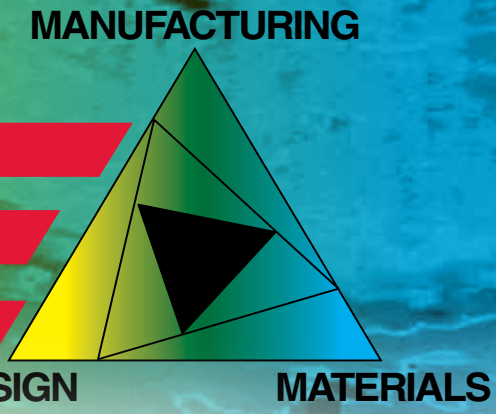
TMS ICME



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.

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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
Exhibition and Break	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
Exhibition and Break	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
Exhibition and Break	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
Exhibition and Break	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
Exhibition and Break	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
Exhibition and Break	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
Exhibition and Break	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 Saal*[1]; [1]Citrine Informatics

8:50 AM Plenary
Advancing ICME Technologies Via Strategic Collaboration while Bridging the Gap Between Academia and Industry: *Ida Berglund*[1]; [1]QuesTek 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 Groeber*[1]; Glenn Daehn[1]; Stephen Niezgoda[1]; Tobias Mahan[1]; Walt Hansen[1]; [1]Ohio State University

10:20 AM
Alloy Evaluation and Flow Forming Process Modeling for Net Shape Aerospace Structures: *Wesley Tayon*[1]; M. Mulvaney[2]; Elizabeth Urig[2]; [1]NASA Langley Research Center; [2]University of Virginia

10:40 AM
Building Explainable Models - Determining Process-structure-property Relationships for Friction Stir Processed Metals: *Moses Yeboah Obiri*[1]; [1]Pacific Northwest National Laboratory

11:00 AM
Simulation of Dynamic Recrystallization in a 316L Stainless Steel Friction Stir Weld with Kinetic Monte Carlo Modeling: *William Frazier*[1]; Lei Li[1]; Ayoub Soulami[1]; Matthew Olszta[1]; Donald Todd[1]; Keerti Kappagantula[1]; Neil Henson[1]; Erin Barker[1]; Eric Smith[1]; [1]Pacific Northwest National Laboratory

11:20 AM
HIP Diffusion Bonding Process Modeling for Fabrication of U-10Mo LEU Fuel: *Taylor Mason*[1]; Patrick Mcneff[1]; Rajib Kalsar[1]; Yucheng Fu[1]; Kriston Brooks[1]; Naveen Karri[1]; Vineet Joshi[1]; [1]Pacific 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 Cherukara*[1]; [1]Argonne National Laboratory

10:20 AM
Microstructure-sensitive Materials Design via Efficient Uncertainty Propagation and Process-structure-property Linkages: *Vahid Attari*[1]; Danial Khatamsaz[1]; Allison Kaye Ituralde Arabelo[1]; Douglas Allaire[1]; Raymundo Arroyave[1]; [1]Texas A&M University

10:40 AM
Deep Learning Enabled Additive Manufacturing (AM) Lattice Segmentation: *Michael Juhasz*[1]; Nick Calta[1]; [1]Lawrence Livermore National Laboratory

11:00 AM
A Deep Learning Approach for Phase Detection in 2D-XRD Patterns of Ti-6Al-4V: *Weiqi Yue*[1]; Pawan Tripathi[1]; Nathaniel Tomczak[1]; Gabriel Ponon[1]; Zhuldyz Ualikhankyzy[1]; Matthew Willard[1]; Vipin Chaudhary[1]; Roger French[1]; [1]Case Western Reserve University

11:20 AM
Understanding Grain Growth Using a Physics-regularized Interpretable Machine Learning Model: Joseph Melville[1]; Vishal Yadav[1]; *Michael Tonks*[1]; Amanda Krause[2]; Joel Harley[1]; [1]University of Florida; [2]Carnegie 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 Brinson*[1]; [1]Duke University

10:20 AM
FAIR Data in PMD: Development of MSE Mid-level and Standard-compliant Application Ontologies: *Markus Schilling*[1]; Bernd Bayerlein[1]; Philipp von Hartrott[2]; Jörg Waitelonis[3]; Henk Birkholz[4]; Jannis Grundmann[4]; Pedro Portella[2]; Birgit Skrotzki[1]; [1]Federal Ministry of Materials Research and Testing; [2]Fraunhofer Institute for Mechanics of Materials; [3]Leibniz Institute for Information Infrastructure; [4]Leibniz-IWT Institut für Werkstofforientierte Technologien

10:40 AM
Automatic Deducing the New Materials Knowledge within the OWL Framework: *Evgeny Blokhin*[1]; [1]Tilde Materials Informatics

11:00 AM
NIST Interatomic Potentials Repository: Discovering, Evaluating and Comparing Interatomic Potentials: *Lucas Hale*[1]; [1]National Institute of Standards and Technology

11:20 AM
Materials Commons and FAIR Data: *Glenn Tarcea*[1]; John Allison[1]; Brian Puchala[1]; Tracy Berman[1]; [1]University 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 Venkatesan*[1]; John Hana[1]; Samuel Owoeye[2]; Ajay Kadiyala[2]; Joseph Lawrence[2]; Ajay Krishnamurthy[1]; [1]Eaton; [2]University of Toledo

1:40 PM
Multi-scale Modeling of Composites Manufacturing Processes: *Huidi Ji*[1]; Ross McLendon[1]; Reinier Akkermans[1]; [1]Dassault Systemes

2:00 PM
Integrated Framework for Cure-informed Progressive Damage and Failure Analysis of Composite Structures: Minh Hoang Nguyen[1]; *Royan Dmello*[1]; Anthony Waas[1]; [1]University of Michigan

2:20 PM
Simulating the Microstructure to Property Relationships with Multiscale Recursive Micromechanics: *Evan Pineda*[1]; Joshua Kemppainen[2]; Jamal Husseini[3]; Brett Bednarcyk[1]; William Pisani[4]; Gregory Odegard[2]; Scott Stapleton[3]; [1]NASA Glenn Research Center; [2]Michigan Technological University; [3]University of Massachusetts, Lowell; [4]U.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 Anderson[1]; Ruth Cardinaels[1]; [1]TU 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]; [1]Northwestern University

1:40 PM
Managing Uncertainty in the Strength of Ceramics: *Eric Walker*[1]; Jason Sun[1]; James Chen[1]; [1]University at Buffalo

2:00 PM
Discovery of Multi-functional Polyimides through High-throughput Screening Using Explainable Machine Learning: *Ying Li*[1]; [1]University 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 Roongta[2]; Martin Diehl[3]; Irene Beyerlein[1]; [1]University of California, Santa Barbara; [2]Max-Planck-Institut für Eisenforschung; [3]Katholieke Universiteit Leuven

2:40 PM
Intelligent Design & Manufacturing of High-performance Iron Castings Using AI/ML: *Jiten Shah*[1]; [1]Product 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 Gopalakrishnan[1]; Ritwik Bandyopadhyay[1]; [1]Purdue University

1:40 PM
ICME Design Approach Based on Multi-scale FEM, Phase-field and Ab-initio Simulations: *Martin Persson*[1]; Luis Reig Buades[1]; Sandeep Kumar[2]; [1]Dassault Systemes, BIOVIA Ltd.; [2]Dassault Systemes Simulia Corp

2:00 PM
Process Chaining to Enable a Material-informed Digital Twin Prototype for Marine Structures: *Charles Fisher*[1]; Thomas Gnaepel-Herold[2]; Suok-Min Na[1]; Kelly Nygren[3]; Armand Beaudoin[3]; [1]Naval Surface Warfare Center - Carderock; [2]National Institute of Standards and Technology; [3]Cornell 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 Chigurupati[1]; Corey O'Connell[1]; [1]PCC Metals

