



7TH WORLD CONGRESS ON
**INTEGRATED COMPUTATIONAL MATERIALS
ENGINEERING (ICME 2023)**

**PRELIMINARY
TECHNICAL PROGRAM**

TMS

This conference is sponsored by
Materials Processing & Manufacturing
Division (MPMD) and the Integrated
Computational Materials Engineering
(ICME) Committee.

SCHEDULE AT A GLANCE • Current as of February 27, 2023 • Subject to change

Sunday, May 21		
	Time	Location
Registration	5:00 p.m. - 7:30 p.m.	Caribbean Reg East
Welcome Reception	6:30 p.m. - 7:30 p.m.	Boca Patio/Pier
Monday, May 22		
	Time	Location
Registration	7:00 a.m. - 4:30 p.m.	Caribbean Reg East
Exhibitor and Poster Installation	7:30 a.m. - 8:30 a.m.	Caribbean V
Plenary Session	8:00 a.m. - 9:30 a.m.	Caribbean VI & VII
<i>Exhibition and Break</i>	9:30 a.m. - 9:50 a.m.	Caribbean V
Technical Sessions	9:50 a.m. - 11:40 a.m.	Caribbean VI & VII, Boca I-III, Boca V-VII
Congress Lunch	11:40 p.m. - 1:10 p.m.	To be announced
Technical Sessions	1:10 p.m. - 4:30 p.m.	Caribbean VI & VII, Boca I-III, Boca V-VII
<i>Exhibition and Break</i>	3:00 p.m. - 3:20 p.m.	Caribbean V
Tuesday, May 23		
	Time	Location
Registration	7:30 a.m. - 5:45 p.m.	Caribbean Reg East
Technical Sessions	8:00 a.m. - 12:00 p.m.	Caribbean VI & VII, Boca I-III, Boca V-VII
<i>Exhibition and Break</i>	9:50 a.m. - 10:10 a.m.	Caribbean V
Lunch	11:50 p.m. - 1:20 p.m.	On your own
Technical Sessions	1:20 p.m. - 4:20 p.m.	Caribbean VI & VII, Boca I-III, Boca V-VII
<i>Exhibition and Break</i>	2:40 p.m. - 3:00 p.m.	Caribbean V
Poster Session and Reception	4:45 p.m. - 5:45 p.m.	Caribbean V
Wednesday, May 24		
	Time	Location
Registration	7:30 a.m. - 4:30 p.m.	Caribbean Reg East
Plenary Session	8:00 a.m. - 9:20 a.m.	Caribbean VI & VII
<i>Exhibition and Break</i>	9:20 a.m. - 9:40 a.m.	Caribbean V
Technical Sessions	9:40 a.m. - 11:30 a.m.	Caribbean VI & VII, Boca I-III, Boca V-VII
Lunch	11:40 p.m. - 1:10 p.m.	On your own
Technical Sessions	1:10 p.m. - 4:30 p.m.	Caribbean VI & VII, Boca I-III, Boca V-VII
TBA Social Function	3:20 p.m. - 4:30 p.m.	Boca V-VII
<i>Exhibition and Break</i>	3:00 p.m. - 3:20 p.m.	Boca V-VII
Exhibitor and Poster Teardown	1:10 p.m. - 4:30 p.m.	Caribbean V
Thursday, May 25		
	Time	Location
Registration	7:30 a.m. - 12:30 p.m.	Caribbean Reg East
Plenary Session	8:00 a.m. - 8:50 a.m.	Caribbean VI & VII
Technical Sessions	9:00 a.m. - 12:30 p.m.	Caribbean VI & VII, Boca I-III, Boca V-VII
<i>Exhibition and Break</i>	10:50 a.m. - 11:10 a.m.	Caribbean V

Plenary Session I

Monday AM
May 22, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: To Be Announced

8:00 AM Introductory Comments

8:10 AM Plenary

Accelerating Development of Materials with Artificial Intelligence: *James Saal¹; ¹Citrine Informatics*

8:50 AM Plenary

Advancing ICME Technologies Via Strategic Collaboration while Bridging the Gap Between Academia and Industry: *Ida Berglund¹; ¹QuesTek Europe AB*

9:30 AM Break

App: AM - Processing I

Monday AM
May 22, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: To Be Announced

9:50 AM Invited

Robotic Blacksmithing: Towards the Autonomous Control of Geometry and Microstructure Via Iterative, Open-die Forming: *Michael Groeber¹; Glenn Daehn¹; Stephen Niezgod¹; Tobias Mahan¹; Walt Hansen¹; ¹Ohio State University*

10:20 AM

Alloy Evaluation and Flow Forming Process Modeling for Net Shape Aerospace Structures: *Wesley Tayon¹; M. Mulvaney²; Elizabeth Urig²; ¹NASA Langley Research Center; ²University of Virginia*

10:40 AM

Building Explainable Models - Determining Process-structure-property Relationships for Friction Stir Processed Metals: *Moses Yeboah Obiri¹; ¹Pacific Northwest National Laboratory*

11:00 AM

Simulation of Dynamic Recrystallization in a 316L Stainless Steel Friction Stir Weld with Kinetic Monte Carlo Modeling: *William Frazier¹; Lei Li¹; Ayoub Soulami¹; Matthew Olszta¹; Donald Todd¹; Keerti Kappagantula¹; Neil Henson¹; Erin Barker¹; Eric Smith¹; ¹Pacific Northwest National Laboratory*

11:20 AM

HIP Diffusion Bonding Process Modeling for Fabrication of U-10Mo LEU Fuel: *Taylor Mason¹; Patrick Mcneff¹; Rajib Kalsar¹; Yucheng Fu¹; Kriston Brooks¹; Naveen Karri¹; Vineet Joshi¹; ¹Pacific Northwest National Laboratory*

AI/ML: Microstructure I

Monday AM
May 22, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: To Be Announced

9:50 AM Invited

HPC+AI@Edge Enabled Real-time Materials Characterization: *Mathew Cherukara¹; ¹Argonne National Laboratory*

10:20 AM

Microstructure-sensitive Materials Design via Efficient Uncertainty Propagation and Process-structure-property Linkages: *Vahid Attari¹; Dania Khatamsaz¹; Allison Kaye Ituralde Arabelo¹; Douglas Allaire¹; Raymundo Arroyave¹; ¹Texas A&M University*

10:40 AM

Deep Learning Enabled Additive Manufacturing (AM) Lattice Segmentation: *Michael Juhasz¹; Nick Calta¹; ¹Lawrence Livermore National Laboratory*

11:00 AM

A Deep Learning Approach for Phase Detection in 2D-XRD Patterns of Ti-6Al-4V: *WeiQi Yue¹; Pawan Tripathi¹; Nathaniel Tomczak¹; Gabriel Pono¹; Zhuldyz Ualikhankyzy¹; Matthew Willard¹; Vipin Chaudhary¹; Roger French¹; ¹Case Western Reserve University*

11:20 AM

Understanding Grain Growth Using a Physics-regularized Interpretable Machine Learning Model: *Joseph Melville¹; Vishal Yadav¹; Michael Tonks¹; Amanda Krause²; Joel Harley¹; ¹University of Florida; ²Carnegie Mellon University*

Mat Data & Platforms: I

Monday AM
May 22, 2023

Room: Boca V-VII
Location: Caribe Royale

Session Chair: To Be Announced

9:50 AM Invited

Materials Data & Informatics: Curation, Frameworks, Access, and Potential for Discovery and Design: *L. Catherine Brinson¹; ¹Duke University*

10:20 AM

FAIR Data in PMD: Development of MSE Mid-level and Standard-compliant Application Ontologies: *Markus Schilling¹; Bernd Bayerlein¹; Philipp von Hartrott²; Jörg Waitelonis³; Henk Birkholz⁴; Jannis Grundmann⁴; Pedro Portella²; Birgit Skrotzki¹; ¹Federal Ministry of Materials Research and Testing; ²Fraunhofer Institute for Mechanics of Materials; ³Leibniz Institute for Information Infrastructure; ⁴Leibniz-IWT Institut für Werkstofforientierte Technologien*

