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7TH WORLD CONGRESS ON

INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING (ICME 2023)

May 21–25, 2023

Caribe Royale Resort | Orlando, Florida, USA

CONGRESS GUIDE AND FINAL TECHNICAL PROGRAM

SPONSORS:

Thermo-Calc Software

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This congress is sponsored by the Materials Processing & Manufacturing Division and the Integrated Computational Materials Engineering Committee.

www.tms.org/ICME2023

SCHEDULE AT A GLANCE • *Current as of April 19, 2023 • Subject to change*

Sunday, May 21	Time	Location
Registration	5:30 p.m. - 7:30 p.m.	Caribbean Registration East
Welcome Reception	6:30 p.m. - 7:30 p.m.	Boca Patio/Pier
Monday, May 22	**Time**	**Location**
Registration	7:30 a.m. - 4:40 p.m.	Caribbean Registration East
Exhibitor and Poster Installation	7:30 a.m. - 9:30 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 IV, Caribbean VI & VII, Boca I-III
Congress Lunch	11:40 p.m. - 1:10 p.m.	Caribbean III
Technical Sessions	1:10 p.m. - 4:40 p.m.	Caribbean IV, Caribbean VI & VII, Boca I-III
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 Registration East
Technical Sessions	8:00 a.m. - 12:00 p.m.	Caribbean IV, Caribbean VI & VII, Boca I-III
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 IV, Caribbean VI & VII, Boca I-III
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. - 4:40 p.m.	Caribbean Registration 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 IV, Caribbean VI & VII, Boca I-III
Lunch	11:40 p.m. - 1:10 p.m.	*On your own*
Technical Sessions	1:10 p.m. - 4:40 p.m.	Caribbean IV, Caribbean VI & VII, Boca I-III
Exhibitor teardown	1:10 p.m. - 4:40 p.m.	Caribbean V
Break	3:00 p.m. - 3:20 p.m.	Caribbean III
Informal Job Fair	3:20 p.m. - 4:40 p.m.	Caribbean III
Poster teardown	3:20 p.m. - 4:40 p.m.	Caribbean V
Thursday, May 25	**Time**	**Location**
Registration	7:30 a.m. - 12:30 p.m.	Caribbean Registration 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 IV, Caribbean VI & VII, Boca I-III
Break	10:50 a.m. - 11:10 a.m.	Caribbean V

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WELCOME

The 7th World Congress on Integrated Computational Materials Engineering (ICME 2023) convenes leading researchers and practitioners to share the latest knowledge and advances in the discipline. This congress is the recognized hub of interaction among software developers and process engineers along the entire production chain, as well as for materials scientists and engineers developing new materials.

ICME 2023 is the only congress dedicated to bringing all stakeholders together from across nations, disciplines, and organizations to focus on integration priorities and gaps that need to be addressed in order to advance the field.

ICME 2023 will benefit researchers, software developers, metallurgists, materials scientists and engineers, process engineers, senior scientists, chief technology officers, and a variety of others working in R&D. Attendees will gain insights on recent advances and discuss opportunities to overcome challenges in the field.

ORGANIZING COMMITTEE

Committee Chair:
Charles Ward, Air Force Research Laboratory (Retired)

Programming Chair:
Heather Murdoch, DEVCOM Army Research Laboratory

Organizing Committee:
- **Durga Ananthanarayanan**, IIT Bombay
- **Austin Mann**, Boeing
- **Victoria Miller**, University of Florida
- **Georg Schmitz**, MICRESS group at ACCESS
- **Kandler Smith**, National Renewable Energy Laboratory
- **Sanjay Sondhi**, GE Research

REGISTRATION

Attendees are required to register. Badges must be worn for admission to technical sessions, the exhibition, and all congress events.

Your registration badge ensures admission to each of these events:
- Technical program
- Refreshment breaks during session intermissions
- Sunday night welcome reception
- Lunch on Monday
- Tuesday night poster reception

Registration Hours
The registration desk will be in Caribbean Reg East at the following times (subject to change):

Sunday, May 21, 5:30 p.m.–7:30 p.m.
Monday, May 22, 7:30 a.m.–5:00 p.m.
Tuesday, May 23, 7:30 a.m.–5:45 p.m.
Wednesday, May 24, 7:30 a.m.–4:40 p.m.
Thursday, May 25, 7:30 a.m.-12:30 p.m.

CONGRESS DETAILS

Technical Sessions

All technical sessions and keynote presentations take place in Caribbean IV, Caribbean VI & VII, and Boca I-III. Poster presentations and the exhibition will be held in Caribbean V. Refer to the technical program for details.

Internet Access

Complimentary internet access is available for attendees in the meeting areas. To access Wi-Fi, sign-in to the following network:

Network: TMS Meeting
Password: ICME2023

Please note the letter case when typing passwords to connect to this Wi-Fi network.

PUBLICATION OPTION

Congress participants are encouraged to submit their work to the TMS journal *Integrating Materials and Manufacturing Innovation*, which will be publishing a topical collection dedicated to the meeting. This collection will take the place of a traditional conference proceedings publication. Only submissions from attendees will be considered for this collection. Submissions will go through the journal's standard peer review process, and there is no guarantee of acceptance. Submissions are due July 31, 2023.

NETWORKING & SOCIAL EVENTS

Welcome Reception
Join us for a welcome reception on Sunday, May 21, from 6:30 p.m. to 7:30 p.m. in Boca Patio/Pier.

All Congress Lunch
Attend the all congress lunch scheduled for Monday, May 22, from 11:40 a.m. to 1:10 p.m. in Caribbean III.