2:40 PM
Model-based Material and Process Definition Application to Aerospace Component Design and Lifing: *Vasisht Venkatesh*[1]; Stephen Barker[1]; Ryan Noraas[1]; Michael McClure[1]; Jean-Philippe Thomas[1]; Sergei Burlatsky[1]; David Furrer[1]; [1]Pratt & 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 Jimenez[1]; Leean Jo[1]; Roger French[1]; Laura Bruckman[1]; [1]Case Western Reserve University

3:40 PM
Multilevel Modelling and Optimization for Large Scale Additive Manufacturing: *Christopher Bock*[1]; Masoud Rais-Rohani[1]; Brett Ellis[1]; [1]University of Maine

4:00 PM
Development of a Computational Framework to Predict Resin Additive Manufacturing for Experimental Design: *Joseph Leonor*[1]; Evan Jones[1]; Cheng Sun[1]; Gregory Wagner[1]; [1]Northwestern 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 Arnold[1]; Marianna Maiaru[2]; [1]NASA Glenn Research Center; [2]University of Massachusetts Lowell

4:40 PM
Design of Manufacturing Process of Polymer Composite Through Multiscale Cure Analysis Using Bayesian Optimization: Yagnik Kalariya[1]; Soban Babu Beemaraj[1]; *Amit Salvi*[1]; [1]Tata Consultancy Services

AI/ML: Properties II

Monday PM
May 22, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: To Be Announced

3:20 PM
A Feasibility Study of Machine Learning-assisted Alloy Design: Yasaman Soofi[1]; Jinling Liu[1]; *Yijia Gu*[1]; [1]Missouri University of Science and Technology

3:40 PM
Machine Intuitive Development of Army Steels - MIDAS: *Heather Murdoch*[1]; Levi McClenny[1]; Benjamin Szajewski[1]; Daniel Field[1]; Berend Rinderspacher[1]; Mulugeta Haile[1]; Krista Limmer[1]; Andrew Garza[2]; [1]U.S. Army Research Laboratory; [2]UC 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 Kalsar[1]; Taylor Mason[1]; Zhijie Xu[1]; Kriston Brooks[1]; Ayoub Soulami[1]; Vineet Joshi[1]; [1]Pacific Northwest National Laboratory

4:20 PM
Microstructural Engineering Towards Alloy Design: *Ramanarayan Hariharaputran*[1]; [1]Institute of High Performance Computing

4:40 PM
Generative Alloy Design Based Framework for In-silico Design of HSLA Steels: *Akash Bhattacharjee*[1]; KV Vamsi[1]; Bilal Muhammed[1]; Amol Joshi[1]; Gerald Tennyson[1]; BP Gautham[1]; [1]TCS Research, Tata Consultancy Services Limited

Mat Data & Platform: II

Monday PM
May 22, 2023

Room: 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 Weber[2]; Samuel Hocker[2]; Brodan Richter[2]; Joshua Pribe[1]; Edward Glaessgen[2]; [1]National Institute of Aerospace; [2]National Aeronautics and Space Administration, Langley Research Center

3:40 PM
Applications of CALPHAD Based Tools to Additive Manufacturing: Amer Malik[1]; Minh Do Quang[1]; Johan Jeppsson[1]; *Andreas Markstrom*[1]; Paul Mason[1]; [1]Thermo-Calc Software

4:00 PM
Databasing Through the AM Pipeline: From Powder to Part: *Srujana Rao Yarasi*[1]; Elizabeth Holm[1]; Amir Barati Farimani[1]; Anthony Rollett[1]; [1]Carnegie Mellon University

4:20 PM
CRADLE a Data Infrastructure for Printable Corrosion-resistant Alloys: *Xiaoli Yan*[1]; Pikee Priya[1]; Phalgun Nelaturu[2]; Dan Thoma[2]; Santanu Chaudhuri[3]; [1]University of Illinois at Chicago; [2]University of Wisconsin–Madison; [3]Argonne National Laboratory

Scientific Workflows for ICME: I (Microstructure)

Tuesday AM
May 23, 2023

Room: 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]; [1]NIST

8:30 AM
Automated Analysis Pipeline to Investigate Bond-wire Corrosion Under Salt-water Exposure: *Jayvic Cristian Jimenez*[1]; Liangyi Huang[2]; Kristen J. Hernandez[1]; Harsha Madiraju[1]; Pawan K. Tripathi[1]; Alp Sehirlioglu[1]; Roger H. French[1]; [1]Case Western Reserve University; [2]Arizona State University

8:50 AM
Microscopy Data Acquisition and Analysis Workflows for Microstructure Quantification: *Michael Uchic*[1]; [1]Air Force Research Laboratory

9:10 AM
Image Processing Pipeline for Fluoroelastomer Crystallite Detection in Atomic Force Microscopy Images: *Mingjian Lu*[1]; Sameera Venkat[1]; Jube Augustino[1]; Jayvic Jimenez[1]; Pawan Tripathi[1]; Yinghui Wu[1]; Roger French[1]; Laura Bruckman[1]; [1]Case Western Reserve University

9:30 AM
Towards Interoperability: Digital Representation of a Material Specific Characterization Method: *Bernd Bayerlein*[1]; Ghezal Ahmad Zia[1]; Markus Schilling[1]; Philipp von Hartrott[2]; Jörg Waitelonis[3]; Thomas Hanke[2]; Birgit Skrotzki[1]; [1]Bundesanstalt für Materialforschung und -prüfung (BAM); [2]Fraunhofer-Institut für Werkstoffmechanik (IWM); [3]Leibniz-Institut für Informationsinfrastruktur (FIZ)

9:50 AM Break

AI/ML: Alloys

Tuesday AM
May 23, 2023

Room: 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]; [1]Texas A&M University

8:30 AM
Elastic Constants Predictions in Multi-principal Element Alloys from DFT and Machine Learning: *Nathan Linton*[1]; Dilpuneet Aidhy[1]; [1]Clemson University

8:50 AM
Charge-density Based Convolutional Neural Networks for Stacking Fault Energy Prediction in Concentrated Alloys: Gaurav Arora[1]; Serveh Kamrava[2]; Pejman Tahmesabi[2]; *Dilpuneet Aidhy*[3]; [1]University of Wyoming; [2]Colorado School of Mines; [3]Clemson 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 Savangouder[1]; [1]Swinburne 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 Wang[1]; Phalgun Nelaturu[2]; Michael Moorehead[3]; Dan Thoma[2]; Santanu Chaudhuri[4]; Jason Hattrick-Simpers[5]; Kumar Sridharan[2]; Adrien Couet[2]; [1]Shanghai Jiaotong University; [2]University Of Wisconsin Madison; [3]Idaho National Laboratory; [4]University of Illinois - Urbana-Champaign; [5]University 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 Fang[1]; Prashant Jadhav[2]; Magnus Anderson[1]; Yu Lu[1]; Lucia Scotti[2]; [1]University of Sheffield; [2]University of Birmingham

8:30 AM
3D Full-field Crystal Plasticity Simulations on an Explicit Microstructure: How accurate are We: *Nikhil Prabhu*[1]; Martin Diehl[1]; [1]KU Leuven

8:50 AM
Validation of Crystal Plasticity Simulations using High-energy X-ray Diffraction Microscopy Measurements: *Saikumar Reddy Yeratapally*[1]; George Weber[2]; Edward Glaessgen[2]; [1]National Institute of Aerospace; [2]NASA 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 Vajragupta[1]; Tatu Pinomaa[1]; Abhishek Biswas[1]; Sicong Ren[1]; Tom Andersson[1]; Anssi Laukkanen[1]; [1]VTT Research Centre of Finland