10:40 AM

Automatic Deducing the New Materials Knowledge within the OWL Framework: *Evgeny Blokhin¹; ¹Tilde Materials Informatics*

11:00 AM

NIST Interatomic Potentials Repository: Discovering, Evaluating and Comparing Interatomic Potentials: *Lucas Hale¹; ¹National Institute of Standards and Technology*

11:20 AM

Materials Commons and FAIR Data: *Glenn Tarcea¹; John Allison¹; Brian Puchala¹; Tracy Berman¹; ¹University of Michigan*

ICME for Non-Metals: I

Monday PM
May 22, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: To Be Announced

1:10 PM Invited

Multiscale Modeling of Structure-property Relationships in Highly Filled Thermoplastic Composites: *Karthik Rajan Venkatesan¹; John Hana¹; Samuel Owoeye²; Ajay Kadiyala²; Joseph Lawrence²; Ajay Krishnamurthy¹; ¹Eaton; ²University of Toledo*

1:40 PM**Multi-scale Modeling of Composites Manufacturing Processes:** *Huidi Ji*¹; Ross McLendon¹; Reinier Akkermans¹; ¹Dassault Systemes**2:00 PM****Integrated Framework for Cure-informed Progressive Damage and Failure Analysis of Composite Structures:** Minh Hoang Nguyen¹; *Royan Dmello*¹; Anthony Waas¹; ¹University of Michigan**2:20 PM****Simulating the Microstructure to Property Relationships with Multiscale Recursive Micromechanics:** *Evan Pineda*¹; Joshua Kempainen²; Jamal Hussein³; Brett Bednarczyk¹; William Pisani⁴; Gregory Odegard²; Scott Stapleton³; ¹NASA Glenn Research Center; ²Michigan Technological University; ³University of Massachusetts, Lowell; ⁴U.S. Army Engineer Research and Development Center**2:40 PM****Design of 3D-printed Nanocomposite Shields for Efficient EMI Shielding via Finite Element Modelling:** *Frederik Van Loock*¹; Patrick Anderson¹; Ruth Cardinaels¹; ¹TU Eindhoven**3:00 PM Break**

AI/ML: Properties I**Monday PM
May 22, 2023****Room: Boca I-III
Location: Caribe Royale***Session Chair:* To Be Announced**1:10 PM Invited****Artificial Intelligence and High-performance Data Mining for Accelerating Materials Discovery and Design:** *Ankit Agrawal*¹; ¹Northwestern University**1:40 PM****Managing Uncertainty in the Strength of Ceramics:** *Eric Walker*¹; Jason Sun¹; James Chen¹; ¹University at Buffalo**2:00 PM****Discovery of Multi-functional Polyimides through High-throughput Screening Using Explainable Machine Learning:** *Ying Li*¹; ¹University of Wisconsin-Madison**2:20 PM****A Machine Learning-based Virtual Lab to Predict Yield Surfaces from Crystal Plasticity Simulation:** *Anderson W Paiva do Nascimento*¹; Sharan Roongta²; Martin Diehl³; Irene Beyerlein¹; ¹University of California, Santa Barbara; ²Max-Planck-Institut für Eisenforschung; ³Katholieke Universiteit Leuven**2:40 PM****Intelligent Design & Manufacturing of High-performance Iron Castings Using AI/ML:** *Jiten Shah*¹; ¹Product Development and Analysis (PDA) LLC**3:00 PM Break**

ICME Des Tools: I**Monday PM
May 22, 2023****Room: Boca V-VII
Location: Caribe Royale***Session Chair:* To Be Announced**1:10 PM Invited****Designing Aerospace Components with Model-based Definitions to Enable Location-specific Tailoring of Properties:** *Michael Sangid*¹; Saikiran Gopalakrishnan¹; Ritwik Bandyopadhyay¹; ¹Purdue University**1:40 PM****ICME Design Approach Based on Multi-scale FEM, Phase-field and Ab-initio Simulations:** *Martin Persson*¹; Luis Reig Buades¹; Sandeep Kumar²; ¹Dassault Systemes, BIOVIA Ltd.; ²Dassault Systemes Simulia Corp**2:00 PM****Process Chaining to Enable a Material-informed Digital Twin Prototype for Marine Structures:** *Charles Fisher*¹; Thomas Gnaepel-Herold²; Suok-Min Na¹; Kelly Nygren³; Armand Beaudoin³; ¹Naval Surface Warfare Center - Carderock; ²National Institute of Standards and Technology; ³Cornell High Energy Synchrotron Source**2:20 PM****Simulated Microstructural Evolution and Tool Chain Development for Process Optimization of Cast & Wrought Nickel-base Superalloy Billet Material:** *Nicholas Krutz*¹; Pavanachand Chigurupati¹; Corey O'Connell¹; ¹PCC Metals**2:40 PM****Model-based Material and Process Definition Application to Aerospace Component Design and Lifting:** *Vasht Venkatesh*¹; Stephen Barker¹; Ryan Noraas¹; Michael McClure¹; Jean-Philippe Thomas¹; Sergei Burlatsky¹; David Furrer¹; ¹Pratt & Whitney**3:00 PM Break**

ICME Non-Metals: II**Monday PM
May 22, 2023****Room: Caribbean VI & VII
Location: Caribe Royale***Session Chair:* To Be Announced**3:20 PM****Data-driven Modeling for Service Lifetime Prediction of Acrylic Polymers:** *Hein Htet Aung*¹; Jayvic Cristian Jimenez²; Leean Jo¹; Roger French¹; Laura Bruckman¹; ¹Case Western Reserve University**3:40 PM****Multilevel Modelling and Optimization for Large Scale Additive Manufacturing:** *Christopher Bock*¹; Masoud Rais-Rohani¹; Brett Ellis¹; ¹University of Maine**4:00 PM****Development of a Computational Framework to Predict Resin Additive Manufacturing for Experimental Design:** *Joseph Leonor*¹; Evan Jones¹; Cheng Sun¹; Gregory Wagner¹; ¹Northwestern University**4:20 PM****Automation of the ICME Workflow Incorporating Material Digital Twins at Different Length Scales Within a Robust Information Management System:** *Brandon Hearley*¹; Steven Arnold¹; Marianna Maiaru²; ¹NASA Glenn Research Center; ²University of Massachusetts Lowell**4:40 PM****Design of Manufacturing Process of Polymer Composite Through Multiscale Cure Analysis Using Bayesian Optimization:** Yagnik Kalariya¹; Soban Babu Beemraj¹; *Amit Salvi*¹; ¹Tata Consultancy Services

AI/ML: Properties IIMonday PM
May 22, 2023Room: Boca I-III
Location: Caribe Royale

Session Chair: To Be Announced

3:20 PM**A Feasibility Study of Machine Learning-assisted Alloy Design:** Yasaman Soofi¹; Jinling Liu²; *Yijia Gu*¹; ¹Missouri University of Science and Technology**3:40 PM****Machine Intuitive Development of Army Steels - MIDAS:** *Heather Murdoch*¹; Levi McClenny¹; Benjamin Szajewski¹; Daniel Field¹; Berend Rinderspacher¹; Mulugeta Haile¹; Krista Limmer¹; Andrew Garza²; ¹U.S. Army Research Laboratory; ²UC Merced**4:00 PM****Analysis of AA6061 Cladding Diffusion Bonding Quality for the U-10Mo Monolithic Fuel Using Multi-fidelity Machine Learning Surrogate:** *Yucheng Fu*¹; Rajib Kalsar¹; Taylor Mason¹; Zhijie Xu¹; Kriston Brooks¹; Ayoub Soulami¹; Vineet Joshi¹; ¹Pacific Northwest National Laboratory**4:20 PM****Microstructural Engineering Towards Alloy Design:** *Ramanarayan Hariharaputran*¹; ¹Institute of High Performance Computing**4:40 PM****Generative Alloy Design Based Framework for In-silico Design of HSLA Steels:** *Akash Bhattacharjee*¹; KV Vamsi¹; Bilal Muhammed¹; Amol Joshi¹; Gerald Tennyson¹; BP Gautham¹; ¹TCS Research, Tata Consultancy Services Limited**Mat Data & Platform: II**Monday PM
May 22, 2023Room: Boca V-VII
Location: Caribe Royale