Poster Reception
Enjoy refreshments and mingle at the reception for poster viewing planned for Tuesday, May 23, from 4:45 p.m. to 5:45 p.m. in Caribbean V.

Informal Job Fair
Meet with organizations looking for their next employee and explore your future employment options at the ICME Job Fair on Wednesday, May 24, from 3:20 p.m. to 4:40 p.m. in Caribbean III.

ABOUT THE VENUE

Caribe Royal Resort
18101 World Center Drive
Orlando, FL 32821
+1 407-238-8000

The Caribe Royale Resort, a AAA Four-Diamond resort, is ideally located in the heart of Orlando, Florida. The Caribe Royale has completed a major renovation and redesign and all suites have been reimagined with a modern style and the comforts of home. The resort's amenities include an outdoor waterfall pool with a waterslide, a two-story fitness center, basketball and tennis courts, jogging trails, and the Island Spa. The Caribe Royale Resort is a Disney Good Neighbor® Hotel and offers scheduled shuttle transportation to all four Disney Theme Parks & Disney Springs®.

The Caribe Royale's location is just 16 miles from the Orlando International Airport (MCO). Transportation options from the airport include taxi, ride-sharing services, and car rental companies.

Upon arriving at the Caribe Royale, parking options include:
- Self-Parking for Overnight Guests: $20 per night
- Self-Parking for Day Guests: $30 per day
- Valet: $35 per day

Hotel guests are encouraged to self-park near their tower for easy access to their vehicle.

The Caribe Royale also offers a shuttle around the resort property. While the shuttle comes frequently, guests can also call +1 407-973-1053 for direct pick up assistance.

EXPLORE THE CARIBE ROYALE RESTAURANTS

The Caribe Royale Resort has seven on-site dining options to suit every palate.

The Venetian Chop House
Hours: Monday-Thursday 6:00 p.m.–10:00 p.m.
Friday-Saturday 5:00 p.m.–10:00 p.m.
Sunday 5:00 p.m.–9:00 p.m.

Tropicale
Hours: Monday-Friday 6:30 a.m.–11:00 a.m.
Saturday-Sunday 7:00 a.m.–12:00 p.m.

Calypso's Pool Bar & Grille
Hours: Open Daily 11:00 a.m.–11:00 p.m.

Café 24
Hours: Open Daily 6:30 a.m.–12:00 a.m.

Rum Bar featuring BACARDÍ® Rum
Hours: Open Daily 4:00 p.m.–12:00 a.m.

Starbucks®
Hours: Open Daily 6:00 a.m.–8:00 p.m.

In-Suite Dining
- **Breakfast**
  Hours: Monday-Thursday 7:00 a.m.–11:00 a.m.; Friday-Sunday 7:00 a.m.–12:00 p.m.
- **All Day Dining**
  Hours: Monday-Thursday 11:00 a.m.–12:00 a.m.; Friday-Sunday 12:00 p.m.–12:00 a.m.
- **Dinner**
  Hours 6:00 p.m.–10:00 p.m.

MEETING POLICIES

Badges
All attendees must wear registration badges at all times during the congress to ensure admission to events included in the paid fee, such as technical sessions and receptions.

Refunds
The deadline for all refunds was April 7, 2023. No refunds will be issued at the congress. Fees and tickets are nonrefundable.

Cell Phone Use

In consideration of attendees and presenters, we kindly request that you minimize disturbances by setting all cell phones and other devices on "silent" while in meeting rooms.

Americans with Disabilities Act

The federal Americans with Disabilities Act (ADA) prohibits discrimination against, and promotes public accessibility for, those with disabilities. In support of, and in compliance with ADA, we ask those requiring specific equipment or services to contact TMS Meeting Services at mtgserv@tms.org or by visiting the registration desk onsite.

Anti-Harassment
In all activities, TMS is committed to providing a professional environment free of harassment, disrespectful behavior, or other unprofessional conduct.

TMS policy prohibits conduct that is disrespectful, unprofessional, or harassing as related to any number of factors including, but not limited to, religion, ethnicity, gender, national origin or ancestry, physical or mental disability, physical appearance, medical condition, partner status, age, sexual orientation, military and veteran status, or any other characteristic protected by relevant federal, state or local law or ordinance or regulation.

Failure to comply with this policy could lead to censure from the TMS Board of Directors, potential legal action, or other actions.

Anyone who witnesses prohibited conduct or who is the target of prohibited verbal or physical conduct should notify a TMS staff member as soon as possible following the incident. It is the duty of the individual reporting the prohibited conduct to make a timely and accurate complaint so that the issue can be resolved swiftly.

Photography and Recording
TMS reserves the right to all audio and video reproduction of presentations at TMS-sponsored meetings. By registering for this meeting, all attendees acknowledge that they may be photographed by TMS personnel while at events and that those photos may be used for promotional purposes, in and on TMS publications and websites, and on social media sites.

Any recording of sessions (audio, video, still photography, etc.) intended for personal use, distribution, publication, or copyright without the express written consent of TMS and the individual authors is strictly prohibited. Attendees violating this policy may be asked to leave the session.

Antitrust Compliance
TMS complies with the antitrust laws of the United States. Attendees are encouraged to consult with their own corporate counsel for further guidance in complying with U.S. and foreign antitrust laws and regulations.

TMS Diversity and Inclusion Statement
TMS is committed to advancing diversity in the minerals, metals, and materials professions, and to promoting an inclusive professional culture that welcomes and engages all who seek to contribute to the field. TMS recognizes that a diverse minerals, metals, and materials workforce is critical to ensuring that all viewpoints, perspectives, and talents are brought to bear in addressing complex science and engineering challenges. To build and nurture this diverse professional community, TMS welcomes and actively engages the participation of underrepresented groups in all of its initiatives and endeavors.