9:30 AM
Multi-scale Modeling of Dislocation Plasticity in Nano-architectected Metals: *Phu Cuong Nguyen*[1]; Ill Ryu[1]; [1]University 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 Pope[1]; Christina Doty[1]; Marissa Gomez Hernandez[1]; [1]PNNL

10:30 AM
Using Unsupervised Learning to Identify Small Crack Characteristics and Link to Fatigue Life: *Katelyn Jones*[1]; Reji John[2]; Paul Shade[2]; William Musinski[3]; Elizabeth Holm[1]; Anthony Rollett[1]; [1]Carnegie Mellon University; [2]Air Force Research Laboratory; [3]University 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 Tripathi[1]; John Lewandowski[1]; Roger French[1]; [1]Case 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 Smith[1]; Yu-Tsen Yi[1]; Brian Simonds[2]; Tao Sun[3]; Anthony Rollett[1]; [1]Carnegie Mellon University; [2]National Institute of Standards and Technology; [3]University of Virginia

11:30 AM
Towards Deep Learning of Dislocations from TEM Images: The Problem of "Never Enough Training Data": *Kishan Govind*[1]; Marc Legros[2]; Stefan Sandfeld[1]; Daniela Oliveros[2]; [1]Institute for Advanced Simulation; [2]CEMES-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 Alman[1]; Saro San[1]; William Trehern[1]; Chantal Sudbrack[1]; Paul Jablonski[1]; Vishnu Raghuraman[2]; Mike Widom[2]; Saket Thapliyal[3]; Michael Kirka[3]; [1]National Energy Technology Laboratory; [2]Carnegie Mellon University; [3]Oak Ridge National Laboratory

10:30 AM
Automated Hierarchical Screening of Refractory Multicomponent Alloys with High Intrinsic Ductility and Surface Passivation Potency: Aditya Sundar[1]; Yong-Jie Hu[2]; *Liang Qi*[1]; [1]University of Michigan; [2]Drexel University

10:50 AM
Examining Phonon Transport in High Entropy Oxides: An Advanced Thermal Barrier Coating Material: *Prince Sharma*[1]; Ganesh Balasubramanian[1]; [1]Lehigh University

11:10 AM
A Computational Tool For Microstructure Development In Multicomponent Alloys During Additive Manufacturing: Christopher Hareland[1]; Gildas Guillemot[2]; Charles-André Gandin[2]; *Peter Voorhees*[1]; [1]Northwestern University; [2]Mines ParisTech Sophia Antipolis

11:30 AM
Optimizing AgAuCuPdPt High Entropy Alloy Compositions as Efficient Catalysts for CO_2 Reduction Reaction: Chinmay Dahale[1]; *Sriram Goverapet Srinivasan*[1]; Beena Rai[1]; [1]Tata 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 Begley[1]; [1]University of Florida

10:30 AM
PRISMS-Indentation: An Open-source Crystal Plasticity Finite Element Virtual Indentation Module: *Aaron Tallman*[1]; Mohammadreza Yaghoobi[2]; [1]Florida International University; [2]University of Michigan

10:50 AM
PRISMS-PF: An Open-source High-performance Phase-field Modeling Framework: *David Montiel*[1]; Vishwas Goel[1]; Mohammadreza Yaghoobi[1]; John Allison[1]; Katsuyo Thornton[1]; [1]University of Michigan

11:10 AM
Uncertainty Reduction of Profilometry-based Indentation Plastometry Using Optical Profilometry: *Astrid Rodriguez Negron*[1]; Denny John[1]; Abhijith Sukumaran[1]; Arvind Agarwal[1]; Aaron Tallman[1]; [1]Florida International University

11:30 AM
Uncertainty Quantification in Internal Stress Distribution Via Integrated High-energy Synchrotron X-ray Experiments and Crystal Plasticity Simulations: *Diwakar Naragani*[1]; Armand Beaudoin[2]; Donald Boyce[2]; Paul Shade[3]; [1]University of Dayton; [2]Cornell University; [3]AFRL

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 Yamanaka*[1]; Masahito Segawa[1]; Shoichiro Nakamura[1]; [1]Tokyo University of Agriculture and Technology

1:40 PM
Microstructure Variability Prediction in Powder Bed Metal Additive Manufacturing: *Aashique Rezwan*[1]; Theron Rodgers[1]; Daniel Moser[1]; [1]Sandia National Laboratories

2:00 PM
Identifying Scaling Laws for Discretization Error in Process-Structure Simulations of Laser Powder Bed Fusion: *Joshua Pribe*[1]; Brodan Richter[2]; Patrick Leser[2]; Edward Glaessgen[2]; [1]National Institute of Aerospace; [2]NASA Langley Research Center

2:20 PM
Prediction of Prior Austenite Structure as a Function of Processing Parameters in Additively Processed High-strength Steel: *Stephen Cluff*[1]; Clara Mock[1]; Brandon Mcwilliams[1]; [1]DEVCOM 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 Barcelos*[1]; Nathaniel Tomczak[1]; Jayvic Jimenez[1]; Sameera Venka[1]; Kristen Hernandez[1]; Raymond Wieser[1]; John Lewandowski[1]; Laura Bruckman[1]; Roger French[1]; [1]CWRU

1:40 PM
On the Applicability of CALPHAD and Process Modelling to Predict Solidification Cracking: *Mustafa Megahed*[1]; Klaus Büßenschütt[2]; Philipp Stich[3]; Markus Apel[4]; Ludo Bautmans[5]; Christian Haase[2]; [1]ESI Group; [2]RWTH Aachen; [3]EOS GmbH; [4]Access Technology; [5]Oerlikon

2:00 PM
A Physics-based Correlation Study of Hot Cracking Phenomenon in the Processes of Additive Manufacturing: *Guannan Tang*[1]; Anthony Rollett[1]; [1]Carnegie Mellon University

2:20 PM
Prediction of Solidification Cracking for Additively Manufactured Rene 80 Superalloy by Directed Energy Deposition: *Hamed Hosseinzadeh*[1]; Lang Yuan[1]; Luke Mohr[2]; Lee Kerwin[2]; Anindya Bhaduri[3]; Arushi Dhakad[3]; Chen Shen[3]; Shenyan Huang[3]; Changjie Sun[3]; Alexander L Kitt[2]; [1]University of South Carolina; [2]Buffalo Engineering Works; [3]General 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 Glaessgen*[1]; Michael Gorelik[2]; [1]NASA Langley Research Center; [2]Federal Aviation Administration

1:40 PM
Accelerating Development and Characterization of Nuclear Materials Processing: An Integrated Methodology: *Erin Barker*[1]; Eric Smith[1]; David Brown[1]; Neil Henson[1]; Keerti Kappagantula[1]; Donald Todd[1]; [1]Pacific Northwest National Laboratory

2:00 PM
Evolution of Model-based Material Definitions: *David Furrer*[1]; Dennis Dimiduck[2]; Charles Ward[3]; [1]Pratt & Whitney; [2]BlueQuartz LLC; [3]IMMI Journal

2:20 PM
Model-based Material and Process Definitions for Additive Component Design and Qualification: *Somnath Ghosh*[1]; Anthony Rollett[2]; David Furrer[3]; [1]Johns Hopkins University; [2]Carnegie Mellon University; [3]Pratt & 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 Jogi*[1]; Markus Stricker[1]; [1]Ruhr-University Bochum