Session Chair: To Be Announced

3:20 PM**Database Design Strategies for Coordinated Simulation and Testing in Additive Manufacturing:** *Andrew Kitahara*¹; George Weber²; Samuel Hocker²; Brodan Richter²; Joshua Pribe¹; Edward Glaessgen²; ¹National Institute of Aerospace; ²National Aeronautics and Space Administration, Langley Research Center**3:40 PM****Applications of CALPHAD Based Tools to Additive Manufacturing:** Amer Malik¹; Minh Do Quang¹; Johan Jeppsson¹; *Andreas Markstrom*¹; Paul Mason¹; ¹Thermo-Calc Software**4:00 PM****Databasing Through the AM Pipeline: From Powder to Part:** *Srujana Rao Yarasi*¹; Elizabeth Holm¹; Amir Barati Farimani¹; Anthony Rollett¹; ¹Carnegie Mellon University**4:20 PM****CRADLE a Data Infrastructure for Printable Corrosion-resistant Alloys:** *Xiaoli Yan*¹; Pikee Priya¹; Phalgun Nelaturu²; Dan Thoma²; Santanu Chaudhuri³; ¹University of Illinois at Chicago; ²University of Wisconsin-Madison; ³Argonne National Laboratory**Scientific Workflows for ICME: I (Microstructure)**Tuesday AM
May 23, 2023Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: To Be Announced

8:00 AM Invited**NexusLIMS: A Laboratory Information Management System for Shared-use Electron Microscopy Facilities:** *June Lau*¹; ¹NIST**8:30 AM****Automated Analysis Pipeline to Investigate Bond-wire Corrosion Under Salt-water Exposure:** *Jayvic Cristian Jimenez*¹; Liangyi Huang²; Kristen J. Hernandez¹; Harsha Madiraju¹; Pawan K. Tripathi¹; Alp Sehrioglu¹; Roger H. French¹; ¹Case Western Reserve University; ²Arizona State University**8:50 AM****Microscopy Data Acquisition and Analysis Workflows for Microstructure Quantification:** *Michael Uchic*¹; ¹Air Force Research Laboratory**9:10 AM****Image Processing Pipeline for Fluoroelastomer Crystallite Detection in Atomic Force Microscopy Images:** *Mingjian Lu*¹; Sameera Venkat¹; Jube Augustino¹; Jayvic Jimenez²; Pawan Tripathi¹; Yinghui Wu¹; Roger French¹; Laura Bruckman¹; ¹Case Western Reserve University**9:30 AM****Towards Interoperability: Digital Representation of a Material Specific Characterization Method:** *Bernd Bayerlein*¹; Ghezal Ahmad Zia¹; Markus Schilling¹; Philipp von Hartrott²; Jörg Waitelonis³; Thomas Hanke²; Birgit Skrotzki¹; ¹Bundesanstalt für Materialforschung und -prüfung (BAM); ²Fraunhofer-Institut für Werkstoffmechanik (IWM); ³Leibniz-Institut für Informationsinfrastruktur (FIZ)**9:50 AM Break****AI/ML: Alloys**Tuesday AM
May 23, 2023Room: Boca I-III
Location: Caribe Royale

Session Chair: To Be Announced

8:00 AM Invited**Batch-wise Improvement in Reduced Design Space Using a Holistic Optimization Technique (BIRDSHOT):** *Raymundo Arroyave*¹; ¹Texas A&M University**8:30 AM****Elastic Constants Predictions in Multi-principal Element Alloys from DFT and Machine Learning:** *Nathan Linton*¹; Dilpuneet Aidhy¹; ¹Clemson University**8:50 AM****Charge-density Based Convolutional Neural Networks for Stacking Fault Energy Prediction in Concentrated Alloys:** Gaurav Arora¹; Serveh Kamrava²; Pejman Tahmesabi²; *Dilpuneet Aidhy*³; ¹University of Wyoming; ²Colorado School of Mines; ³Clemson University**9:10 AM****Predicting Mechanical Properties of Multicomponent Alloys Via a Hybrid Scheme of Heuristic Algorithms and Artificial Neural Network:** *Novana Hutasoit*¹; Ravindra Savangouder¹; ¹Swinburne University of Technology

9:30 AM

An Interpretable Machine Learning Model to Predict Molten Salt Corrosion of Compositionally Complex Alloys and Facilitate Understanding of Novel Corrosion Mechanisms: *Bonita Goh*; Yafei Wang¹; Phalgun Nelaturu²; Michael Moorehead³; Dan Thoma²; Santanu Chaudhuri⁴; Jason Hattrick-Simpers⁵; Kumar Sridharan²; Adrien Couet²; ¹Shanghai Jiaotong University; ²University of Wisconsin Madison; ³Idaho National Laboratory; ⁴University of Illinois - Urbana-Champaign; ⁵University of Toronto

9:50 AM Break

Linkages: Deformation I

Tuesday AM
May 23, 2023

Room: Boca V-VII
Location: Caribe Royale

Session Chair: To Be Announced

8:00 AM Invited

Computationally Derived Correlations for Process-induced Cracking During AM of Nickel-based Superalloys: *Hector Basoalto*¹; Chizhou Fang¹; Prashant Jadhav²; Magnus Anderson¹; Yu Lu¹; Lucia Scotti²; ¹University of Sheffield; ²University of Birmingham

8:30 AM

3D Full-field Crystal Plasticity Simulations on an Explicit Microstructure: How accurate are We: *Nikhil Prabhu*¹; Martin Diehl¹; ¹KU Leuven

8:50 AM

Validation of Crystal Plasticity Simulations using High-energy X-ray Diffraction Microscopy Measurements: *Saikumar Reddy Yeratapally*¹; George Weber²; Edward Glaessgen²; ¹National Institute of Aerospace; ²NASA Langley Research Center

9:10 AM

Integrated Computational Materials Engineering Toolkit to Understand Process-structure-property Relationships of Additively Manufactured Metals: *Matti Lindroos*¹; Napat Vajragupta¹; Tatu Pinomaa¹; Abhishek Biswas¹; Sicong Ren¹; Tom Andersson¹; Anssi Laukkanen¹; ¹VTT Research Centre of Finland

9:30 AM

Multi-scale Modeling of Dislocation Plasticity in Nano-architected Metals: *Phu Cuong Nguyen*¹; Ill Ryu¹; ¹University of Texas at Dallas

9:50 AM Break

AI/ML: Microstructure II

Tuesday AM
May 23, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: To Be Announced

10:10 AM

Microstructural Analysis of Stainless Steel SEM Images by Combining EBSD Data and Deep Learning: *Julia Nguyen*¹; Jenna Pope¹; Christina Doty¹; Marissa Gomez Hernandez¹; ¹PNNL

10:30 AM

Using Unsupervised Learning to Identify Small Crack Characteristics and Link to Fatigue Life: *Katelyn Jones*¹; Reji John²; Paul Shade²; William Musinski³; Elizabeth Holm¹; Anthony Rollett¹; ¹Carnegie Mellon University; ²Air Force Research Laboratory; ³University of Wisconsin Milwaukee

10:50 AM

Spatiotemporal Feature Extraction Using Deep Learning for Stress Corrosion Cracking in X-ray Computed Tomography Scans of Al-Mg Alloys: *Thomas Ciardi*¹; Pawan Tripathi¹; John Lewandowski¹; Roger French¹; ¹Case Western Reserve University