PLENARY SPEAKERS

Andrew Bobel, General Motors Global Research & Development MPMD ICME Industry Implementation Award Recipient Representative
Presentation: "Multi-scale Approach for Developing a High Silicon Al-Si-Cu Alloy for Additive Manufacturing Supercharger Rotors"

Ida Berglund, QuesTek Europe AB
Presentation: "Advancing ICME Technologies via Strategic Collaboration while Bridging the Gap between Academia and Industry"

Laurent Capolungo, Los Alamos National Laboratory
Presentation: "ExtremeMat Quantification of the Effect of Microstructure and Composition on the Creep Rupture Life of Steels"

Adam Kopper, Mercury Marine
Presentation: "The Multiple Facets of ICME in Modern Manufacturing at Brunswick Boat Group and Mercury Marine"

James Saal, Citrine Informatics
Presentation: "Accelerating Development of Materials with Artificial Intelligence"

EMERGENCY PROCEDURES

The chances of an emergency situation occurring at ICME 2023 are quite small. However, being prepared to react effectively in case of an incident is the most critical step in ensuring the health and safety of yourself and those around you. Please take a few moments to review the maps of the Caribe Royale Resort printed on the back cover of this program. When you enter the building, familiarize yourself with the exits and the stairs leading to those exits. When you arrive at your session or event location, look for the emergency exits that are in closest proximity to you.

IN AN EMERGENCY, DIAL 911.

Please use the following local safety and security contact information if you or someone near you is experiencing an emergency.

Nearest Police Department:
Orlando Police Department
1250 W South Street
Orlando, FL 32805
+1 321-235-5300
www.orlando.gov/Our-Government/Departments-Offices/Orlando-Police-Department

Nearest Fire Department:
Orange County Fire Station 56
13303 International Drive
Orlando, FL 32821
+1 407-836-3111
www.ocfl.net/emergencysafety/firerescue.aspx#.ZEAU_HbMKUk

Nearest Hospital:
AdventHealth Celebration Hospital
400 Celebration Place
Kissimmee, FL 34747
+1 407-303-4000
www.adventhealth.com/hospital/adventhealth-celebration

Urgent Care:
Buena Vista Urgent Care
8200 World Center Drive
Orlando, FL 32821
+1 407-465-1110
www.buenavistaurgentcare.com/

TMS UPCOMING MEETINGS

TMS offers programming that spans the technical interests of the global minerals, metals, and materials community.

October 1–4, 2023
Columbus, Ohio, USA
www.tms.org/TMSFall2023

November 12–15, 2023
Pittsburgh, Pennsylvania, USA
www.tms.org/HEA2023

March 3–7, 2024
Orlando, Florida, USA
www.tms.org/TMS2024

June 16-20, 2024
Cleveland, Ohio, USA
www.tms.org/SpecialtyCongress/2024

September 8–12, 2024
Champion, Pennsylvania, USA
www.tms.org/Superalloys2024

March 23–27, 2025
Las Vegas, Nevada, USA
www.tms.org/TMS2025

June 15-19, 2025
Anaheim, California, USA
www.tms.org/SpecialtyCongress/2025

November 16–20, 2025
Phoenix, Arizona, USA
www.extractionmeeting.org/2025

For a complete listing of upcoming meetings, scan this QR code or visit www.tms.org/UpcomingMeetings

TMS UPCOMING COURSES

TMS offers a variety of online and in-person courses that span the technical interests of the global minerals, metals, and materials community.

For a complete listing of upcoming courses and other professional development events, scan this QR code or visit www.tms.org/UpcomingPDEvents

CORPORATE SPONSOR

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TMS SPECIALTY CONGRESS 2024

JUNE 16-20, 2024

Cleveland Hilton | Cleveland, Ohio, USA

#TMSSpecialtyCongress

SAVE THE DATE

ONE REGISTRATION. THREE MEETINGS. COUNTLESS BENEFITS.

The TMS Specialty Congress annually convenes the Society's recurring specialty meetings under one roof with a single registration fee. Explore your technical interest in a focused, small event environment, while also having access to cross-disciplinary learning and collaboration opportunities with aligned materials communities. **Call for abstracts opens June 2023.**

PLAN TO JOIN US AT OUR INAUGURAL CONGRESS IN 2024!

2024 CO-LOCATED MEETINGS

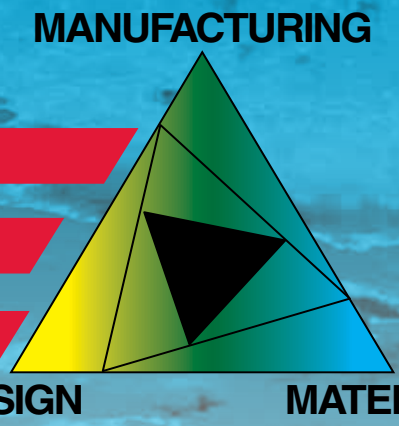
Key issues and future pathways in the implementation of artificial intelligence.

Science and technology associated with numerically controlled forming methodologies.

Cutting edge R&D efforts surrounding mechanical behavior over a wide range of material types.