3:20 PM
Phase Field Modeling Investigation of Polycrystalline Grain Growth Using a Spherical-Gaussian-based 5-D Computational Approach: *Lenissongui Yeo*[1]; Michael Costa[1]; Jacob Bair[1]; [1]Oklahoma 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]; [1]University 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-Tamayo[1]; Krishna Pitike[1]; Lei Li[1]; Benjamin Schuessler[1]; Sridhar Niverty[1]; Vineet Joshi[1]; [1]Pacific Northwest National Laboratory

Linkages: Processing I

Tuesday PM **Room: Boca I-III**
May 23, 2023 **Location: Caribe Royale**

Session Chair: To Be Announced

3:00 PM
Modeling Defect Generation During Production of Single Crystal Sapphire: *Peter Raninger*[1]; Masoud Sistaninia[1]; Werner Eßl[1]; Georg Reiss[1]; Sina Lohrasbi[2]; Christoph Gammer[3]; [1]Materials Center Leoben Forschung GmbH; [2]FAMETEC GmbH; [3]Erich 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 Renderos[2]; Eva Anglada[1]; Franck Girot[2]; Maider Garcia de Cortazar[1]; [1]TECNALIA, Basque Research and Technology Alliance (BRTA); [2]University of the Basque Country (UPV/EHU)

3:40 PM
Cellular Automaton Simulation of Microstructure and Porosity Formation During Solidification Processing of Aluminum Alloys: Michael Moodispaw[1]; Buwei Chen[1]; Nicole Trometer[1]; *Alan Luo*[1]; [1]Ohio State University

4:00 PM
On the Origin of Dendrite Misorientation in Ni-based Single Crystal Superalloy: *Huxiang Xia*[1]; Qingyan Xu[1]; [1]Tsinghua University

ICME Design Tools: III

Tuesday PM **Room: Boca V-VII**
May 23, 2023 **Location: Caribe Royale**

Session Chair: To Be Announced

3:00 PM
The Alloy Optimization Software (TAOS): Application to HEAs: *Aurelien Perron*[1]; Brandon Bocklund[1]; Vincenzo Lordi[1]; [1]Lawrence Livermore National Laboratory

3:20 PM
Digital Transformation of Materials Enabled and Accelerated by ICME: *Jason Sebastian*[1]; [1]QuesTek Innovations LLC

3:40 PM
The Role of Computational Materials Design in the Circular Economy of Materials: *Paul Mason*[1]; Anders Engstrom[1]; [1]Thermo-Calc Software

4:00 PM
An ICME Framework for Design of Hot-rolled Nb,Ti Microalloyed Steels: *Surya Ardham*[1]; Akash Bhattacharjee[1]; Sandeep Pusuluri[1]; Srimannarayana Pusuluri[1]; Harisankar R[1]; Pravin Kumar[1]; Sarbari Ganguly[2]; Yadvendra[2]; Appa Rao Chintha[2]; Monojit Dutta[2]; Gautham BP[1]; Gerald Tennyson[1]; [1]TCS research; [2]Tata Steel

Plenary Session II

Wednesday AM **Room: Caribbean VI & VII**
May 24, 2023 **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]; [1]Mercury 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 Kumar[1]; Ricardo Lebensohn[1]; Andrea Rovinelli[1]; Paul Christodoulou[2]; Yuki Yamamoto[3]; [1]Los Alamos National Laboratory; [2]UCSB; [3]ORNL

9:20 AM Break

Linkages: Microstructure II

Wednesday AM **Room: Caribbean VI & VII**
May 24, 2023 **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 Rezwan[1]; Ill Ryu[2]; Hojun Lim[1]; [1]Sandia National Laboratories; [2]The 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 Capolungo[1]; [1]Los Alamos National Laboratory

10:20 AM
Nanoscale Precipitation Strengthening Mechanisms in CoCrNi-based Medium Entropy Alloys: *Ning Zhang*[1]; Charles Matlock[1]; [1]Baylor University

10:40 AM
An ICME Workflow to Assess the Process Sensitivity of the Heat Treatment of IN718: Taiwu Yu[1]; Thomas Barkar[1]; Carl-Magnus Lancelot[1]; *Paul Mason*[1]; [1]Thermo-Calc Software

11:00 AM
A New AI/ML Framework for Materials Innovation: *Surya Kalidindi*[1]; [1]Georgia Institute of Technology

AI/ML: Microstructure III

Wednesday AM **Room: Boca I-III**
May 24, 2023 **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 Farizhandi[1]; [1]Boise 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 Steinbach[1]; [1]Ruhr University Bochum

10:20 AM
Predicting Laser Powder Bed Fusion Microstructures Using Machine Learning: *Gregory Wong*[1]; Anthony Rollett[1]; Gregory Rohrer[1]; [1]Carnegie 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 Copp[1]; July Reyes[1]; Steven Zinkle[1]; [1]University of Tennessee and Oak Ridge National Laboratory

11:00 AM
ICME for DNA-templated Dye Aggregate Design for Quantum Information Applications: *Lan Li*[1]; [1]Boise State University

New & Emerging

Wednesday AM **Room: Boca V-VII**
May 24, 2023 **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 Chadwick[1]; Peter Voorhees[1]; [1]Northwestern 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 Tonks[1]; Will Gardner[2]; Marina Sessim[2]; [1]University of Florida; [2]QuantumScape

10:20 AM
Machine Learning Driven Prediction of Capacity Fade in Lithium-ion Batteries: *Abhinand Ayyaswamy*[1]; Bairav Sabarish Vishnugopi[1]; Partha P Mukherjee[1]; [1]Purdue University

10:40 AM
From Li Atom to Battery Pack: Integrated Multiscale Simulation: *Felix Hanke*[1]; Nils Modrow[1]; Victor Oancea[1]; Hamidreza Hajiyani[1]; Nehzat Safaei[1]; Johan Carlsson[1]; [1]Dassault Systemes

11:00 AM
Molecular Modelling of Locally Concentrated Electrolytes for Lithium-ion Batteries: *Mahesh Mynam*[1]; Saurav Chandel[1]; Beena Rai[1]; [1]TCS 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 Chandel[1]; *Vamsi Krishna Garapati*[1]; Naga Neehar Dingari[1]; Mahesh Mynam[1]; Beena Rai[1]; [1]Tata Consultancy Services (TCS) Research

Linkages: Deformation II

Wednesday PM **Room: Caribbean VI & VII**
May 24, 2023 **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 Park[1]; Aaditya Lakshmanan[1]; Sazol Das[1]; [1]Novelis

1:40 PM
The Through-process Texture Analysis of Non-grain-oriented Electrical Steel: *Masoud Sistaninia*[1]; Peter Raninger[1]; Petri Prevedel[1]; Paul Angerer[1]; Herbert Kreuzer[2]; Thomas Antretter[3]; [1]Materials Center Leoben Forschung Gmbh; [2]voestalpine Stahl GmbH; [3]Montanuniversitaet 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 Soulami[1]; Donald Todd[1]; Neil Henson[1]; Erin Barker[1]; Eric Smith[1]; [1]Pacific Northwest National Laboratory

2:20 PM
Microstructural Evolution During Closed Die Forging of UDIMET720 and Prediction of Mechanical Properties: *Christian Gruber*[1]; Flora Godor[1]; Aleksandar Stanojevic[1]; Jürgen Krobath[2]; Peter Raninger[2]; Martin Stockinger[3]; [1]voestalpine BÖHLER Aerospace GmbH & Co KG; [2]Materials Center Leoben Forschung GmbH; [3]Montanuniversität Leoben

2:40 PM
ICME and ML Framework to Predict the Microstructure During U-10Mo Fuel Fabrication: *Ayoub Soulami*[1]; Yucheng Fu[1]; William Frazier[1]; Kyoo Sil Choi[1]; Lei Li[1]; Zhijie Xu[1]; Curt Lavender[1]; Vineet Joshi[1]; [1]Pacific Northwest National Laboratory