11:10 AM

Vapor Depression Segmentation and Absorptivity Prediction from Synchrotron X-ray Images Using Deep Neural Networks: *Runbo Jiang*¹; John Smith¹; Yu-Tsen Yi¹; Brian Simonds²; Tao Sun³; Anthony Rollett¹; ¹Carnegie Mellon University; ²National Institute of Standards and Technology; ³University of Virginia

11:30 AM

Towards Deep Learning of Dislocations from TEM Images: The Problem of "Never Enough Training Data": *Kishan Govind*¹; Marc Legros²; Stefan Sandfeld¹; Daniela Oliveros²; ¹Institute for Advanced Simulation; ²CEMES-CNRS

App: Alloy Des. I

Tuesday AM
May 23, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: To Be Announced

10:10 AM

Rapid Design of High-performance Refractory High Entropy Alloys Aided by Multiscale Modeling and Additive Manufacturing: *Michael Gao*¹; David Alman¹; Saro San¹; William Trehern¹; Chantal Sudbrack¹; Paul Jablonski¹; Vishnu Raghuraman²; Mike Widom²; Saket Thapliyal³; Michael Kirka³; ¹National Energy Technology Laboratory; ²Carnegie Mellon University; ³Oak Ridge National Laboratory

10:30 AM

Automated Hierarchical Screening of Refractory Multicomponent Alloys with High Intrinsic Ductility and Surface Passivation Potency: Aditya Sundar¹; Yong-Jie Hu²; *Liang Qi*¹; ¹University of Michigan; ²Drexel University

10:50 AM

Examining Phonon Transport in High Entropy Oxides: An Advanced Thermal Barrier Coating Material: *Prince Sharma*¹; Ganesh Balasubramanian¹; ¹Lehigh University

11:10 AM

A Computational Tool For Microstructure Development In Multicomponent Alloys During Additive Manufacturing: Christopher Hareland¹; Gildas Guillemot²; Charles-André Gandin²; *Peter Voorhees*¹; ¹Northwestern University; ²Mines ParisTech Sophia Antipolis

11:30 AM

Optimizing AgAuCuPdPt High Entropy Alloy Compositions as Efficient Catalysts for CO₂ Reduction Reaction: Chinmay Dahale¹; *Sriram Goverapet Srinivasan*¹; Beena Rai¹; ¹Tata Consultancy Services Ltd.

Sci Workflow: II

Tuesday AM
May 23, 2023

Room: Boca V-VII
Location: Caribe Royale

Session Chair: To Be Announced

10:10 AM

VPSC's New Clothes: Developing a Modern MATLAB API for Automating High-throughput VPSC Experiments: *Victoria Miller*¹; Benjamin Begley¹; ¹University of Florida

10:30 AM

PRISMS-Indentation: An Open-source Crystal Plasticity Finite Element Virtual Indentation Module: Aaron Tallman¹; Mohammadreza Yaghoobi²; ¹Florida International University; ²University of Michigan

10:50 AM

PRISMS-PF: An Open-source High-performance Phase-field Modeling Framework: David Montiel¹; Vishwas Goel¹; Mohammadreza Yaghoobi¹; John Allison¹; Katsuyo Thornton¹; ¹University of Michigan

11:10 AM

Uncertainty Reduction of Profilometry-based Indentation Plastometry Using Optical Profilometry: Astrid Rodriguez Negron¹; Denny John¹; Abhijith Sukumaran¹; Arvind Agarwal¹; Aaron Tallman¹; ¹Florida International University

11:30 AM

Uncertainty Quantification in Internal Stress Distribution Via Integrated High-energy Synchrotron X-ray Experiments and Crystal Plasticity Simulations: Divakar Naragan¹; Armand Beaudoin²; Donald Boyce²; Paul Shade³; ¹University of Dayton; ²Cornell University; ³AFRL

App.: AM Microstructure I

Tuesday PM
May 23, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: To Be Announced

1:20 PM

Multi-phase-field Simulation of Rapid Solidification in SUS316L Stainless Steel Using Artificial Neural Network-based Thermodynamic Calculation: Akinori Yamanaka¹; Masahito Segawa¹; Shoichiro Nakamura¹; ¹Tokyo University of Agriculture and Technology

1:40 PM

Microstructure Variability Prediction in Powder Bed Metal Additive Manufacturing: Aashique Rezwani¹; Theron Rodgers³; Daniel Moser¹; ¹Sandia National Laboratories

2:00 PM

Identifying Scaling Laws for Discretization Error in Process-Structure Simulations of Laser Powder Bed Fusion: Joshua Pribe¹; Brodan Richter²; Patrick Leser²; Edward Glaesgen²; ¹National Institute of Aerospace; ²NASA Langley Research Center

2:20 PM

Prediction of Prior Austenite Structure as a Function of Processing Parameters in Additively Processed High-strength Steel: Stephen Cluff¹; Clara Mock¹; Brandon McWilliams¹; ¹DEVCOM Army Research Laboratory

2:40 PM Break

App.: AM Processing II

Tuesday PM
May 23, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: To Be Announced

1:20 PM

Statistical Learning Approaches for Predicting Pore Formation from In-situ Characterization for Additive Manufacturing of SS 316L Using Laser Powder Bed Fusion: Erika Barcelos¹; Nathaniel Tomczak¹; Jayvic Jimenez¹; Sameera Venka¹; Kristen Hernandez²; Raymond Wieser¹; John Lewandowski¹; Laura Bruckman¹; Roger French¹; ¹CWRU

1:40 PM

On the Applicability of CALPHAD and Process Modelling to Predict Solidification Cracking: Mustafa Megahed¹; Klaus Büßenschütt²; Philipp Stich³; Markus Apel⁴; Ludo Bautmans⁵; Christian Haase²; ¹ESI Group; ²RWTH Aachen; ³EOS GmbH; ⁴Access Technology; ⁵Oerlikon

2:00 PM

A Physics-based Correlation Study of Hot Cracking Phenomenon in the Processes of Additive Manufacturing: Guannan Tang¹; Anthony Rollett¹; ¹Carnegie Mellon University

2:20 PM

Prediction of Solidification Cracking for Additively Manufactured Rene 80 Superalloy by Directed Energy Deposition: Hamed Hosseinzadeh¹; Lang Yuan¹; Luke Mohr²; Lee Kerwin²; Anindya Bhaduri³; Arushi Dhakad³; Chen Shen³; Shenyan Huang³; Changjie Sun³; Alexander L Kitt²; ¹University of South Carolina; ²Buffalo Engineering Works; ³General Electric Research

2:40 PM Break

ICME Design Tools: II

Tuesday PM
May 23, 2023

Room: Boca V-VII
Location: Caribe Royale

Session Chair: To Be Announced

1:20 PM

Development of a Roadmap for Computational Materials-informed Qualification and Certification of Process Intensive Metallic Materials: Edward Glaesgen¹; Michael Gorelik²; ¹NASA Langley Research Center; ²Federal Aviation Administration

1:40 PM

Accelerating Development and Characterization of Nuclear Materials Processing: An Integrated Methodology: Erin Barker¹; Eric Smith¹; David Brown¹; Neil Henson¹; Keerti Kappagantula¹; Donald Todd¹; ¹Pacific Northwest National Laboratory

2:00 PM

Evolution of Model-based Material Definitions: David Furrer¹; Dennis Dimiduck²; Charles Ward³; ¹Pratt & Whitney; ²BlueQuartz LLC; ³IMMI Journal

2:20 PM

Model-based Material and Process Definitions for Additive Component Design and Qualification: Somnath Ghosh¹; Anthony Rollett²; David Furrer³; ¹Johns Hopkins University; ²Carnegie Mellon University; ³Pratt & Whitney

2:40 PM Break

Linkages: Microstructure I

Tuesday PM
May 23, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: To Be Announced

