>Jaime Marian*, Xinran Zhou, Sicong He, Stephanie Taylor</i>	Symposium 7 Strengthening due to localized obstacles in bcc alloys <i>Yuri Osetsky*</i>	Dislocation, Twinning, Phase Transformation, Phonon, Diffusion, and Their Interactions in Materials Manufacturing, Processing, and Testing, Chair(s): Anas Abu-Odeh Composition and Stress-Orientation Dependence of Lomer and Lomer-Cottrell Dislocation Behavior <i>Anas Abu-Odeh*, Tarun Allaparti, Mark Asta</i>		
			Elucidating the mechanism of nucleation and growth of {11-22} twins <i>Ritu Verma*, Andriy Ostapovets, Anna Serra</i>	Micromechanical behavior of martensite influenced thermal expansion <i>Daniel Savage*, Donald Brown, Bjorn Clausen, Sean Agnew, Sven Vogel</i>

Thursday Afternoon, October 6 / TECHNICAL PROGRAM

1:45 PM	2:15 PM	2:35 PM	2:55 PM	3:15 PM
5th Floor Maryland Ballroom E Keynote presentation: Multi-Phase-Field Modeling and Large-Scale Simulations for Solid-State Sintering <i>Tomohiro Takaki*</i>	Symposium 10 Phase-field Cosserat Crystal Plasticity towards Modelling Nucleation in Recrystallization <i>Flavien Ghiglione*, Anna Ask, Kais Ammar, Benoit Appolaire, Samuel Forest</i>	Interface-Driven Phenomena in Materials: Thermodynamics, Kinetics, and Chemistry, Chair(s): Jaime Marian Atomistically informed Phase Field model to investigate grain boundary migration in FCC polycrystals <i>Etienne Ngenzi, Sylvain Queyreau*, Jaime Marian</i>	Phase-Field Modeling of Zr-O Binary System Phase Separation: Zirconium Alpha and Beta Phase <i>Jiho Kim*, Kunok Chang</i>	A Generalized 3D Elastic Model for Nanoscale, Self-assembled Oxide-metal Thin Films with Pillar-in-matrix Configurations <i>Kyle Starkey, Ahmad Ahmad*, Juanjuan Lu, Haiyan Wang, Anter El-Azab, Sreekar Annadanam</i>
5th Floor Maryland Ballroom D Keynote presentation: On the Dynamics of Curved Dislocation Ensembles <i>Istvan Groma*, Péter Dusán Ispánovity, Thomas Hochrainer</i>	Symposium 12 Phenomenology and statistical thermodynamics of dislocation plasticity <i>Victor Berdichevsky*</i>	Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem, Chair(s): Wei Cai An Action Principle for Nonlinear Dislocation Dynamics <i>Amit Acharya*</i>	Correlations and effective stress fields in vector density continuum dislocation dynamics <i>Joseph Anderson*, Vignesh Vivekanandan, Anter El-Azab</i>	Adaptive grids for FFT based Field Dislocation Mechanics <i>Rodrigo Santos-Güemes*, Gonzalo Álvarez, Javier Segurado</i>
5th Floor Maryland Ballroom F Keynote presentation: Investigation of Toughness Increase at the Macroscale due to Competing Mechanisms of Crack-Tip Shielding and Toughness Change from Induced Damage Evolution at the Microscale via Material Inhomogeneities <i>Samit Roy*</i>	Symposium 17 Mesoscale Modeling of Heterogeneous and Additively Manufactured Materials <i>Maryam Shakiba*</i>	Multiscale and Multifield Modeling of Composites: from Atomic to Continuum Scale, Chair(s): Sanjib Chowdhury Data-driven Parametrically-Upscaled Continuum Damage Mechanics (PUCDM) Model for Composites <i>Xiaofan Zhang*, Somnath Ghosh</i>		
6th Floor Kent Room Keynote presentation: Electronic Structure of Incommensurate 2D Heterostructures with Mechanical Relaxation <i>Daniel Massatt*, Stephen Carr, Mitchell Luskín</i>	Symposium 18 Towards Understanding the Optical Properties of Two-Dimensional Materials <i>Nicholas Pike*, Ruth Pachter</i>	An integrated machine learning – first principles approach for the study of chiral matter <i>Amartya Banerjee*, Hsuan Ming Yu, Shashank Pathrudkar, Susanta Ghosh</i>	Optimization of 2D Transition Metal Dichalcogenides using Electronic Structure and Thermoelectric Coefficient Calculations <i>Isaiah Chen*, Paulette Clancy</i>	Synergistic coupling in ab initio-machine learning simulations of dislocations <i>Petr Grigorev, Thomas Swinburne*</i>