3:00 PM Break

App.: AM Microstructure II

Wednesday PM **Room: Boca I-III**
May 24, 2023 **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 Spangenberger[1]; Diana Lados[1]; [1]Worcester 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 Steinbach[1]; [1]Ruhr University Bochum

2:00 PM
The Potency of Alloy Composition on the 316L Solidification Path in Fusion-based Additive Manufacturing: *Joseph Aroh*[1]; Anthony Rollett[1]; [1]Carnegie Mellon University

2:20 PM
Columnar to Equiaxed Transition During Solidification Under Additive Manufacturing Conditions: *Bala Radhakrishnan*[1]; Tahany El-Wardany[2]; Ranadip Acharya[3]; [1]Oak Ridge National Laboratory; [2]Raytheon Technologies Research Center; [3]Collins 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 Panwisawas[2]; [1]Shimane University; [2]Queen 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 Shanthraj[2]; Martin Diehl[3]; Franz Roters[1]; [1]Max-Planck-Institut für Eisenforschung; [2]University of Manchester; [3]KU Leuven

3:40 PM
Microstructure Informed Modelling of Ductile-to-brittle Transition in Ferritic Steels: *Sicong Ren*[1]; Bernard Marini[2]; Pierre Forget[2]; Matti Lindroos[1]; Anssi Laukkanen[1]; [1]VTT Technical Research Centre of Finland Ltd.; [2]CEA 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 Foster[1]; Ryan Sills[2]; [1]Sandia National Laboratories; [2]Rutgers University

4:20 PM
Multi-scale Microstructure Evolution Informed Constitutive Behavior Modeling of Cast Iron: *Ujjal Tewary*[1]; Shyamprasad Karagadde[2]; Alankar Alankar[2]; Goutam Mohapatra[1]; Satyam Sahay[1]; Indradev Samajdar[2]; [1]John Deere India Pvt. Ltd.; [2]Indian 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 Lee[1]; Yeon Su Lee[1]; Gun jin Yun[1]; [1]Seoul National University

3:40 PM
Coupled Thermal-solidification Process Simulation of Sapphire Growth: *Raluca Trasca*[1]; Werner Eßl[1]; Georg Reiss[1]; Sina Lohrasbi[2]; [1]Materials Center Leoben Forschung GmbH; [2]FAMETEC GmbH

4:00 PM
Multiscale Modeling of Metal Vaporization/Condensation in Manufacturing Processes: *Scott Muller*[1]; Andrew Ritzmann[1]; Floyd Hilty[1]; W Rosenthal[1]; Lance Hubbard[1]; Matthew Olszta[1]; [1]Pacific 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 Pribe[2]; Edward Glaessgen[1]; [1]NASA Langley Research Center; [2]National 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 Kim[2]; Lee Casalena[3]; Anil Sachdev[1]; [1]General Motors Corporation; [2]Populus Group; [3]Thermo 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]; [1]Johns Hopkins University

9:30 AM
True Multiscale Simulations of Virtual Coupon Tests in Composites.: *Kedar Malusare*[1]; Kennedy Neves[1]; Luiz Lima[1]; Flavio Souza[1]; [1]Siemens

9:50 AM
Damage Prediction of Sintered a-SiC Using Thermo-mechanical Coupled Fracture Model: *Jason Sun*[1]; Joseph Marziale[1]; James Chen[1]; [1]University at Buffalo

10:10 AM
Machine-learned Structural Descriptors for Metallic and Covalent Glassy Materials: *Thomas Hardin*[1]; [1]Sandia 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 Olubambi[1]; [1]University 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 Tari[1]; John Foltz[1]; Ramesh Minisandram[1]; [1]ATI Specialty Materials

9:30 AM
ICME Modeling of Can Body Stock: Waqas Muhammad[1]; Abhijit Brahme[1]; Kaan Inal[1]; *Chal Park*[2]; Aaditya Lakshmanan[2]; Sazol Das[2]; [1]University of Waterloo; [2]Novelis

9:50 AM
Digital Threads for FAST Processing: *Lucia Scotti*[1]; Martin Jackson[1]; Oliver Levano Blanch[2]; Beatriz Fernandez Silva[2]; Sam Lister[1]; Prashant Jadhav[1]; Hugh Banes[1]; Magnus Anderson[1]; Hector Basoalto[1]; [1]University of Sheffield; [2]Rolls-Royce Plc

10:10 AM
Machine Learning-enhanced Robust Co-design Exploration for Many Objective, Multilevel Materials Design Problems: *Anand Balu Nellippallil*[1]; Mathew Baby[1]; Rashmi Rama Sushil[2]; Palaniappan Ramu[2]; Janet K. Allen[3]; Farrokh Mistree[3]; [1]Florida Institute of Technology; [2]IIT Madras; [3]University of Oklahoma

10:30 AM
Integrating Crystal Plasticity and Thermo-mechanical Constitutive Modeling: *Anderson W Paiva do Nascimento*[1]; Akhilesh Pedgaonkar[2]; Curt Bronkhorst[2]; Irene Beyerlein[1]; [1]University of California, Santa Barbara; [2]University of Wisconsin-Madison

10:50 AM Break

App: Alloy Des. II

Thursday AM
May 25, 2023

Room: Boca V-VII
Location: Caribe Royale

Session Chair: To Be Announced

9:00 AM Invited
Crudden_PLACEHOLDER: *David Crudden*[1]; [1]Alloyed Inc.

9:30 AM
Material And Process Parameter Optimization for Additive Manufacturing Using High-throughput Kinetic Simulations: *Evgeniya Kabliman*[1]; Nora Barschkett[1]; Sebastian Tonatiuh Carrion Ständer[1]; [1]Technical University of Munich

9:50 AM
Computational Modeling of the Microstructure Evolution in the Mo-V Binary Alloy System: *Abhishek Thakur*[1]; Sasa Kovacevic[2]; Krishna Muralidharan[3]; [1]The University of Arizona; [2]Imperial College London; [3]University of Arizona

10:10 AM
Sustainable Aluminum Alloy Design Using Physics-informed Machine Learning: *Fatih Sen*[1]; Marat Latypov[1]; Heath Murphy[1]; Dasha Artsykhovska[1]; Kyle Haines[1]; Shruthi Raj[1]; Aurele Mariaux[1]; Sazol Das[1]; Yudie Yuan[1]; Vishwanath Hegadekatte[1]; [1]Novelis

10:30 AM
ICMD: ICME-based Genomic Materials Design: *Jiadong Gong*[1]; [1]Questek Innovations LLC

10:50 AM Break

Linkages: Deformation III

Thursday AM
May 25, 2023

Room: 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]; [1]Johns Hopkins University

11:30 AM
Designing Fatigue Resistance of Metallic Alloys with a Hybrid of Deep Learning and Micromechanics: *Anssi Laukkanen*[1]; Matti Lindroos[1]; Tom Andersson[1]; Napat Vajragupta[1]; Tatu Pinomaa[1]; Sicong Ren[1]; Abhishek Biswas[1]; Tomi Suhonen[1]; [1]VTT 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]; [1]NLR

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]; [1]Tata Consultancy Services Limited

App: AM Microstructure III

Thursday AM
May 25, 2023

Room: 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]; [1]University 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 Chung[1]; Yeon Su Lee[1]; Gun Jin Yun[1]; [1]Seoul National University

11:50 AM
Development of Digital Model Predicting Mechanical Properties of Inconel 718 for Powder Based Additive Manufacturing: *Parimal Maity*[1]; Mohit Singhal[1]; Jacob Kallivayalil[2]; [1]Eaton India Innovation Center; [2]Eaton 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]; [1]Indian Institute of Technology Gandhinagar; [2]m4p material solutions GmbH; [3]Indian Institute of Technology Bombay