3:00 PM

Simulations Showing the Formation of Grooves and Ledges Over \947' Precipitates During High-temperature Creep: A Dynamically Coupled Discrete Dislocation Dynamics and Phase-field Model: Tushar Jog¹; Markus Stricker¹; ¹Ruhr-University Bochum

3:20 PM

Phase Field Modeling Investigation of Polycrystalline Grain Growth Using a Spherical-Gaussian-based 5-D Computational Approach: Lenissongui Yeo¹; Michael Costa¹; Jacob Bair¹; ¹Oklahoma State University

3:40 PM

Unravelling the Ultrahigh Modulus of Resilience of Core-shell SU-8 Nanocomposite Nanopillars Fabricated by Vapor-Phase Infiltration: *Ying Li*¹; ¹University of Wisconsin-Madison

4:00 PM

Predicting the Metallurgical Bond at the Interface Between Two Aluminum Sheets Joined Using High-velocity Riveting Through Finite Element and Molecular Dynamics: *Ayoub Soulami*¹; Daniel Ramirez-Tamayo¹; Krishna Pitike¹; Lei Li¹; Benjamin Schuessler¹; Sridhar Niverty¹; Vineet Joshi¹; ¹Pacific Northwest National Laboratory

Linkages: Processing I

Tuesday PM
May 23, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: To Be Announced

3:00 PM

Modeling Defect Generation During Production of Single Crystal Sapphire: *Peter Raninger*¹; Masoud Sistaninia¹; Werner Ebl¹; Georg Reiss¹; Sina Lohrasbi²; Christoph Gammer³; ¹Materials Center Leoben Forschung GmbH; ²FAMETEC GmbH; ³Erich Schmid Institute of Materials Science, Austrian Academy of Sciences

3:20 PM

Study of the Critical Angle for Nucleation of Different Shape of Nanoparticles in an Aluminium Alloy: *Ane Jimenez*¹; Mario Alfredo Renderos²; Eva Anglada¹; Franck Giroit²; Maider Garcia de Cortazar¹; ¹TECNALIA, Basque Research and Technology Alliance (BRTA); ²University of the Basque Country (UPV/EHU)

3:40 PM

Cellular Automaton Simulation of Microstructure and Porosity Formation During Solidification Processing of Aluminum Alloys: Michael Moodispaw¹; Buwei Chen¹; Nicole Trometer¹; *Alan Luo*¹; ¹Ohio State University

4:00 PM

On the Origin of Dendrite Misorientation in Ni-based Single Crystal Superalloy: *Huxiang Xia*¹; Qingyan Xu¹; ¹Tsinghua University

ICME Design Tools: III

Tuesday PM
May 23, 2023

Room: Boca V-VII
Location: Caribe Royale

Session Chair: To Be Announced

3:00 PM

The Alloy Optimization Software (TAOS): Application to HEAs: *Aurelien Perron*¹; Brandon Bocklund¹; Vincenzo Lordi¹; ¹Lawrence Livermore National Laboratory

3:20 PM

Digital Transformation of Materials Enabled and Accelerated by ICME: *Jason Sebastian*¹; ¹QuesTek Innovations LLC

3:40 PM

The Role of Computational Materials Design in the Circular Economy of Materials: *Paul Mason*¹; Anders Engstrom¹; ¹Thermo-Calc Software

4:00 PM

An ICME Framework for Design of Hot-rolled Nb,Ti Microalloyed Steels: *Surya Ardham*¹; Akash Bhattacharjee¹; Sandeep Pusuluri¹; Srimannarayana Pusuluri¹; Harisankar R¹; Pravin Kumar¹; Sarbari Ganguly²; Yadvendra²; Appa Rao Chintha²; Monojit Dutta²; Gautham BP¹; Gerald Tennyson¹; ¹TCS research; ²Tata Steel

Plenary Session II

Wednesday AM
May 24, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: To Be Announced

8:00 AM Plenary

The Multiple Facets of ICME in Modern Manufacturing at Brunswick Boat Group and Mercury Marine: *Adam Kopper*¹; ¹Mercury Marine

8:40 AM Plenary

ExtremeMat: Quantification of the Effect of Microstructure and Composition on the Creep Rupture Life of Steels: *Laurent Capolungo*¹; Arul Kumar¹; Ricardo Lebensohn¹; Andrea Rovinelli¹; Paul Christodoulou²; Yuki Yamamoto³; ¹Los Alamos National Laboratory; ²UCSB; ³ORNL

9:20 AM Break

Linkages: Microstructure II

Wednesday AM
May 24, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: To Be Announced

9:40 AM

Plastic Deformation and Failure Predictions of Al-6061 With Inhomogeneities Using Finite Element Modeling Techniques Across Different Length Scales: *Nicole Aragon*¹; Aashique Rezwani¹; Ill Ryu²; Hojun Lim¹; ¹Sandia National Laboratories; ²The University of Texas at Dallas

10:00 AM

Numerical Characterization of the Effect of Precipitates on the Creep Responses of Steel Alloys: *Mariyappan Arul Kumar*¹; Laurent Capolungo¹; ¹Los Alamos National Laboratory

10:20 AM

Nanoscale Precipitation Strengthening Mechanisms in CoCrNi-based Medium Entropy Alloys: *Ning Zhang*¹; Charles Matlock¹; ¹Baylor University

10:40 AM

An ICME Workflow to Assess the Process Sensitivity of the Heat Treatment of IN718: Taiwu Yu¹; Thomas Barkar¹; Carl-Magnus Lancelot¹; *Paul Mason*¹; ¹Thermo-Calc Software

11:00 AM

A New AI/ML Framework for Materials Innovation: *Surya Kalidindi*¹; ¹Georgia Institute of Technology

AI/ML: Microstructure III

Wednesday AM
May 24, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: To Be Announced

9:40 AM

Chemistry and Processing Prediction for Targeted Microstructure Morphology: *Mahmood Mamivand*¹; Amir Abbas Kazemzadeh Farizhandi¹; ¹Boise State University

10:00 AM

A Data-driven Approach for Estimating Three-dimensional Microstructural Features of Bainitic Steels Using Phase-field Simulation Results: *Dhanunjaya Kumar Nerella*¹; Ingo Steinbach¹; ¹Ruhr University Bochum

10:20 AM

Predicting Laser Powder Bed Fusion Microstructures Using Machine Learning: *Gregory Wong*¹; Anthony Rollett¹; Gregory Rohrer¹; ¹Carnegie Mellon University

10:40 AM

Application of Deep Learning Object Detection and Image Segmentation Code Such as YOLO and U-Net for Detection of Helium Bubbles and Voids in Nuclear Reactor Materials: *Shradha Agarwal*¹; Sydney Copp¹; July Reyes¹; Steven Zinkle¹; ¹University of Tennessee and Oak Ridge National Laboratory

11:00 AM

ICME for DNA-templated Dye Aggregate Design for Quantum Information Applications: *Lan Li*¹; ¹Boise State University

New & Emerging

Wednesday AM
May 24, 2023

Room: Boca V-VII
Location: Caribe Royale

Session Chair: To Be Announced

9:40 AM

A Quantitative Phase Field Tool for Lithium-metal Battery Design: *Jin Zhang*¹; Alexander Chadwick¹; Peter Voorhees¹; ¹Northwestern University

10:00 AM

Influence Of Interfacial Voids And Grain Boundary Conductivity On Depletion Kinetics Of Sodium Metal Anodes In All-solid-state Batteries: *Sourav Chatterjee*¹; Michael Tonks¹; Will Gardner²; Marina Sessim²; ¹University of Florida; ²QuantumScape

10:20 AM

Machine Learning Driven Prediction of Capacity Fade in Lithium-ion Batteries: *Abhinand Ayyaswamy*¹; Bairav Sabarish Vishnugopi¹; Partha P Mukherjee¹; ¹Purdue University

10:40 AM

From Li Atom to Battery Pack: Integrated Multiscale Simulation: *Felix Hanke*¹; Nils Modrow¹; Victor Oancea¹; Hamidreza Hajiyani¹; Nehzat Safaei¹; Johan Carlsson¹; ¹Dassault Systemes

11:00 AM

Molecular Modelling of Locally Concentrated Electrolytes for Lithium-ion Batteries: *Mahesh Mynam*¹; Saurav Chandel¹; Beena Rai¹; ¹TCS Research, Tata Consultancy Services Ltd.