For details and to sign up for updates, visit:
www.tms.org/SpecialtyCongress/2024

TMS ICME



7TH WORLD CONGRESS ON

INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING (ICME 2023)

May 21–25, 2023

Caribe Royale Resort | Orlando, Florida, USA

FINAL TECHNICAL PROGRAM

www.tms.org/ICME2023

Plenary Session I

Monday AM
May 22, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: Chuck Ward; *IMMI* Journal

8:00 AM Introductory Comments

8:10 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

Structural steels utilized for power generation applications are subjected to complex loading conditions (e.g. stresses, temperatures). A robust knowledge of the evolution of the performance steels, both austenitic and ferritic, with service conditions relies on the degree to which one can establish firm bridges between the microstructure, composition and material performance: such is one of the primary goals of the consortium ExtremeMat. To quantify the impact of microstructure on the material creep rupture life, we introduce a new spectral based model predicting the primary, secondary and tertiary creep response of ferritic and austenitic steels. The framework is found to satisfactorily predict the effects of temperature and stress on the creep rupture life rupture of 347H (austenitic) and Gr91 (ferritic) steels. Finally, leveraging the numerical efficiency of the EVPFFT platform the roles of initial dislocation and precipitate content on the creep rupture life of the material is studied.

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

The benefits to industry in applying ICME are many, including a science-informed understanding of the challenges observed in material manufacturing, rapid optimization of chemistry and heat treatment, and an accelerated qualification of new materials enabling improved component performance. This presentation will exemplify how QuesTek has leveraged its ICME technologies to understand and worked to resolve the most pressing materials related issues to combine manufacturability and performance in various alloy systems. Emphasis will be placed on how QuesTek utilize expertise and interact with entities across the value chain, from producers and manufacturers to end-users, and in collaboration with research institutes and universities. This workflow inherently helps to bridge the gap between academia and industry. Technical examples from collaboration projects in Europe and USA will be presented, and general challenges discussed.

9:30 AM Break

Applications: Advanced Manufacturing - Processing I

Monday AM
May 22, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: Raymundo Arroyave; Texas A&M University

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]The Ohio State University

The use of advanced incremental forming has been validated by blacksmiths and parts can be made that are much larger than a given available press. Systems with large robots and modestly-sized presses can develop these large forgings and in a fraction of the current time as dies do not need to be designed or built. Beyond these practical advantages, the goal of this work is to produce components where location-specific material properties/performance metrics are met in addition to the geometry requirements. We will present an initial robotic system - both its cyber and physical components. We will also highlight initial results in achieving required component geometries with desired microstructural characteristics. We will also present the details of the control algorithms developed for the system to operate in a semi-autonomous manner.

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

Over the past decade, NASA Langley Research Center (LaRC) has led several manufacturing demonstration projects exploiting flow forming technology. The work has resulted in the commercial-scale manufacture of 10-ft. diameter single-piece, integrally stiffened cylinders. Near-net-shape flow forming offers simplified manufacturing schedules and cost savings through reduced part count. Reduction or elimination of machining, welding, and/or riveting can also lead to significant performance gains.NASA LaRC recently established a flow forming research facility to investigate new alloys and stiffener geometries for fuselage and launch vehicle cryotank applications. Candidate aluminum alloys and heat treatment combinations have been characterized through advanced mechanical testing and microscopy to maximize workability during flow forming trials. Elasto-plastic deformation simulations of the forming process have been performed using the finite element software DEFORM and correlated with forming trial results. The overall objective is to optimize structural performance through a combination of innovative materials, processes, and designs.

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

Friction stir processing (FSP) is a technique for altering the microstructure of a material via concentrated plastic deformation and typically leads to improved mechanical, fatigue, and wear performance. The deformation is created by forcibly inserting a non-consumable tool into the workpiece and rotating it while pushing it laterally. To enhance performance attributes such as hardness, and yield strength, the relationship between process parameters and microstructural features are being researched. Numerous process variables are known to influence the microstructure and properties of the FSP material; however, the exact relationships between process variables, and microstructure and performance properties have yet to be completely studied. Using response surface approaches, we create explainable polynomial models for describing process-microstructure-property relationships in this effort that are corroborated as necessary by high fidelity physics models. In addition, parametric and non-parametric techniques are employed to quantify uncertainty, and subsequent experiments are designed using quasi-Monte Carlo Spacefilling techniques.

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

In order to improve upon existing predictive capabilities for the evolution of alloy microstructures subjected to friction stir processing (FSP), an approach was developed integrating a Kinetic Monte Carlo (KMC) Potts Model of recrystallization and grain growth with macroscale Smoothed Particle Hydrodynamics (SPH) simulations of a 316L stainless steel plate. To this end, the KMC Potts Model used the thermomechanical data provided by SPH calculations of the FSP process in order to predict the recrystallization behavior, final grain size, and grain size distribution within the processed region as a function of position. Potts Model simulations were thus able to predict microstructure as a function of 316L stainless steel thermomechanical history and FSP process parameters. Simulation results were validated through experimental comparison with scanning electron microscopy data obtained by 316L stainless steel samples subjected to corresponding process parameters. The fidelity of our results to these experiments are discussed.

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

Uranium-10Mo alloy has been identified as a promising low enriched uranium (LEU) fuel candidate to replace high enriched uranium oxide dispersion fuel (HEU) for use in United States high performance research reactors. Aluminum alloy 6061 (AA6061) cladding encapsulates the U-10Mo fuel foil and is diffusion bonded using hot isostatic pressing (HIP). Limited research has been performed to understand the effect of key HIP parameters on the minimum cladding thickness and strength of the cladding bond. This research has combined finite element modeling with experimental studies on a range of HIP can assembly configurations to evaluate their resulting fuel cladding properties. The experimental work informed the thermal and stress finite element models to predict and elucidate the effect of differing HIP can assembly configurations and process parameters on resulting U-10Mo LEU fuel product. This work identified the main factors for inhibiting heat transfer and producing min clad within the fuel product.