App.: AM Processing IV

Thursday AM
May 25, 2023

Room: 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 Vela[1]; Pejman Honarmandi[1]; Peter Morcos[1]; David Shoukr[1]; Abdelrahman Kotb[1]; Ibrahim Karaman[1]; Alaa Karaman[1]; Raymundo Arroyave[1]; [1]Texas A&M University

11:30 AM
Computational Design and Modelling of Nickel-based Alumindes High Entropy Alloys: *Peter Odetola*[1]; Peter Olubambi[1]; [1]University 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 Halder*[1]; Seunghee Oh[1]; Anthony Rollett[1]; Andrew Chuang[2]; [1]Carnegie Mellon University; [2]Argonne National Laboratory

12:10 PM
An Integrated Process-structure-property Framework for In-silico Design of Additively Manufactured 18Ni-300 Maraging Steels: *Akash Bhattacharjee*[1]; Pravin Kumar[1]; Himanshu Nirgudkar[1]; Surya Ardham[1]; Pramod Zagade[1]; Gerald Tennyson[1]; BP Gautham[1]; [1]TCS 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 Baby*[1]; Anand Balu Nellippallil[1]; [1]Florida Institute of Technology

A Software Approach to Predict Creep Behavior in Time and Temperature Dependent Materials: *Abdullah Kose*[1]; Irina Viktorova[1]; Muhammed Kose[1]; Garrett Pataky[1]; Sofya Alekseeva[1]; Leo Rebholz[1]; [1]Clemson University

Automated Characterization of Generated Meltpool from High Speed Camera: *Kristen Hernandez*[1]; John Lewandowski[1]; Roger French[1]; Laura Bruckman[1]; Jayvic Jimenez[1]; Thomas Ciardi[1]; Sameera Venkat[1]; [1]Case Western Reserve University

Computational Simulations on Behavior of UHPC Subjected to Chloride Ingress: Jun Wang[1]; *Yail Jimmy Kim*[1]; [1]University of Colorado Denver

A Generative Adversarial Network for the Creation of Complex 3D Bimodal Polycrystalline Microstructures: Application to Cold-spray Al7050 Alloy: *Brayan Murgas*[1]; Joshua Stickel[1]; Somnath Ghosh[1]; [1]Johns Hopkins University

Ab-initio Modelling of Phonon Transport in 2D High Entropy MXene Layers: *Prince Sharma*[1]; Ganesh Balasubramanian[1]; [1]Lehigh University

Decision Support System for Device Fabrication: Neelanshi Wadhwa[1]; Sapan Shah[1]; *Deepak Jain*[1]; Sreedhar Reddy[1]; Beena Rai[1]; [1]Tata Consultancy Services

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

Material Data Scraping and Automatic Curation: *Vinod Kumar Mannaru*[1]; Shrikant Tarte[1]; Om Singh[2]; [1]Eaton; [2]NIT Trichy

Joining of Dissimilar Metals for High-speed Electric Motor Applications: A Molecular Dynamics Study: *Jiayi Chen*[1]; Johannes Nokelainen[2]; Bernardo Barbiellini[2]; Hemantha Yeddu[1]; [1]LUT University; [2]Northeastern University

Development of a Fully Anisotropic Monte Carlo Potts Model to Study Grain Growth: *Lin Yang*[1]; Vishal Yadav[1]; Michael Tonks[1]; [1]University of Florida

Micromechanical Modeling of Cyclic Damage in Metallic Materials: *Gururaj Gopal Rao*[1]; Leslie T Mushongera[1]; [1]University of Nevada, Reno

Irradiance Simulation of Real World Field for PV Backsheets Degradation: *Zelin Li*[1]; Raymond Wieser[1]; Xuanji Yu[1]; Laura Bruckman[1]; [1]Case Western Reserve University

Fluoroelastomer Crystallization Kinetics Studied by Deep Learning Segmentation of Atomic Force Microscopy Images: *Sameera Nalin Venkat*[1]; Thomas Ciardi[1]; Jube Augustino[1]; Jayvic Jimenez[1]; Peter Schlueter[1]; Mingjian Lu[1]; Frank Ernst[1]; Yinghui Wu[1]; Roger French[1]; Laura Bruckman[1]; [1]Case Western Reserve University

Geospatiotemporal Modeling of Near Subsurface Temperatures of the Continental United States for Assessment of Materials Degradation: *Deepa Bhuvanagiri*[1]; Hope Omodolor[1]; Erika Barcelos[1]; Vibha Mandayam[1]; Sameera Nalin Venkat[1]; R. Mohan Srivastava[1]; Roger French[1]; Jeffrey Yarus[1]; [1]Case Western Reserve University

Discriminative Object Tracking by Domain Contrast: *Huayue Cai*[1]; Xiang Zhang[1]; Long Lan[1]; Changcheng Xiao[1]; Chuanfu Xu[1]; Jie Liu[1]; Zhigang Luo[1]; [1]National University of Defense Technology

Effects of Surface Segregations in Catalytic AgAuCuPdPt High Entropy Alloy: Chinmay Dahale[1]; *Soumyadipta Maiti*[1]; Sriram Srinivasan[1]; Beena Rai[1]; [1]TCS Research, TRDDC

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

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

First-principles and Data-driven Discovery of High-entropy Alloys for Corrosion Protection: Andrew Neils[1]; Nathan Post[1]; *Cheng Zeng*[1]; Jack Lesko[1]; [1]The Roux Institute at Northeastern University

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Phase Field Simulation of Heat Treatment Process for Single Crystal Ni-based Superalloy: *Yeyuan Hu*[1]; Qingyan Xu[1]; [1]Tsinghua University

Ontology-based Digital Representations of Materials Testing in the MaterialDigital Initiative: *Hossein Beygi Nasrabadi*[1]; Thomas Hanke[2]; Miriam Eisenbart[3]; Matthias Weber[2]; Roy Meissner[4]; Gordian Dziwis[4]; Yue Chen[1]; Birgit Skrotzki[1]; [1]Bundesanstalt für Materialforschung und -prüfung (BAM); [2]Fraunhofer-Institut für Werkstoffmechanik (IWM); [3]Forschungsinstitut Edelmetalle + Metallchemie (fem); [4]Institut für Angewandte Informatik (InfAI)

Predicting the Performance Degradation of Advanced Devices Exposed to Ionizing Radiation: *Xiaoyu Guan*[1]; Michael Tonks[1]; [1]University of Florida

Tensile Loading Modelling of Laser-deposited AlCoCrFeNiCu High Entropy Alloy Using Comsol Multiphysics: *Modupeola Dada*[1]; Patricia Popoola[1]; [1]Tshwane University of Technology

The Effects of Orientation and Temperature on Deformation Mechanisms in Single-crystalline CrCoNi: *Charles Matlock*[1]; Ning Zhang[1]; [1]Baylor University

Modeling the Effects of Short Range Order on Initial Passivation in Binary Alloys: *Alex Tai*[1]; John Cavin[1]; Ian McCue[1]; Karl Sieradzki[2]; [1]Northwestern University; [2]Arizona State University

Predicting Grain Morphology in LBPF Haynes 282 with Complex Geometry via ICME Approach: *Yu-Tsen Yi*[1]; Junwon Seo[1]; Anthony Rollett[1]; [1]Carnegie Mellon University

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

Modelling of Carbides in Irradiated Steel Microstructure: *Andris Freimanis*[1]; Matti Lindroos[1]; Anssi Laukkanen[1]; Sicong Ren[1]; [1]VTT 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]; [1]Indian Institute of Science; [2]Indian Institute of Technology