11:20 AM

Multiscale Study of the Influence of Electrolyte on the System Level Performance of Na Ion Batteries: Saurav Chandel¹; *Vamsi Krishna Garapati*¹; Naga Neehar Dingari¹; Mahesh Mynam¹; Beena Rai¹; ¹Tata Consultancy Services (TCS) Research

Linkages: Deformation II

Wednesday PM
May 24, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: To Be Announced

1:10 PM Invited

Simulating Phenomena of Industrial Rolling via Gleeble Compression for Calibration of an Aluminum Processing Model: *Jeffrey Tschirhart*¹; Chal Park¹; Aaditya Lakshmanan¹; Sazol Das¹; ¹Novelis

1:40 PM

The Through-process Texture Analysis of Non-grain-oriented Electrical Steel: *Masoud Sistaninia*¹; Peter Raninger¹; Petri Prevedel¹; Paul Angerer¹; Herbert Kreuzer²; Thomas Antretter³; ¹Materials Center Leoben Forschung GmbH; ²voestalpine Stahl GmbH; ³Montanuniversitaet Leoben

2:00 PM

Smoothed Particle Hydrodynamics Model for Friction Stir Processing of 316 L Stainless Steel: Process Modeling and Microstructure Prediction: *Lei Li*¹; Ayoub Soulami¹; Donald Todd¹; Neil Henson¹; Erin Barker¹; Eric Smith¹; ¹Pacific Northwest National Laboratory

2:20 PM

Microstructural Evolution During Closed Die Forging of UDIMET720 and Prediction of Mechanical Properties: *Christian Gruber*¹; Flora Godor¹; Aleksandar Stanojevic¹; Jürgen Krobath²; Peter Raninger²; Martin Stockinger³; ¹voestalpine BÖHLER Aerospace GmbH & Co KG; ²Materials Center Leoben Forschung GmbH; ³Montanuniversität Leoben

2:40 PM

ICME and ML Framework to Predict the Microstructure During U-10Mo Fuel Fabrication: *Ayoub Soulami*¹; Yucheng Fu¹; William Frazier¹; Kyoo Sil Choi¹; Lei Li¹; Zhijie Xu¹; Curt Lavender¹; Vineet Joshi¹; ¹Pacific Northwest National Laboratory

3:00 PM Break

App.: AM Microstructure II

Wednesday PM
May 24, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: To Be Announced

1:10 PM Invited

Multi-scale Microstructure Predictions and Phase Transformations in Additively Manufactured Ti-6Al-4V Using a Hybrid Kinetic Monte Carlo – Phase Field Method: *Bonnie Whitney*¹; Anthony Spangenberg¹; Diana Lados¹; ¹Worcester Polytechnic Institute

1:40 PM

3D Phase-field Modelling of Microstructure Evolution During Additive Manufacturing of Multi-component Single Crystal Ni-based Super Alloys: *Murali Uddagiri*¹; Ingo Steinbach¹; ¹Ruhr University Bochum

2:00 PM

The Potency of Alloy Composition on the 316L Solidification Path in Fusion-based Additive Manufacturing: *Joseph Aroh*¹; Anthony Rollett¹; ¹Carnegie Mellon University

2:20 PM

Columnar to Equiaxed Transition During Solidification Under Additive Manufacturing Conditions: *Bala Radhakrishnan*¹; Tahany EL-Wardany²; Ranadip Acharya³; ¹Oak Ridge National Laboratory; ²Raytheon Technologies Research Center; ³Collins Aerospace

2:40 PM

Composition-microstructure Control of in-situ Alloying Using Laser Powder-bed Fusion Additive Manufacturing: High-fidelity Thermal-chemical-fluid-microstructure Modelling: *Junji Shinjo*¹; Chinnapat Panwisawas²; ¹Shimane University; ²Queen Mary University of London

3:00 PM Break

Linkages: Microstructure III

Wednesday PM
May 24, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: To Be Announced

3:20 PM

Modeling Coupled Chemo-mechanical Fracture in DAMASK: *Sharan Roongta*¹; Pratheek Shanthraj²; Martin Diehl³; Franz Roters¹; ¹Max-Planck-Institut für Eisenforschung; ²University of Manchester; ³KU Leuven

3:40 PM

Microstructure Informed Modelling of Ductile-to-brittle Transition in Ferritic Steels: *Sicong Ren*¹; Bernard Marini²; Pierre Forget²; Matti Lindroos¹; Anssi Laukkanen¹; ¹VTT Technical Research Centre of Finland Ltd.; ²CEA Paris-Saclay

4:00 PM

Enabling Molecular Dynamics Simulations of Helium Bubble Formation in Tritium-containing Austenitic Stainless Steels: An Fe-Ni-Cr-H-He Potential: *Xiaowang Zhou*¹; Michael Foster¹; Ryan Sills²; ¹Sandia National Laboratories; ²Rutgers University

4:20 PM

Multi-scale Microstructure Evolution Informed Constitutive Behavior Modeling of Cast Iron: *Ujjal Tewary*¹; Shyamprasad Karagadde²; Alankar Alankar²; Goutam Mohapatra¹; Satyam Sahay¹; Indradev Samajdar²; ¹John Deere India Pvt. Ltd.; ²Indian Institute of Technology Bombay

App.: AM Processing III

Wednesday PM
May 24, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: To Be Announced

3:20 PM

Multiphysics Modeling of Ti-based Composite Direct Energy Deposition for Analyzing the Dynamics of Nano-sized Reinforcing Particles: *Mingyu Chung*¹; Kang Hyun Lee¹; Yeon Su Lee¹; Gun jin Yun¹; ¹Seoul National University

3:40 PM

Coupled Thermal-solidification Process Simulation of Sapphire Growth: *Raluca Trasca*¹; Werner Ebl¹; Georg Reiss¹; Sina Lohrasbi²; ¹Materials Center Leoben Forschung GmbH; ²FAMETEC GmbH

4:00 PM

Multiscale Modeling of Metal Vaporization/Condensation in Manufacturing Processes: *Scott Muller*¹; Andrew Ritzmann¹; Floyd Hilty¹; W Rosenthal¹; Lance Hubbard¹; Matthew Olszta¹; ¹Pacific Northwest National Laboratory

4:20 PM

Impact of Dendrite Tip Velocity Formulation on Simulated Microstructures of Powder Bed Fusion Ti-6Al-4V: *Brodan Richter*¹; Joshua Pribe²; Edward Glaessgen¹; ¹NASA Langley Research Center; ²National Institute of Aerospace

Plenary Session III

Thursday AM
May 25, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: To Be Announced

8:00 AM Introductory Comments

8:10 AM Plenary

MPMD ICME Industry Implementation Award: Multi-scale Approach for Developing a High Silicon Al-Si-Cu Alloy for Additive Manufacturing Supercharger Rotors: *Andrew Bobel*¹; Yoojin Kim²; Lee Casalena³; Anil Sachdev¹; ¹General Motors Corporation; ²Populus Group; ³Thermo Fisher Scientific

8:50 AM Break

ICME for Non-Metals: III

Thursday AM
May 25, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: To Be Announced

9:00 AM Invited

Multiscale Modeling and Machine Learning-based Digital Twin for Piezocomposite Damage Sensing: *Somnath Ghosh*¹; ¹Johns Hopkins University