Artificial Intelligence /Machine Learning: Microstructure I

Monday AM
May 22, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: Shankarjee Krishnamoorthi; ATI Specialty Materials

9:50 AM Invited
HPC+AI@Edge Enabled Real-time Materials Characterization: *Mathew Cherukara*[1]; [1]Argonne National Laboratory

The capabilities provided by next generation light sources such as the APSU along with the development of new characterization techniques and detector advances are expected to revolutionize materials characterization (metrology) by providing the ability to perform scale-bridging, multi-modal materials characterization under in-situ and operando conditions. For example, providing the ability to image in 3D large fields of view (~mm3) at high resolution (<10 nm), while simultaneously acquiring information about structure, strain, elemental composition, oxidation state, photovoltaic response etc. However, these novel capabilities dramatically increase the complexity and volume of data generated by instruments at the new light sources. Conventional data processing and analysis methodologies become infeasible in the face of such large and varied data streams. The use of AI/ML methods is becoming indispensable for real-time analysis, data abstraction and decision making at advanced synchrotron light sources such as the APS. I will describe the use of high-performance computing (HPC) along with AI on edge devices to enable real-time analysis of streaming data from x-ray imaging instruments at the APS.

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

The field of Integrated Computational Materials Engineering (ICME) combines a broad range of methods to study materials' responses over a spectrum of length scales. A relatively unexplored aspect of microstructure-sensitive materials design is uncertainty propagation and quantification (UP/UQ) of materials' microstructure, as well as establishing process-structure-property (PSP) relationships. An accurate UP technique built on the idea of changing probability measures for microstructure-based problems is proposed. Probability measures are used to represent microstructure space, and Wasserstein metrics are used to test the efficiency of the method. By using Variational AutoEncoder (VAE), we identify the correlations between the material/process parameters and the thermal conductivity of heterogeneous microstructures. Through high-throughput screening, UQ/UP, and deep-generative learning methods, PSP relationships that are too complicated/complex can be revealed through high-throughput exploitation of the materials' design space with an emphasis on microstructures.

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

Ex-situ computed tomography (CT) analysis of Additive Manufacturing (AM) produced parts is commonplace as a means of Non-Destructive Evaluation (NDE) quality assurance. Most CT examinations focus on porosity, both from keyholing or entrained gas. With the recent acceleration in image processing enabled through Deep Learning/Machine Learning (ML/DL), this presentation suggests expanding CT analysis of AM parts to extend beyond porosity analysis to encompass the study of other requirement-driven, critical geometries. As a case study, AM produced lattices underwent CT and were subsequently segmented into component pieces. These segmented components can be examined individually or as a larger subset where statistics can be taken, with an eye to drawing comparison and correlation to both ex-situ mechanical properties and in-situ process signatures. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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

Beamline 2-D X-ray diffraction (XRD) diffractograms play an important role in determining properties associated with crystal structure such as crystalline phase, texture, and chemistry. Deep learning techniques help create an efficient and accurate solution capable of processing large amounts of image data. Herein, we analyzed patterns of a Ti-6Al-4V (Ti-64) alloy that was heat treated throughout capture of the diffraction patterns. We designed a convolutional neural network (CNN) to predict the titanium beta phase volume percentage during the temperature fluctuations. Images were pre-processed to remove bias in the XRD patterns and prevent loss of information. The 2-D XRD patterns were input directly into the CNN model instead of traditional 1-D XRD peak patterns. The model was trained using an experimental dataset that contains 3,012 XRD images and was tested with another 1,102 experimental XRD images, achieving a mean square error (MSE) of 0.076%.

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

Physics-based mesoscale models of grain growth have been unable to accurately represent the grain growth behavior of real materials. We are developing the Physics Regularized Interpretable Machine Learning Microstructure Evolution (PRIMME) model that can learn to predict grain growth directly from experimental data. The PRIMME algorithm uses a multi-level neural network to predict grain growth in a voxelated domain. It uses a regularization function that encourages evolution that decreases the number of nearest neighbor voxels assigned to different grains. PRIMME helps to interpret and understand its learned grain growth behavior by determining the likelihood of a voxel changing to the grain of neighboring voxels. PRIMME was originally trained using data from 2D isotropic simulation results. It is now being extended to 3D isotropic and 2D anisotropic behavior. It will begin to be trained using experimental data rather than just simulation results in the near future.

Materials Databases & Platforms: I

Monday AM
May 22, 2023

Room: Caribbean IV
Location: Caribe Royale

Session Chair: Fatih G. Sen; Novelis

9:50 AM Invited
Materials Data & Informatics: Curation, Frameworks, Access, and Potential for Discovery and Design: *L. Catherine Brinson*[1]; [1]Duke University

With the advent of the materials genome initiative (MGI) in the United States and a similar focus on materials data around the world, numerous materials data resources and associated vocabularies, tools, and repositories have been developed. While the majority of these systems focus on slices of computational data with an emphasis on crystallographic materials, platforms for organic materials and their composites, especially those incorporating experimental data, have been quite limited. We will discuss the unique aspects of tackling data assembly and informatics associated with experimental organic materials data, with focus on our experiences creating an open-source data resource, NanoMine, part of MaterialsMine. Our goal has been to curate, annotate and store widely varying experimental data on polymer nanocomposites (polymers doped with nanofiller) and providing access to characterization and analysis tools with the long-term objective of promoting facile nanocomposite design. The challenges and promises associated with data curation, ontology and vocabulary development, standardization and interoperability, and data visualization and analysis tools will be discussed. Several case studies will be presented, including use of natural language processing for archival data curation, coupling of experimental and computational data for materials design, and development of machine learning tools for rapid property screening and inference. Overall, we focus on the promise of this new approach to tackle materials design principles for the complex, high dimensional problems inherent in the multi-phase polymer space.