Thursday Afternoon, October 6 / TECHNICAL PROGRAM

1:45 PM	2:15 PM	2:35 PM	2:55 PM	3:15 PM
5th Floor Fells Point Room	Symposium 20	Multiscale Modeling of Battery Materials, Chair(s): Elham Sahraei		
<p>Keynote presentation: Mechanistic Interactions in Solid-State Battery Interfaces and Architectures</p> <p><i>Partha Mukherjee, Bairav Vishnugopi*</i></p>	<p>On the tradeoff of the Ion Exchange induced residual compressive stress to prevent Lithium filament growth, and the Lithium Ion transport in solid state electrolytes</p> <p><i>Harsh Jagad*, Stephen Harris, Yue Qi, Brian Sheldon</i></p>	<p>Phase-Field Modeling of Lithium Dendrite Growth and Fracture in Solid Electrolytes</p> <p><i>Sulin Zhang, Dingchuan Xue*, Ruyue Fang</i></p>	<p>From Short to Long Time and Length Scales: A MultiScale Methodology for Ionic Diffusion in Solid-State Electrolytes for Solid Batteries</p> <p><i>Mahmoud Attia, Said Yagoubi, Jean-Paul Crocombette, Thibault Charpentier</i></p>	
5th Floor Guilford Room	Symposium 23	Scale Bridging in Materials Science, Chair(s): Hojun Lim		
<p>Keynote presentation: Scale Bridging in the Inelastic Mechanical Response of BCC Metals</p> <p><i>Christopher Weinberger*, Anik Faisal, Hojun Lim, Lucas Hale, Hunter Brumblay, Jonathan Zimmerman, Corbett Battaile</i></p>	<p>Atomistic Simulations Reveal Effects of Gas Bubbles on Metal Strength</p> <p><i>Sylvie Aubry*, Nicolas R. Bertin, Vasily V. Bulatov</i></p>	<p>Dynamical Correlations and Collective Deformation Modes in Discrete Dislocation Dynamics Simulations</p> <p><i>Gábor Péterffy*, Peter Michael Derlet, Dénes Berta, Péter Dusan Ispánovity</i></p>		
5th Floor Federal Hill Room	Symposium 25	Uncertainty Quantification, Sensitivity Analysis, and Machine Learning in Materials Modeling, Chair(s): Jaroslav Knap		
<p>Keynote presentation: Reducing Uncertainties in Materials Modeling and Design via Data Fusion</p> <p><i>Mehdi Shishehbor, Ramin Bostanabad*</i></p>	<p>Insights on the robustness, sensitivity and expressivity of simple many-body potentials: application to alpha-Zr</p> <p><i>Alessandra Del Masto*, Céline Varvenne, Jean Baccou, Guy Tréglia, Fabienne Ribeiro</i></p>	<p>Nonlinear Microstructure Material Design with Reduced-Order Modeling</p> <p><i>David Brandyberry, Xiang Zhang*, Philippe Geubelle</i></p>	<p>Transverse Cracks Initiation to Formation in a Fiber-Reinforced Composite Through Sensitivity Analysis</p> <p><i>Maryam Shakiba*</i></p>	<p>An Evaluation of Machining Learning Models for Material Microstructure Reconstructions.</p> <p><i>Noah Wade*, Ashwini Gupta, Lori Graham-Brady</i></p>
5th Floor Pride of Baltimore Room	Symposium 27	The Physics of Metal Plasticity: A Memorial Symposium in Honor of Professor Hussein Zbib, Chair(s): Niaz Abdolrahim		
<p>Keynote presentation: Interface size effects in strong and deformable bimetallics</p> <p><i>Irene Beyerlein*, Shuozi Xu, Nathan Mara, Justin Cheng</i></p>	<p>Simulations and modelling of the high temperature yield behavior of compositionally complex concentrated BCC alloys</p> <p><i>Satish Rao*, Brahim Akdim, Oleg Senkov, Eric Payton</i></p>	<p>A threshold density of helium bubbles induces a ductile-to-brittle transition at a grain boundary in nickel</p> <p><i>Michael Demkowicz*</i></p>	<p>Mass transport in nanoparticle sintering. Meso- and macro-scale models.</p> <p><i>Sandra Ritchie, Sasa Kovacevic, Prithviraj Deshmukh, Sinisa Mesarovic*, Rahul Panat</i></p>	<p>Stress-assisted structural transformation and plasticity enhancement in Mo/Cu bicontinuous intertwined composites</p> <p><i>Niaz Abdolrahim*, Lijie He, Linh Vu, Zheming Guo, Ali Shargh</i></p>