9:30 AM

True Multiscale Simulations of Virtual Coupon Tests in Composites.: *Kedar Malusare*¹; Kennedy Neves¹; Luiz Lima¹; Flavio Souza¹; ¹Siemens

9:50 AM

Damage Prediction of Sintered a-SiC Using Thermo-mechanical Coupled Fracture Model: *Jason Sun*¹; Joseph Marziale¹; James Chen¹; ¹University at Buffalo

10:10 AM

Machine-learned Structural Descriptors for Metallic and Covalent Glassy Materials: *Thomas Hardin*¹; ¹Sandia National Laboratories

10:30 AM

Design of Titanium Aluminum Reinforced with TiB₂ Composite for Powder Manufacturing Using Integrated Computational Materials Engineering: *Ayodeji Afolabi*¹; Peter Olubambi¹; ¹University of Johannesburg

10:50 AM Break

ICME Des Tools: IV

Thursday AM
May 25, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: To Be Announced

9:00 AM Invited

An ICME Based Approach for Improving High-strength Ni Alloy Process Yield: *Shankarjee Krishnamoorthi*¹; Vahid Tari¹; John Foltz¹; Ramesh Minisandram¹; ¹ATI Specialty Materials

9:30 AM

ICME Modeling of Can Body Stock: Waqas Muhammad¹; Abhijit Brahme¹; Kaan Inal¹; *Chal Park*²; Aaditya Lakshmanan²; Sazol Das²; ¹University of Waterloo; ²Novelis

9:50 AM

Digital Threads for FAST Processing: *Lucia Scott*¹; Martin Jackson¹; Oliver Levano Blanch²; Beatriz Fernandez Silva²; Sam Lister¹; Prashant Jadhav¹; Hugh Banes¹; Magnus Anderson¹; Hector Basoalto¹; ¹University of Sheffield; ²Rolls-Royce Plc

10:10 AM

Machine Learning-enhanced Robust Co-design Exploration for Many Objective, Multilevel Materials Design Problems: *Anand Balu Nellippallil*¹; Mathew Baby¹; Rashmi Rama Sushil²; Palaniappan Ramu²; Janet K. Allen³; Farrokh Mistree³; ¹Florida Institute of Technology; ²IIT Madras; ³University of Oklahoma

10:30 AM

Integrating Crystal Plasticity and Thermo-mechanical Constitutive Modeling: *Anderson W Paiva do Nascimento*¹; Akhilesh Pedgaonkar²; Curt Bronkhorst²; Irene Beyerlein¹; ¹University of California, Santa Barbara; ²University of Wisconsin-Madison

10:50 AM Break

App: Alloy Des. II

Thursday AM
May 25, 2023Room: Boca V-VII
Location: Caribe Royale

Session Chair: To Be Announced

9:00 AM Invited

Cruden_PLACEHOLDER: *David Cruden*¹; ¹Alloyed Inc.

9:30 AM

Material And Process Parameter Optimization for Additive Manufacturing Using High-throughput Kinetic Simulations: *Evgeniya Kabliman*¹; Nora Barschkett¹; Sebastian Tonatiuh Carrion Ständer¹; ¹Technical University of Munich

9:50 AM

Computational Modeling of the Microstructure Evolution in the Mo-V Binary Alloy System: *Abhishek Thakur*¹; Sasa Kovacevic²; Krishna Muralidharan³; ¹The University of Arizona; ²Imperial College London; ³University of Arizona

10:10 AM

Sustainable Aluminum Alloy Design Using Physics-informed Machine Learning: *Fatih Sen*¹; Marat Latypov¹; Heath Murphy¹; Dasha Artsykhovska¹; Kyle Haines¹; Shruthi Raj¹; Aurele Mariaux¹; Sazol Das¹; Yudie Yuan¹; Vishwanath Hegadekatte¹; ¹Novelis

10:30 AM

ICMD: ICME-based Genomic Materials Design: *Jiadong Gong*¹; ¹Questek Innovations LLC

10:50 AM Break

Linkages: Deformation III

Thursday AM
May 25, 2023Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: To Be Announced

11:10 AM

Parametrically-upscaled Crack Nucleation Model(PUCNM) for Fatigue Nucleation in Ti Alloys Containing Micro-texture Regions: *Somnath Ghosh*¹; ¹Johns Hopkins University

11:30 AM

Designing Fatigue Resistance of Metallic Alloys with a Hybrid of Deep Learning and Micromechanics: *Anssi Laukkanen*¹; Matti Lindroos¹; Tom Andersson¹; Napat Vajragupta¹; Tatu Pinomaa¹; Sicong Ren¹; Abhishek Biswas¹; Tomi Suhonen¹; ¹VTT Technical Research Center of Finland

11:50 AM

A Phenomenological Model for the Relationship Between Fatigue Life and Mechanical Properties: *Emiel Amsterdam*¹; *Borit Zwerink*¹; ¹NLR

12:10 PM

Evaluation of Stochastic Safe Life of a DP Steel Component Subjected to Fatigue Using a Micromechanics Based Approach: *Srimannarayana P*¹; *Harisankar K.R.*¹; *Akash Gupta*¹; *K.V. Vamsi*¹; *Gerald Tennyson*¹; *B.P. Gautham*¹; ¹Tata Consultancy Services Limited

App: AM Microstructure III

Thursday AM
May 25, 2023Room: Boca I-III
Location: Caribe Royale

Session Chair: To Be Announced

11:10 AM

Discrete Dislocation Dynamics Simulation Analysis of Plasticity and Size Effect in Additive Manufactured Metals: *Caizhi Zhou*¹; ¹University of South Carolina

11:30 AM

A Physics-Informed Multimodal Conditional Generative Model for Linking Process and Microstructure in Metal Additive Manufacturing: *Kang-Hyun Lee*¹; Min Gyu Chung¹; Yeon Su Lee²; Gun Jin Yun¹; ¹Seoul National University

11:50 AM

Development of Digital Model Predicting Mechanical Properties of Inconel 718 for Powder Based Additive Manufacturing: *Parimal Maity*¹; Mohit Singhal¹; Jacob Kallivayalil²; ¹Eaton India Innovation Center; ²Eaton Corporation

12:10 PM

Directed Energy Deposition of Al-0.5Sc-0.5Si Alloy: Effect of Thermal Cycles in Microstructure and Mechanical Properties: *Amit Singh*¹; *Yasham Mundada*¹; *Priyanshu Bajaj*²; *Sushil Mishra*³; *Amit Arora*¹; ¹Indian Institute of Technology Gandhinagar; ²m4p material solutions GmbH; ³Indian Institute of Technology Bombay

App.: AM Processing IV

Thursday AM
May 25, 2023Room: Boca V-VII
Location: Caribe Royale

Session Chair: To Be Announced

11:10 AM

High-throughput Computation and Process Design for Metal Additive Manufacturing: *Sofia Sheikh*¹; Brent Vela¹; Pejman Honarmandi¹; Peter Morcos¹; David Shoukr¹; Abdelrahman Kotb¹; Ibrahim Karaman¹; Alaa Karaman¹; Raymundo Arroyave¹; ¹Texas A&M University

11:30 AM

Computational Design and Modelling of Nickel-based Alumindes High Entropy Alloys: *Peter Odetola*¹; Peter Olubambi¹; ¹University of Johannesburg

11:50 AM

Effect of Cooling Rates on the Evolution of Microstructure, Phase Transformation, and Strain in Ti-6Al-4V Studied by High Speed Synchrotron X-ray Diffraction: *Rajib Halder¹; Seunghye Oh¹; Anthony Rollett¹; Andrew Chuang²; ¹Carnegie Mellon University; ²Argonne National Laboratory*

12:10 PM

An Integrated Process-structure-property Framework for In-silico Design of Additively Manufactured 18Ni-300 Maraging Steels: *Akash Bhattacharjee¹; Pravin Kumar¹; Himanshu Nirgudkar¹; Surya Ardham¹; Pramod Zagade¹; Gerald Tennyson¹; BP Gautham¹; ¹TCS Research, Tata Consultancy Services Limited*