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[5]; 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; [5]Leibniz-IWT Institut für Werkstofforientierte Technologien

The efforts taken within the project 'platform MaterialDigital' (PMD, materialdigital.de) to store FAIR data in accordance with a standard-compliant ontological representation ('application ontology') of a tensile test of metals at room temperature (ISO 6892-1:2019-11) will be presented. This includes the path from developing an ontology in accordance with the respective standard, converting ordinary data obtained from standard tests into the interoperable RDF format, up to connecting the ontology and data. The semantic connection of the ontology and data leads to interoperability and an enhanced ability of querying. For further reusability of data and knowledge semantically stored, the PMD core ontology (PMDco) was developed, which is a mid-level ontology in the field of MSE. The semantic connection of the tensile test application ontology to the PMDco is also presented. Moreover, Ontopanel, a tool for domain experts facilitating visual ontology development and mapping for FAIR data sharing in MSE, is introduced briefly.

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

The computer ontologies ("ashes from the fire of human thinking") can be practically thought as the advanced databases. Their OWL standard was developed with the aim to mathematically guarantee, that the logical reasoning succeeds in finite time. In this work I benchmark the modern Python tools to work with several established nowadays OWL materials ontologies, such as EMMO and PMD. I also present our own in-house effort called MPDS. The highly inter-linked MPDS data graph consists of approximately 5M nodes and 150M edges. All the assertions were taken from the world's published literature in materials science (about 0.5M publications since 1891), as curated by the Pauling Files project, see www.mpds.io. Also the MPDS data graph can be greatly expanded with our in-house ab initio simulations data, which will be produced high-throughput in the cloud fully automatically, controlled with the ontology reasoning engine.

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

Classical atomistic calculations provide a means of exploring the important linkages between atomic structures and larger scale dynamic properties and behaviors. However, the calculation predictions are strongly dependent on the choice of interatomic potential used. The NIST Interatomic Potentials Repository contains citation listings and parameter files for known potentials, as well as a large collection of computed crystalline and crystal defect properties specific to each potential. This not only makes it easy to discover existing potentials, but helps users select which potentials are best suited for their interests. All calculation methods, underlying tools, and high throughput capabilities are available as open-source Python code. The entire calculation framework is designed to be extensible and accessible to users at all levels of interaction.

11:20 AM
Materials Commons and FAIR Data: *Glenn Tarcea*[1]; John Allison[1]; Brian Puchala[1]; Tracy Berman[1]; [1]University of Michigan

The Materials Commons is a data repository for the materials sciences. We describe how Materials Commons conforms to FAIR Data and discuss some of the challenges and needs to make data reusable. The FAIR Data principles of Findable, Accessible, Interoperable and Reusable provide a framework for data reuse, but there is still a large gap to achieving true reusability and understandability. Materials Commons has been extending the ideas of FAIR to help close this gap. We discuss the need for cultural and funding agency changes in order to achieve the larger goal of reuse. We look into how technology, as well as incentives from research funding agencies, can help make published data more reusable.

ICME for Non-Metals: I

Monday PM
May 22, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: See Session Sheets

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

A synergistic multi-scale modeling framework that captures multi-filler interactions at the microstructural level is developed to establish the structure-property relationships of injection-molded thermoplastics with graphite and carbon fiber reinforcements. Representative volumetric elements (RVEs) of the material samples are generated based on known geometrical features extracted using raw images obtained from optical and electron microscopy. Geometrical parameters such as filler orientation and size distribution are calibrated using two baseline samples containing only graphite and carbon fiber fillers, respectively. These parameters are systematically correlated to the differences in viscosities of the molded samples. The calibrated parameters and modeling strategies are then used to generate the combined filler system microstructures to capture the synergistic effects of integrating graphite and carbon fiber. The predicted mechanical and thermal properties are verified and validated for various graphite and carbon fiber weight fractions. Future pathways to improve model prediction capabilities and accuracies are presented.

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

In this work we present the simulation of various composite manufacturing processes using multi-scale modeling techniques in Abaqus to predict how these processes impact the final composite component. Plastic injection molding is simulated to predict fiber dispersion which is imported into Abaqus FE analyses to predict warpage and performance under service loads. Additionally, compression molding is simulated to predict fiber reorientation due to large deformations during the compression process. These forming results including fiber orientation and residual stresses are mapped into subsequent FE analyses for warpage analyses. Finally, the cure process is simulated at small length scales to predict both the homogeneous composite cure response and evaluate how the residual stress field in the composite microstructure interacts with mechanically-induced stresses.

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

We present a finite element (FE) - based framework to perform integrated cure and progressive failure analyses of fiber-reinforced polymers. This framework goes beyond the unit cell and is applicable to laminate scales with various layups, geometries and loading cases. Cure residual stresses are calculated using a coupled chemo-thermo-mechanical analysis, where a data-driven CHILE (cure-hardening/ instantaneous linear elastic) constitutive model is used to capture the evolution of the matrix properties (Nguyen, Dmello and Waas, Archive of Applied Mechanics, 2022). After the residual stresses are calculated, a progressive failure analysis step is performed based on the semi-discrete modeling technique (Nguyen and Waas, Composites Part C, 2020). It comprises a smart meshing strategy, a failure separation, a probabilistic modeling approach, and a mesh-objective constitutive model. The enhanced semi-discrete damage model (eSD2M) can capture multiple failure modes and their interactions as well as predict failure loads with reasonable accuracy.