Thursday Evening, October 6 / TECHNICAL PROGRAM

4:00 PM	4:30 PM	4:50 PM	5:10 PM
5th Floor Baltimore Ballroom A Keynote presentation: Polynomial Machine Learning Potentials and Crystal Structure Optimization Using Machine Learning <i>Atsuto Seko*</i>	Symposium 5 Predicting Material Properties of Si Electrodes for Multivalent Cations by Ensembling Convolutional Neural Network with Support Vector Regression <i>Joy Datta*, Dibakar Datta</i>	Data-Driven and Physics-Informed Multiscale Materials Modelling, Chair(s): Erik Bitzek CEGAN: Crystal Edge Graph Attention Network for multiscale classification of materials environment <i>Suvo Banik*, Sukriti Manna, Debdas Dhabal, Henry Chan, Valeria Molinero, Subramanian Sankaranarayanan</i>	
		Autobahn: Constructing Neural Networks from Molecular Substructures <i>Erik Thiede*, Wenda Zhou, Risi Kondor</i>	
5th Floor Baltimore Ballroom B Keynote presentation: A General Method for Calculating Local Stress and Elastic Constants for Arbitrary Many-Body Interaction Potentials in LAMMPS <i>Aidan Thompson*, Germain Clavier, Steve Plimpton</i>	Symposium 7 Deformation, Dislocation Evolution, Instability and the Non-Schmid Effect in Single- and Polycrystalline Tantalum <i>Seunghyeon Lee*, Hansohl Cho, Curt Bronkhorst</i>	Dislocation, Twinning, Phase Transformation, Phonon, Diffusion, and Their Interactions in Materials Manufacturing, Processing, and Testing, Chair(s): Alex Selimov Atomistic Modeling of Peierls Barriers to Dislocation Glide in Metals <i>Yipin Si*, David McDowell, Ting Zhu</i>	
		Concurrent Atomistic-Continuum studies of confined layer slip in Cu/Ni nanolaminates <i>Alex Selimov*, Youping Chen, David McDowell</i>	
5th Floor Maryland Ballroom E Keynote presentation: Bayesian Data Assimilation for Phase-Field Simulation of Microstructure Evolution <i>Akinori Yamanaka*, Eisuke Miyoshi, Akimitsu Ishii</i>	Symposium 10 Combined Bayesian inference and phase-field modelling for evaluating triple-junction drag on grain boundary migration <i>Eisuke Miyoshi*, Munekazu Ohno, Yasushi Shibuta, Akinori Yamanaka, Tomohiro Takaki</i>	Interface-Driven Phenomena in Materials: Thermodynamics, Kinetics, and Chemistry, Chair(s): Tomoaki Suzudo Automated Atomistic Analysis of Disconnections during Martensitic Transformations using a Novel Interfacial Defect Analysis Approach <i>Nipal Deka*, Alexander Stukowski, Ryan Sills</i>	
		Simulation of Nanomaterials and Composites from Atoms to Micrometers in Order of Magnitude Higher Accuracy: Models, Examples, and Applications <i>Cheng ZhuBiswa, Hendrik Heinz*</i>	
5th Floor Maryland Ballroom D Keynote presentation: 3D DD Simulations of Ni and Co Superalloys: Investigation of the Tension-Compression Asymmetry During Creep Under Low Stress <i>Marc Fivel*, Jean-Loup Strudel</i>	Symposium 12 Dislocation-Obstacle interactions: the influence of obstacle size and distribution on the Orowan bypass stress <i>Benjamin Szajewski*, Joshua Crone, Jaroslaw Knap</i>	Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem, Chair(s): Istvan Groma Effects of Surface Curvature on the Uniaxial Compression of Micropillars by Discrete Dislocation Dynamics <i>Fabrizio Rovaris*, Stefanos Papanikolaou, Mikko Alava</i>	
		Investigating the Influence of the Internal Stress State due to Precipitates on Strengthening Mechanisms in Mg Alloys Using Phase-Field Simulations <i>Darshan Bamney*, Laurent Capolungo</i>	