Poster Session

Tuesday PM
May 23, 2023

Room: Caribbean V
Location: Caribe Royale

Session Chair: To Be Announced

A Framework for Multilevel Robust Co-design of Material and Product Systems: *Mathew Baby¹; Anand Balu Nellippallil¹; ¹Florida Institute of Technology*

A Software Approach to Predict Creep Behavior in Time and Temperature Dependent Materials: *Abdullah Kose¹; Irina Viktorova¹; Muhammed Kose¹; Garrett Pataky¹; Sofya Alekseeva¹; Leo Rebholz¹; ¹Clemson University*

Automated Characterization of Generated Meltpool from High Speed Camera: *Kristen Hernandez¹; John Lewandowski¹; Roger French¹; Laura Bruckman¹; Jayvic Jimenez¹; Thomas Ciardi¹; Sameera Venkat¹; ¹Case Western Reserve University*

Computational Simulations on Behavior of UHPC Subjected to Chloride Ingress: *Jun Wang¹; Yail Jimmy Kim¹; ¹University of Colorado Denver*

A Generative Adversarial Network for the Creation of Complex 3D Bimodal Polycrystalline Microstructures: Application to Cold-spray Al7050 Alloy: *Brayan Murgas¹; Joshua Stickel¹; Somnath Ghosh¹; ¹Johns Hopkins University*

Ab-initio Modelling of Phonon Transport in 2D High Entropy MXene Layers: *Prince Sharma¹; Ganesh Balasubramanian¹; ¹Lehigh University*

Decision Support System for Device Fabrication: *Neelanshi Wadhwa¹; Sapan Shah¹; Deepak Jain¹; Sreedhar Reddy¹; Beena Rai¹; ¹Tata Consultancy Services*

Deformation Behavior in Core-Shell Heterostructured Materials: *Hyoung Seop Kim¹; ¹Pohang University of Science and Technology*

Material Data Scraping and Automatic Curation: *Vinod Kumar Mannaru¹; Shrikant Tarte¹; Om Singh²; Eaton¹; ²NIT Trichy*

Joining of Dissimilar Metals for High-speed Electric Motor Applications: A Molecular Dynamics Study: *Jiayi Chen¹; Johannes Nokelainen²; Bernardo Barbiellini²; Hemantha Yeddu¹; ¹LUT University; ²Northeastern University*

Development of a Fully Anisotropic Monte Carlo Potts Model to Study Grain Growth: *Lin Yang¹; Vishal Yadav¹; Michael Tonks¹; ¹University of Florida*

Micromechanical Modeling of Cyclic Damage in Metallic Materials: *Gururaj Gopal Rao¹; Leslie T Mushongera¹; ¹University of Nevada, Reno*

Irradiance Simulation of Real World Field for PV Backsheets Degradation: *Zelin Li¹; Raymond Wieser¹; Xuanji Yu¹; Laura Bruckman¹; ¹Case Western Reserve University*

Fluoroelastomer Crystallization Kinetics Studied by Deep Learning Segmentation of Atomic Force Microscopy Images: *Sameera Nalin Venkat¹; Thomas Ciardi¹; Jube Augustino¹; Jayvic Jimenez¹; Peter Schlueter¹; Mingjian Lu¹; Frank Ernst¹; Yinghui Wu¹; Roger French¹; Laura Bruckman¹; ¹Case Western Reserve University*

Geospatiotemporal Modeling of Near Subsurface Temperatures of the Continental United States for Assessment of Materials Degradation: *Deepa Bhuvanagiri¹; Hope Omodolor¹; Erika Barcelos¹; Vibha Mandayam¹; Sameera Nalin Venkat¹; R. Mohan Srivastava¹; Roger French¹; Jeffrey Yarus¹; ¹Case Western Reserve University*

Discriminative Object Tracking by Domain Contrast: *Huayue Cai¹; Xiang Zhang¹; Long Lan¹; Changcheng Xiao¹; Chuanfu Xu¹; Jie Liu¹; Zhigang Luo¹; ¹National University of Defense Technology*

Effects of Surface Segregations in Catalytic AgAuCuPdPt High Entropy Alloy: *Chinmay Dahale¹; Soumyadipta Maiti¹; Sriram Srinivasan¹; Beena Rai¹; ¹TCS Research, TRDDC*

Finite Volume Based Multi-contact Modeling to Study Detailed Mechanical Response of an Elastic Material: *Ranjan Dhakal¹; Philip Cardiff²; ¹Graz University of Technology; ²University College Dublin*

Enhancement of Grain Refinement and Heat Resistance in Tib2-Reinforced Tial Matrix Composite Powder Manufactured by Spark Plasma Sintering: *Ayodeji Afolabi¹; Peter Olubambi¹; ¹University of Johannesburg*

First-principles and Data-driven Discovery of High-entropy Alloys for Corrosion Protection: *Andrew Neils¹; Nathan Post¹; Cheng Zeng¹; Jack Lesko¹; ¹The Roux Institute at Northeastern University*

Microstructure-based Modelling Approach to Determine Hydrogen Diffusion and Trapping in Steels: *Maribel Arribas¹; Ana Rosa Carrillo¹; Ane Jimenez¹; Jean Baptiste Jorcin¹; ¹Tecnalia Research & Innovation*

Phase Field Simulation of Heat Treatment Process for Single Crystal Ni-based Superalloy: *Yeyuan Hu¹; Qingyan Xu¹; ¹Tsinghua University*

Ontology-based Digital Representations of Materials Testing in the Material Digital Initiative: *Hossein Beygi Nasrabadi¹; Thomas Hanke²; Miriam Eisenbart³; Matthias Weber²; Roy Meissner⁴; Gordian Dziwis⁴; Yue Chen¹; Birgit Skrotzki¹; ¹Bundesanstalt für Materialforschung und -prüfung (BAM); ²Fraunhofer-Institut für Werkstoffmechanik (IWM); ³Forschungsinstitut Edelmetalle + Metallchemie (fem); ⁴Institut für Angewandte Informatik (InfAI)*

Predicting the Performance Degradation of Advanced Devices Exposed to Ionizing Radiation: *Xiaoyu Guan¹; Michael Tonks¹; ¹University of Florida*

Tensile Loading Modelling of Laser-deposited AlCoCrFeNiCu High Entropy Alloy Using Comsol Multiphysics: *Modupeola Dada¹; Patricia Popoola¹; ¹Tshwane University of Technology*

The Effects of Orientation and Temperature on Deformation Mechanisms in Single-crystalline CrCoNi: *Charles Matlock¹; Ning Zhang¹; ¹Baylor University*

Modeling the Effects of Short Range Order on Initial Passivation in Binary Alloys: *Alex Tai¹; John Cavin¹; Ian McCue¹; Karl Sieradzki²; ¹Northwestern University; ²Arizona State University*

Predicting Grain Morphology in LBPF Haynes 282 with Complex Geometry via ICME Approach: *Yu-Tsen Yi¹; Junwon Seo¹; Anthony Rollett¹; ¹Carnegie Mellon University*

Quantitative Precipitate Analysis of an Age-hardenable Aluminium Alloy Using a Deep Learning Approach: *Ghezal Ahmad Jan Zia¹; ¹BAM*

Modelling of Carbides in Irradiated Steel Microstructure: *Andris Freimanis*¹; *Matti Lindroos*¹; *Anssi Laukkanen*¹; *Sicong Ren*¹; ¹VTT Technical research center of Finland

Pushing the Limits of Deep Learning for Synthetic Image Generation of Titanium Alloy Microstructures in Limited Data Regime: *Gowtham Nimmal Haribabu*¹; *Jeyapriya J*¹; *Chiranjib Bhattacharya*²; *Bikramjit Basu*¹; ¹Indian Institute of Science; ²Indian Institute of Technology

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 Agrawal, A. 4
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