INDEX

A

Acharya, R....9
Afolabi, A....10, 12
Agarwal, A....7
Agarwal, S....9
Agrawal, A....4
Aidhy, D....5
Akkermans, R....4
Alankar, A....10
Alekseeva, S....12
Allaire, D....3
Allen, J....11
Allison, J....3, 7
Alman, D....6
Amsterdam, E....11
Anderson, M....6, 11
Anderson, P....4
andersson, t....11
Andersson, T....6
Angerer, P....9
Anglada, E....8
Antretter, T....9
Apel, M....7
Arabelo, A....3
Aragon, N....8
Ardham, S....8, 12
Arnold, S....4
Aroh, J....9
Arora, A....11
Arora, G....5
Arribas, M....12
Arroyave, R....3, 5, 11
Artsykhovska, D....11
Arul Kumar, M....8
Attari, V....3
Augustino, J....5, 12
Aung, H....4
Ayyaswamy, A....9

B

Baby, M....11, 12
Bair, J....7
Bajaj, P....11
Balasubramanian, G....6, 12
Bandyopadhyay, R....4
Banes, H....11
Barbiellini, B....12
Barcelos, E....7, 12
Barkar, T....8
Barker, E....3, 7, 9
Barker, S....4
Barschkett, N....11
Basoalto, H....6, 11
Basu, B....13
Bautmans, L....7
Bayerlein, B....3, 5
Beaudoin, A....4, 7
Bednarcyk, B....4
Beemaraj, S....4
Begley, B....6
Berglund, I....3
Berman, T....3
Beyerlein, I....4, 11
Beygi Nasrabadi, H....12
Bhaduri, A....7
Bhattacharjee, A....5, 8, 12
Bhattacharya, C....13
Bhuvanagiri, D....12
Birkholz, H....3
biswas, a....11
Biswas, A....6
Blokhin, E....3
Bobel, A....10
Bock, C....4
Bocklund, B....8
Boyce, D....7
BP, G....8
Brahme, A....10
Brinson, L....3
Bronkhorst, C....11
Brooks, K....3, 5
Brown, D....7
Bruckman, L....4, 5, 7, 12
Burlatsky, S....4
Büßenschütt, K....7

C

Cai, H....12
Calta, N....3
Capolungo, L....8
Cardiff, P....12
Cardinaels, R....4
Carlsson, J....9
Carrillo, A....12
Carrion Ständer, S....11
Casalena, L....10
Cavin, J....12
Chadwick, A....9
Chandel, S....9
Chatterjee, S....9
Chaudhary, V....3
Chaudhuri, S....5, 6
Chen, B....8
Chen, J....4, 10, 12
Chen, Y....12
Cherukara, M....3
Chigurupati, P....4
Chintha, A....8
Choi, K....9
Christodoulou, P....8
Chuang, A....12
Chung, M....10, 11
Ciardi, T....6, 12
Cluff, S....7
Copp, S....9
Costa, M....7
Couet, A....6
Crudden, D....11

D

Dada, M....12
Daehn, G....3
Dahale, C....6, 12
Das, S....9, 10, 11
Dhakad, A....7
Dhakal, R....12
Diehl, M....4, 6, 10
Dimiduck, D....7
Dingari, N....9
Dmello, R....4
Doty, C....6
Dutta, M....8
Dziwis, G....12

E

Eisenbart, M....12
Ellis, B....4
El-Wardany, T....9
Engstrom, A....8
Ernst, F....12
Eßl, W....8, 10

F

Fang, C....6
Farimani, A....5
Fernandez Silva, B....11
Field, D....5
Fisher, C....4
Foltz, J....10
Forget, P....10
Foster, M....10
Frazier, W....3, 9
Freimanis, A....13
French, R....3, 4, 5, 6, 7, 12
Furrer, D....4, 7
Fu, Y....3, 5, 9

G

Gammer, C....8
Gandin, C....6
Ganguly, S....8
Gao, M....6
Garapati, V....9
Garcia de Cortazar, M....8
Gardner, W....9
Garza, A....5
Gautham, B....5, 11, 12
Ghosh, S....7, 10, 11, 12
Girot, F....8
Glaessgen, E....5, 6, 7, 10
Gnaepel-Herold, T....4
Godor, F....9
Goel, V....7

Goh, B 6
Gomez Hernandez, M 6
Gong, J 11
Gopalakrishnan, S 4
Gopal Rao, G. 12
Gorelik, M 7
Goverapet Srinivasan, S. 6
Govind, K 6
Groeber, M 3
Gruber, C. 9
Grundmann, J. 3
Guan, X 12
Guillemot, G 6
Gupta, A. 11
Gu, Y 5

H

Haase, C. 7
Haile, M 5
Haines, K 11
Hajiyani, H 9
Halder, R 12
Hale, L 3
Hana, J 3
Hanke, F. 9
Hanke, T 5, 12
Hansen, W. 3
Hardin, T 10
Hareland, C 6
Hariharaputran, R 5
Harley, J 3
Hattrick-Simpers, J. 6
Hearley, B. 4
Hegadekatte, V 11
Henson, N 3, 7, 9
Hernandez, K 5, 7, 12
Hilty, F 10
Hocker, S 5
Holm, E 5, 6
Honarmandi, P 11
Hosseinzadeh, H. 7
Huang, L 5
Huang, S. 7
Hubbard, L 10
Husseini, J 4
Hutasoit, N 5
Hu, Y 6, 12

I

Inal, K. 10

J

Jablonski, P 6
Jackson, M 11
Jadhav, P. 6, 11
Jain, D. 12
Jeppsson, J 5
Jiang, R. 6
Ji, H. 4
Jimenez, A 8, 12
Jimenez, J. 4, 5, 7, 12
J, J 13
Jogi, T. 7
John, D. 7
John, R 6
Jo, L. 4
Jones, E. 4
Jones, K 6
Jorcin, J. 12
Joshi, A. 5
Joshi, V. 3, 5, 8, 9
Juhasz, M 3

K

Kabliman, E. 11
Kadiyala, A 3
Kalariya, Y. 4
Kalidindi, S 8
Kallivayalil, J 11
Kalsar, R. 3, 5
Kamrava, S. 5
Kappagantula, K. 3, 7
Karagadde, S 10
Karaman, A 11
Karaman, I. 11
Karri, N 3
Kazemzadeh Farizhandi, A 8
Kemppainen, J. 4
Kerwin, L. 7
Khatamsaz, D 3
Kim, H 12
Kim, Y 10, 12
Kirka, M. 6
Kitahara, A 5
Kitt, A. 7
Kopper, A. 8
Kose, A. 12
Kose, M 12
Kotb, A. 11
Kovacevic, S. 11
Krause, A 3
Kreuzer, H 9
K.R., H 11
Krishnamoorthi, S 10
Krishnamurthy, A. 3
Krobath, J. 9
Krutz, N. 4
Kumar, A 8
Kumar, P 8, 12
Kumar, S. 4

L

Lados, D. 9
Lakshmanan, A. 9, 10
Lancelot, C. 8
Lan, L 12
Latypov, M. 11
Lau, J. 5
Laukkanen, A 6, 10, 11, 13
Lavender, C 9
Lawrence, J 3
Lebensohn, R 8
Lee, K 10, 11
Lee, Y 10, 11
Legros, M. 6
Leonor, J. 4
Leser, P. 7
Lesko, J. 12
Levano Blanch, O 11
Lewandowski, J. 6, 7, 12
Li, L. 3, 8, 9
Lima, L. 10
Lim, H 8
Limmer, K 5
lindroos, m 11
Lindroos, M. 6, 10, 13
Linton, N 5
Lister, S. 11
Liu, J 5, 12
Li, Y 4, 8
Li, Z 12
Lohrasbi, S. 8, 10
Lordi, V 8
Lu, M 5, 12
Luo, A. 8
Luo, Z. 12
Lu, Y. 6