Thursday Evening, October 6 / TECHNICAL PROGRAM

4:00 PM	4:30 PM	4:50 PM	5:10 PM
6th Floor Kent Room	Symposium 18	Multiscale Materials Modeling Using Ab-Initio Accuracy Methods, Chair(s): Vikram Gavini	
Keynote presentation: Equivariant Analytical Mapping of First Principles Hamiltonians to Accurate and Transferable Materials Models <i>Liwei Zhang, Berk Onat, Geneviève Dussou, Gautam Anand, Reinhard Maurer, James Kermode*</i>	Predicting the Energetics and Kinetics of Cr Atoms in Fe-Ni-Cr Alloys via Physics-based Machine Learning <i>Yuchu Wang*, Yue Fan</i>	Exploring the behavior of MoNbTaTi refractory CCAs across composition space using a machine learned interatomic potential <i>Megan McCarthy*, Jacob Startt, Remi Dingreville, Aidan Thompson, Mitchell Wood</i>	
5th Floor Fells Point Room	Symposium 20	Multiscale Modeling of Battery Materials, Chair(s): Gorakh M. Pawar	
Keynote presentation: Electrochemical-Mechanical Coupling at Li Metal / Solid Electrolyte Interfaces <i>Paul Albertus*</i>	Influence of Mechanics on Lithium Dendrite Growth in Solid State Batteries: A Phase Field Study <i>Feifei Fan*, Jun Liu</i>	Unraveling and Characterizing the Multiscale Nature of the Interfacial Contact between Lithium Metal and Solid Electrolytes in Solid-State Batteries under Stack Pressure <i>Min Feng*, Xing Liu, Brian Sheldon, Yue Qi</i>	Prediction of Interface Instability of all Solid-State Batteries: Phase-Field Model Integrating Creep/Contact Mechanics (Invited) <i>Lei Chen, Hanghang Yan, Karpiwat Tantratian*</i>
5th Floor Guilford Room	Symposium 23	Scale Bridging in Materials Science, Chair(s): Coleman Alleman	
Keynote presentation: Predicting the unobserved: a statistical mechanics framework for non-equilibrium material response with quantified uncertainty <i>Celia Reina*, Shenglin Huang, Ian Graham, Robert Riggelman, Paulo Arratia, Steve Fitzgerald</i>	Multiscale Material Modeling: Application in Structural Topology Optimization <i>Rowin Bol, Payam Poorolajou*, Hèrm Hofmeyer, Akke Suiker</i>	A Multi Time Domain Algorithm for Nonlinear Impact Phenomena in a Novel Concurrent Multiscale Framework <i>Kin Fung Chan*, Nicola Bombace, Duygu Sap, Nik Petrinic</i>	
5th Floor Federal Hill Room	Symposium 25	Uncertainty Quantification, Sensitivity Analysis, and Machine Learning in Materials Modeling, Chair(s): Michael Shields	
Keynote presentation: Deep Learning Enhanced Uncertainty Quantification <i>Ting Wang*, Jaroslaw Knap</i>	Constructing Training Sets for Transferable Moment Tensor Potentials: Application to Defects in Bulk Mg <i>Marvin Poul*, Liam Huber, Erik Bitzek, Jörg Neugebauer</i>	A Manifold Learning Model for the Deformation of Multiwalled Carbon Nanotubes under Torsion and Bending <i>Upendra Yadav, Shashank Pathrudkar*, Susanta Ghosh</i>	Predicting the Dynamics of Fracture in Crystalline Solids using Deep Neural Network <i>Yu-Chuan Hsu*, Markus Buehler</i>

Thursday Evening, October 6 / TECHNICAL PROGRAM

4:00 PM	4:30 PM	4:50 PM	5:10 PM
5th Floor Pride of Baltimore Room	Symposium 27	The Physics of Metal Plasticity: A Memorial Symposium in Honor of Professor Hussein Zbib, Chair(s): Joshua Robbins	
<p>Keynote presentation: An Irradiation-Dependent Internal State Variable Elastoviscoplasticity-Damage Model for Polycrystalline Metals</p> <p><i>Heechen Cho*, Mark Horstemeyer</i></p>	<p>Invited Talk: Advances in Phase-Field Modeling of Ductile Fracture</p> <p><i>Mohsen Asle Zaeem*, William Huber</i></p>	<p>On the Mechanical Response and Microstructure Evolution in Martensitic Steel: Discrete Dislocation Dynamics Investigation</p> <p><i>Ossama Abou Ali Modad, Mutasem Shehadeh*</i></p>	<p>Gradient-based design optimization with material strength awareness</p> <p><i>Joshua Robbins*, Karl Garbrecht, Miguel Aguilo, Jacob Hochhalter</i></p>