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

Thermoplastic materials, including polyether ether ketone (PEEK) and polyether ketone ketone (PEKK) are high-performance semi-crystalline polymers ideal for aerospace applications because of their excellent properties, toughness, resistance to aging, manufacturability and "tailorability." Understanding the linkages between the microstructure of the material and its properties facilitate designing of the material itself. A multiscale recursive micromechanics (MsRM) model has been developed and implemented in the NASA Multiscale Analysis Tool (NASMAT). The microstructure of the thermoplastic is modeled using MsRM over three integrated scales (spherulite, lamellar stacks, granular crystal blocks). Inputs for the base constituents are obtained from molecular dynamics calculations. With this computational tool, the effects of microstructure to property relationships are simulated through parametric studies on crystallinity, spherulite packing, and morphology of the microstructure.

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

Electronic devices emit electromagnetic (EM) waves, which may interfere with neighboring electronic components, a phenomenon known as electromagnetic interference (EMI). Conventional metallic shields exhibit high shielding effectiveness values. Yet, most of the power is reflected, resulting in secondary EM pollution. Instead, one can make use of polymer nanocomposite shields which are able to partially absorb the incident power. The challenge is to produce polymer-based shields of high shielding effectiveness where most of the power is absorbed instead of reflected. In this work, we explore the use of 3D gradients in electromagnetic properties within a nanocomposite layer to fill this gap in material property space. An efficient 3D finite element model is constructed to predict the shielding performance as a function of EM property gradient and geometric design of the layer. After validation with experimental data for uniform nanocomposite layers, we use the model to identify optimal material design cases.

3:00 PM Break

Artificial Intelligence /Machine Learning: Properties I

Monday PM
May 22, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: Shankarjee Krishnamoorthi; ATI Specialty Materials

1:10 PM Invited
Artificial Intelligence and High-performance Data Mining for Accelerating Materials Discovery and Design: *Ankit Agrawal*[1]; [1]Northwestern University

The increasing availability of data from the first three paradigms of science (experiments, theory, and simulations), along with advances in artificial intelligence and machine learning (AI/ML) techniques has offered unprecedented opportunities for data-driven science and discovery, which is the fourth paradigm of science. Within the arena of AI/ML, deep learning (DL) has emerged as a game-changing technique in recent years with its ability to effectively work on raw big data, bypassing the (otherwise crucial) manual feature engineering step traditionally required for building accurate ML models, thus enabling numerous real-world applications, such as autonomous driving. In this talk, I will present ongoing AI research in our group with illustrative applications in materials science. In particular, we will discuss approaches to gainfully apply AI/ML/DL on big data as well as small data in the context of materials science. I will also demonstrate some of the materials informatics tools developed in our group.

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

A known challenge in decision-based manufacturing of ceramics is that there are input uncertainties from data, models and model parameters. In a decision-based manufacturing environment, it is critical to know the probability that a ceramic will have a flexural strength below an acceptable limit. Regarding the flexural strength of silicon carbide (\945-SiC), an absolute error bound of ±15% was set as a baseline previously in literature. However, this is inadequate because the uncertainty can shift both in its mean and standard deviation due to manufacturing-caused changes in microstructure and porosity. A Bayesian-based approach is proposed to dynamically and precisely provide a live uncertainty quantification (UQ) in a smart manufacturing environment. Five scenarios with variably perturbed flexural strength data are demonstrated. Across the scenarios the goodness-of-fit to the mean, as measured by R^2, is improved by a range from 0.12-0.61. Also, uncertainty is reduced from ±15% to ±12-±8% depending upon scenario.

2:00 PM
Discovery of Multi-functional Polyimides through High-throughput Screening using Explainable Machine Learning: *Ying Li*[1]; [1]University of Wisconsin-Madison

Aiming to expedite the discovery of high-performance polyimides, we utilize computational methods of machine learning (ML) and molecular dynamics (MD) simulations. We first build a comprehensive library of more than 8 million hypothetical polyimides based on the polycondensation of existing dianhydride and diamine/diisocyanate molecules. Then we establish multiple ML models for the thermal and mechanical properties of polyimides based on their experimentally reported values, including glass transition temperature, Young's modulus, and tensile yield strength. The obtained ML models demonstrate excellent predictive performance in identifying the key chemical substructures influencing the thermal and mechanical properties of polyimides. Applying the well-trained ML models, we obtain property predictions of the 8 million hypothetical polyimides. Then, we screen the whole hypothetical dataset and identify three (3) best-performing novel polyimides that have better-combined properties than existing ones through Pareto frontier analysis.

2:20 PM
A Machine Learning-based Virtual Lab to Predict Yield Surfaces from Crystal Plasticity Simulation: *Anderson 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

At the continuum level, the plastic anisotropy of a wide range of metals and alloys is well described by advanced phenomenological yield surfaces. Relevant difficulties in their usage, however, are associated with the non-trivial parameter identification process and the non-uniqueness of the anisotropy coefficients. Alternative avenues for plastic flow prediction have been studied, and machine learning based approaches have gained notoriety due to their high fitting capabilities. We present a Machine Learning Virtual Lab for yield surface prediction, a framework that integrates crystal plasticity with deep neural network models and provides performance comparable to 3D yield functions. Important features such as well-defined flow vector, convexity, and multi-axial yield prediction are analyzed and compared against benchmark yield criteria.