M

Madiraju, H. 5
Mahan, T 3
Maiaru, M 4
Maiti, S. 12
Maity, P 11
Malik, A 5
Malusare, K 10
Mamivand, M 8
Mandayam, V 12
Mannaru, V. 12
Mariaux, A. 11
Marini, B 10
Markstrom, A 5
Marziale, J 10
Mason, P 5, 8
Mason, T 3, 5
Matlock, C. 8, 12
McClenny, L 5
McClure, M. 4
McCue, I 12
McLendon, R. 4
Mcneff, P 3
Mcwilliams, B 7
Megahed, M 7
Meissner, R 12

Melville, J. 3
Miller, V. 6
Minisandram, R 10
Mishra, S 11
Mistree, F. 11
Mock, C 7
Modrow, N 9
Mohapatra, G 10
Mohr, L 7
Montiel, D 7
Moodispaw, M 8
Moorehead, M 6
Morcos, P. 11
Moser, D 7
Muhammad, W. 10
Muhammed, B 5
Mukherjee, P. 9
Muller, S. 10
Mulvaney, M 3
Mundada, Y. 11
Muralidharan, K. 11
Murdoch, H. 5
Murgas, B. 12
Murphy, H. 11
Musinski, W 6
Mynam, M. 9

N

Nakamura, S 7
Nalin Venkat, S 12
Naragani, D 7
Na, S 4
Neils, A. 12
Nelaturu, P 5, 6
Nellippallil, A 11, 12
Nerella, D. 8
Neves, K. 10
Nguyen, J 6
Nguyen, M. 4
Nguyen, P 6
Niezgoda, S 3
Nimmal Haribabu, G. 13
Nirgudkar, H. 12
Niverty, S 8
Nokelainen, J. 12
Noraas, R 4
Nygren, K. 4

O

Oancea, V 9
Obiri, M 3
O'Connell, C 4
Odegard, G 4
Odetola, P 11
Oh, S. 12
Oliveros, D 6
Olszta, M 3, 10
Olubambi, P 10, 11, 12
Omodolor, H. 12
Owoeye, S 3

P

Paiva do Nascimento, A. 4, 11
Panwisawas, C. 9
Park, C 9, 10
Pataky, G 12
Pedgaonkar, A. 11
Perron, A 8
Persson, M. 4
Pineda, E 4
pinomaa, t 11
Pinomaa, T 6
Pisani, W 4
Pitike, K 8
Ponon, G 3
Pope, J 6
Popoola, P 12
Portella, P. 3
Post, N 12
Prabhu, N. 6
Prevedel, P. 9
Pribe, J 5, 7, 10
Priya, P. 5
P, S. 11
Puchala, B 3
Pusuluri, S 8

Q

Qi, L 6
Quang, M. 5

R

Radhakrishnan, B. 9
Raghuraman, V. 6
Rai, B 6, 9, 12
Rais-Rohani, M. 4
Raj, S. 11
Rama Sushil, R 11
Ramirez-Tamayo, D 8
Ramu, P 11
Raninger, P 8, 9
Rebholz, L 12
Reddy, S 12
Reig Buades, L. 4
Reiss, G 8, 10
Renderos, M 8
ren, s. 11
Ren, S 6, 10, 13
Reyes, J. 9
Rezwan, A 7, 8
R, H 8
Richter, B 5, 7, 10
Rinderspacher, B. 5
Ritzmann, A 10
Rodgers, T 7
Rodriguez Negron, A. 7
Rohrer, G 9
Rollett, A 5, 6, 7, 9, 12
Roongta, S 4, 10
Rosenthal, W. 10
Roters, F. 10
Rovinelli, A 8
Ryu, I 6, 8

S

Saal, J 3
Sachdev, A 10
Safaei, N. 9
Sahay, S. 10
Salvi, A. 4
Samajdar, I. 10
Sandfeld, S 6
Sangid, M. 4
San, S 6
Savangouder, R 5
Schilling, M 3, 5
Schlueter, P 12
Schuessler, B 8
Scotti, L 6, 11
Sebastian, J 8
Segawa, M 7
Sehirlioglu, A 5
Sen, F 11
Seo, J. 12
Sessim, M. 9
Shade, P 6, 7
Shah, J 4
Shah, S 12
Shanthraj, P 10
Sharma, P. 6, 12
Sheikh, S 11
Shen, C. 7
Shinjo, J 9
Shoukr, D. 11
Sieradzki, K 12
Sills, R. 10
Simonds, B. 6
Singh, A 11
Singhal, M 11
Singh, O 12
Sistaninia, M 8, 9
Skrotzki, B 3, 5, 12
Smith, E 3, 7, 9
Smith, J. 6
Soofi, Y. 5
Soulami, A. 3, 5, 8, 9
Souza, F 10
Spangenberger, A 9
Sridharan, K 6
Srinivasan, S 12
Srivastava, R 12
Stanojevic, A 9
Stapleton, S 4
Steinbach, I 8, 9

Stich, P 7
Stickel, J 12
Stockinger, M 9
Stricker, M 7
Sudbrack, C 6
suhonen, t 11
Sukumaran, A 7
Sun, C 4, 7
Sundar, A 6
Sun, J 4, 10
Sun, T 6
Szajewski, B 5

T

Tahmesabi, P 5
Tai, A 12
Tallman, A 7
Tang, G 7
Tarcea, G 3
Tari, V 10
Tarte, S 12
Tayon, W 3
Tennyson, G 5, 8, 11, 12
Tewary, U 10
Thakur, A 11
Thapliyal, S 6
Thoma, D 5, 6
Thomas, J 4
Thornton, K 7
T Mushongera, L 12
Todd, D 3, 7, 9
Tomczak, N 3, 7
Tonks, M 3, 9, 12
Trasca, R 10
Trehern, W 6
Tripathi, P 3, 5, 6
Trometer, N 8
Tschirhart, J 9

U

Ualikhankyzy, Z 3
Uchic, M 5
Uddagiri, M 9
Urig, E 3

V

vajragupta, n 11
Vajragupta, N 6
Vamsi, K 5, 11
Van Loock, F 4
Vela, B 11
Venka, S 7
Venkatesan, K 3
Venkatesh, V 4
Venkat, S 5, 12
Viktorova, I 12
Vishnugopi, B 9
von Hartrott, P 3, 5
Voorhees, P 6, 9

W

Waas, A 4
Wadhwa, N 12
Wagner, G 4
Waitelonis, J 3, 5
Walker, E 4
Wang, J 12
Wang, Y 6
Ward, C 7
Weber, G 5, 6
Weber, M 12
Whitney, B 9
Widom, M 6
Wieser, R 7, 12
Willard, M 3
Wong, G 9
Wu, Y 5, 12

X

Xia, H 8
Xiao, C 12
Xu, C 12
Xu, Q 8, 12
Xu, Z 5, 9

Y

Yadav, V 3, 12
Yaghoobi, M 7
Yamamoto, Y 8
Yamanaka, A 7
Yang, L 12
Yan, X 5
Yarasi, S 5
Yarus, J 12
Yeddu, H 12
Yeo, L 7
Yeratapally, S 6
Yi, Y 6, 12
Yuan, L 7
Yuan, Y 11
Yue, W 3
Yun, G 10, 11
Yu, T 8
Yu, X 12

Z

Zagade, P 12
Zeng, C 12
Zhang, J 9
Zhang, N 8, 12
Zhang, X 12
Zhou, C 11
Zhou, X 10
Zia, G 5, 12
Zinkle, S 9
Zwerink, B 11