POSTER SESSION - TUESDAY, OCTOBER 4 / MARYLAND AND BALTIMORE FOYERS, 5:45-7:30PM

Number	Title	Symposium	Author	Affiliation
1	Phase-Field Simulations Two-Step Mechanism of Macromolecular Nucleation and Crystallization	1 - Advances in Methods for Bridging Spatiotemporal Scales in Soft Matter, Polymer and Network Materials	Alexander R. Umantsev	Fayetteville State University
2	Coarse-Grained Potentials for Fluids	1 - Advances in Methods for Bridging Spatiotemporal Scales in Soft Matter, Polymer and Network Materials	Siwei Luo	University of British Columbia
3	Revealing the Polyelectrolyte Valency of Nanoparticles Using Dissipative Particle Dynamics Simulations	1 - Advances in Methods for Bridging Spatiotemporal Scales in Soft Matter, Polymer and Network Materials	Yinong Zhao	Johns Hopkins University
4	Development of Data Assimilation System with Phase-Field Simulation for 3D Columnar Dendrite Growth	10 - Interface-Driven Phenomena in Materials: Thermodynamics, Kinetics, and Chemistry	Ayano Yamamura	Kyoto Institute of Technology
5	Mechanistic Understanding of Lead Chalcogenide Quantum Dot Assembly and Attachment on Fluid Interfaces	10 - Interface-Driven Phenomena in Materials: Thermodynamics, Kinetics, and Chemistry	Wenxin Qi	Johns Hopkins University
6	An Elastic Model of Lattice Distortions in High Entropy Alloys	12 - Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem	David Rodney	University Lyon 1
7	Nickel Intergranular Fracture Prediction with Multi-Scale Simulations	12 - Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem	Laurent Van Brutzel	CEA
8	Acoustic Emissions-Based Approach to Quantify Characteristics of Dislocation Avalanches in Metals.	12 - Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem	Mostafa Omar	Johns Hopkins University
9	Dislocation Evolution in Copper During Nanoindentation	12 - Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem	Wurong Jian	Stanford University
10	Representative Volume Element in Discrete Dislocation Dynamics Conceptualization and Implementation of Bulk Boundary Conditions	12 - Mechanics and Physics of Defects in Crystals: A Symposium in Honor of Professor Nasr Ghoniem	Yash Pachaury	Purdue University

POSTER SESSION - TUESDAY, OCTOBER 4 / MARYLAND AND BALTIMORE FOYERS, 5:45-7:30PM

Number	Title	Symposium	Author	Affiliation
11	Adaptive Wavelet-Enhanced Cohesive Zone Phase-Field FE Model for Crack Evolution in Piezoelectric Composites	13 - Mechanics and Physics of Material Failure	Saikat Dan	Johns Hopkins University
12	Load Versus Displacement Controlled Nanomechanics: Insights from Atomistic Simulations	14 - Metals at the Nanoscale and Metals-Based Nanoparticles: Environmental, Mechanical and Kinetic Properties	Jonathan Amodeo	CNRS
13	Helium diffusion and clustering in tungsten borides: A first-principles study	18 - Multiscale Materials Modeling Using Ab-Initio Accuracy Methods	Li Yang	University of Tennessee
14	Solution Energy of Hydrogen at the Tungsten / Copper Interface from Density Functional Theory Calculations.	18 - Multiscale Materials Modeling Using Ab-Initio Accuracy Methods	Yves Ferro	Aix-Marseille Université / CNRS
15	The Interaction Between a Single Dislocation and Atomic Hydrogen in Tungsten: Atomistic Study	2 - Bridging Scales in the Microstructure Modeling of Nuclear Materials	Hyoungryul Park	Yonsei University
16	Conversion of Stacking Fault Tetrahedra to Bubbles in Dual (Kr, He)-Beam Irradiated Copper	2 - Bridging Scales in the Microstructure Modeling of Nuclear Materials	Sreekar Annadanam	Purdue University
17	Stress-Dependent Activation Entropy in Thermally Activated Cross-Slip of Dislocations	2 - Bridging Scales in the Microstructure Modeling of Nuclear Materials	Yifan Wang	Stanford University
18	Accurately modeling dynamical heterogeneity in glassforming liquids across a wide range of spatial dimensions	21 - Multiscale Modeling of Glasses and Structurally Disordered Materials	Robert Hoy	University of South Florida
19	3D MPF-LB Model and Simulations for Equiaxed Solidification Structures	22 - Multiscale Solidification Modeling	Namito Yamanaka	Kyoto Institute of Technology

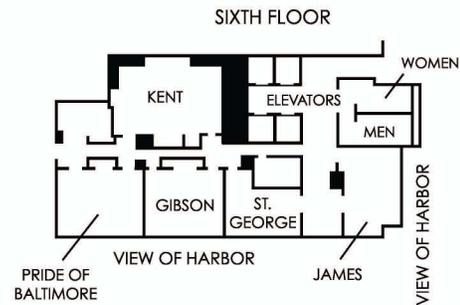
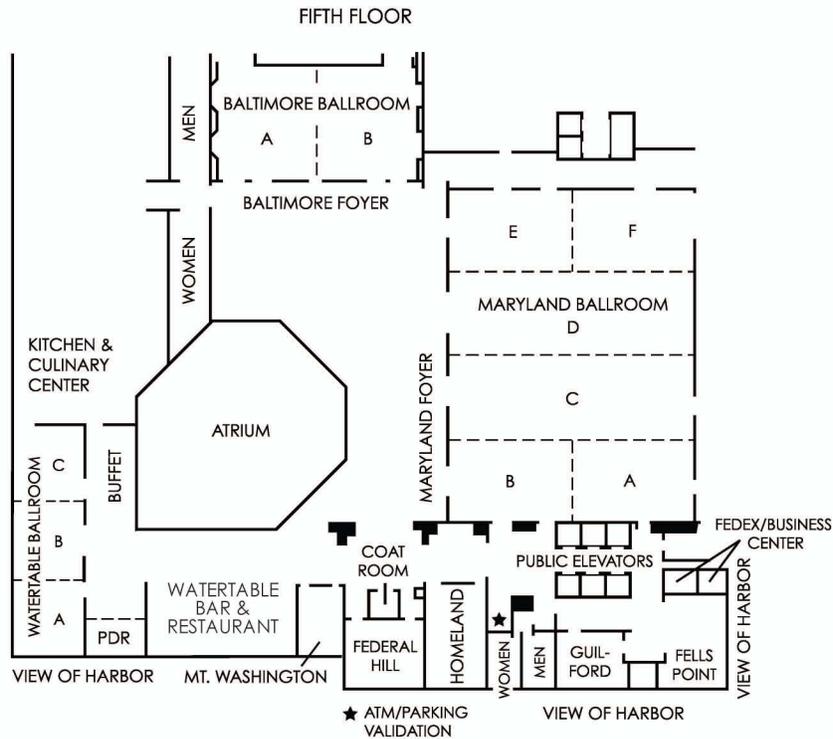
POSTER SESSION - WEDNESDAY, OCTOBER 5 / MARYLAND AND BALTIMORE FOYERS, 5:45-7:30PM

Number	Title	Symposium	Author	Affiliation
21	Nanomechanical Analysis of Coronavirus Spike proteins and Correlation with Infectivity and Lethality	23 - Scale Bridging in Materials Science	Yiwen Hu	MIT
22	Thermal Super-Jogs Control High-Temperature Strength in Nb-Mo-Ta-W Alloys	24 - Stochastic Methods in Materials Simulation	Sicong He	University of California, Los Angeles
23	A Deep Learning Approach to Model Composites at Multiple Scale	25 - Uncertainty Quantification, Sensitivity Analysis, and Machine Learning in Materials Modeling	Ashwini Gupta	Johns Hopkins University
24	Atomistic Insights on the Core Properties and Mobility of <100> Dislocations in Body-Centered Cubic Transition Metals	27 - The Physics of Metal Plasticity: A Memorial Symposium in Honor of Professor Hussein Zbib	Baptiste Bienvenu	CEA Saclay
25	Thermodynamic maps and nanoparticle cooling rates in laser ablation of FeNi in liquid	3 - Computer Modeling of Laser and Ion Beam Interactions with Materials	Chaobo Chen	University of Virginia
26	Laser Fragmentation of Gold Nanoparticles in Water: Phase Explosion, Nanoscale Inverse Leidenfrost Effect, and Evaporation-driven Nanobubble	3 - Computer Modeling of Laser and Ion Beam Interactions with Materials	Leonid Zhigilei	University of Virginia
27	Atomistic Modelling of Femtosecond Laser Melting of Pb Nanoparticles Embedded into Al Film	3 - Computer Modeling of Laser and Ion Beam Interactions with Materials	Mikhail I. Arefev	University of Virginia
28	Molecular Dynamics Study of the Stresses and Atomic Structures of DLC Films According to Deposition Conditions	3 - Computer Modeling of Laser and Ion Beam Interactions with Materials	Nortsugu Kametani	Kyoto Institute of Technology
29	CASTING – A Continuous Action Space Tree Search for INverse Design	5 - Data-Driven and Physics-Informed Multiscale Materials Modelling	Suvo Banik	University of Illinois at Chicago
30	Quantifying Chemical Ordering in Chemically Complex Alloys	6 - Defects and Microstructure Complexity in Materials: Experiments and Multiscale Modeling	Annie Barnett	Johns Hopkins University
31	Multi-Scale Microstructure Evolution of Tungsten Under Neutron and Plasma Loads	6 - Defects and Microstructure Complexity in Materials: Experiments and Multiscale Modeling	Francesco Maresca	University of Groningen
32	Vacancy Energetics in the equiatomic Nb-Ta-Mo-W	6 - Defects and Microstructure Complexity in Materials: Experiments and Multiscale Modeling	Xinran Zhou	UCLA

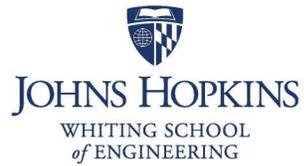
POSTER SESSION - WEDNESDAY, OCTOBER 5 / MARYLAND AND BALTIMORE FOYERS, 5:45-7:30PM

Number	Title	Symposium	Author	Affiliation
33	Dislocation bias and loop bias in fcc copper and bcc iron	6 - Defects and Microstructure Complexity in Materials: Experiments and Multiscale Modeling	Ziang Yu	The University of Tennessee, Knoxville
34	Theory and modelling of the austenite-martensite interface structure and glissile transformation of lath martensite in steels	7 - Dislocation, Twinning, Phase Transformation, Phonon, Diffusion, and Their Interactions in Materials Manufacturing, Processing, and Testing	Francesco Maresca	University of Groningen
35	Computational Approaches for Studying the Nucleation of Voids at the Nanoscale	7 - Dislocation, Twinning, Phase Transformation, Phonon, Diffusion, and Their Interactions in Materials Manufacturing, Processing, and Testing	Vicente Munizaga	Johns Hopkins University
36	Polymorphism in Medium Entropy Alloy CoCrNi Under Quasi-Isentropic Compression	7 - Dislocation, Twinning, Phase Transformation, Phonon, Diffusion, and Their Interactions in Materials Manufacturing, Processing, and Testing	Zhuocheng Xie	South China University of Technology
37	Coupled Crystal Plasticity Phase-Field Model for Ductile Fracture in Polycrystalline Microstructures	8 - Fatigue and Fracture of Materials: from Micro to Macroscale Modeling and Experimentation	Thirupathi Maloth	Johns Hopkins University
38	Parametrically Upscaled Coupled Constitutive Model (PUCCM) for Nonuniform Unidirectional Multifunctional Composites from Micromechanical Analysis	9 - Integrated Multiscale/Multiphysics Modeling of Structural Materials	Preetam Tarafder	Johns Hopkins University
39	Atomic Simulation of Chemical Ordering Effect on Irradiation Resistance and Defect Diffusion in High/Medium-entropy Alloys	9 - Integrated Multiscale/Multiphysics Modeling of Structural Materials	Yangen Li	Osaka University
40	El-Numodis, a New Tool to Model Dislocation Versus Surface Interactions: Application to Nanoparticle Mechanics	14 - Metals at the Nanoscale and Metals-Based Nanoparticles: Environmental, Mechanical and Kinetic Properties	Jonathan Amodeo	CNRS

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