2:40 PM
Intelligent Design & Manufacturing of High-performance Iron Castings Using AI/ML: *Jiten Shah*[1]; [1]Product Development and Analysis (PDA) LLC

High performance iron castings design and manufacturing have many variables with uncertainty impacting the casting quality and performance. A framework is developed for building meta models utilizing historical data and generating required missing data under controlled experiments and ICME based predictions. Author will present the meta models developed using AI/ML for predicting properties and porosity for sand cast ductile iron castings. For the design community, models assist predicting properties as a function of section thickness, feature orientation with respect to gravity and type of mold media coupled with processing parameters that will be presented. These meta models are demonstrated for a near real time intelligent processing of the castings in a production environment.

3:00 PM Break

ICME Design Tools: I

Monday PM
May 22, 2023

Room: Caribbean IV
Location: Caribe Royale

Session Chair: Katherine M Sebeck; US Army Combat Capabilities Development Command Ground Vehicle Systems Center

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

The geometric design of components traditionally consider the material as a monolithic structure, therefore not accounting for microstructural gradients that occur during the manufacturing process. The resulting material design allowables are conservative and associated with large uncertainty bounds. To improve precision in the life estimates, a location-specific lifing framework is developed, which tracks manufacturing processes and retrieves microstructural information at distinct locations for use within a crystal plasticity fatigue life prediction model. These approaches are used within a model-based feature information network to link the geometric features with material's simulation and analyses to streamline the product lifecycle management. A use case for microstructural-sensitive fatigue predictions of a dual microstructure heat treated turbine disk component is demonstrated near the bore (fine grains) and rim (coarse grains) regions. The proposed location-specific lifing framework presents new opportunities for simultaneously designing the component and tailoring the microstructures to meet the targeted performance.

1:40 PM

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

We present a workflow that combines atomistic, phase-field and FEM simulations to study the effects of alloy composition and of manufacturing process on the working performance of a component. In this approach, a component-scale FEM model of the manufacturing process captures the effect of process parameters and produces the inputs for a phase-field simulation of microstructural evolution. From the phase field method, an RVE of the microstructure is generated and introduced into an FEM micro-mechanical simulation to assess the mechanical potential of the microstructure produced. The workflow also produces homogenized properties for a macro-scale structural performance analysis of the component. We use first-principle calculations to assess the effects of alloy composition on performance by calculating the properties needed in the macro and meso-scale manufacturing simulations. We illustrate the workflow by simulating additive manufacturing of stable Titanium alloys.

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

Residual stress from fabrication can severely degrade structural performance over a ship's lifecycle. However, the evolution of the residual stress distribution throughout the shipbuilding process is not well understood. ICME techniques enable linking disparate software codes across multiple length scales, thereby facilitating simulation of the entire material lifecycle. This project pairs computational simulation with physical measurement for verification and validation (V&V) of the linked finite-element analysis (FEA) tools. The linked FEA tools, in a technique referred to as process chaining, enable simulation of a representative marine structure. Concurrently, the residual stress in an analogous physical structure was measured through each step of the fabrication process: incoming plate, cutting, and welded assembly. The effort followed specific areas within the component to understand the effects of fabrication on residual stress magnitude and distribution. This fabrication-cycle material information is essential to understand marine structures as the industry moves towards a digital twin standard.

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

The microstructure evolution of Nickel-base Superalloy ingot material through final melt and initial ingot breakdown is simulated using a multi-step simulation workflow. The local solidification rates predicted during the final melt are treated as inputs to predict the local grain features within the ingot. The sensitivity of the as-cast flow stress to local segregation predictions is evaluated. The data obtained from the melt simulation is mapped onto the element centroids of a continuum Finite Element simulation to evaluate the microstructure evolution during initial stages of ingot breakdown. The breakdown forging sequence is coupled to a mean field recrystallization model capable of capturing dynamic and post-dynamic recrystallization which updates the flow stress of the material point within the given simulation time step. The effect of grain orientation as implemented is evaluated. The simulation results are compared to laboratory data. The relative sensitivities of the inputs are identified to a first-order approximation.

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

Traditional approaches to define materials and associated manufacturing processes have been successful for many decades. These approaches rely on large quantities of experimental data to assess material properties, sensitivity to manufacturing processing paths, and potential sources for variation. As materials, processes and component designs are more exacting relative to definition of capabilities a new approach as part of integrated computational materials engineering has been established and successfully demonstrated with a range of materials and processes. The ability to predict component location-specific properties as a function of manufacturing path and operational utilization enables enhanced capability to predict component damage accumulation and life. The framework for model-based material and process definitions will be reviewed along with examples of how it can augment and greatly improve the traditional approaches based simply on empirical testing to establish critical material design curves.

3:00 PM Break

ICME Non-Metals: II

Monday PM
May 22, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: Karthik Rajan Venkatesan; Eaton

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

Polymethyl methacrylate (PMMA) is a thermoplastic polymer known for its optical clarity and hardness, among other properties, making it a commodity polymer. However, PMMA is susceptible to degradation arising from environmental factors such as UV, heat, and humidity. These stressors lead to performance loss and reduced lifetime service. In our work, six different formulations of PMMA containing various UV absorbers and stabilizers are exposed under three accelerated conditions, as per ASTM G154 and G155, in a longitudinal stepwise manner. We then quantified their performance metrics using colorimetric methods such as the Yellowness Index and obtaining UV-vis, fluorescence and Fourier-transform infrared (FTIR) spectra. The data collected are then modeled with netSEM (Network Structural Equation Modeling), which provides inferential and predictive data-driven models. These data-driven models are selected based on adjusted R2 values and stepwise regression is performed using either Akaike (AIC) or Bayesian (BIC) Information Criteria to avoid complexity and overfitting.

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

Large scale additive manufacturing (LSAM) of thermoplastics is a manufacturing process that is being adopted by industry for different manufacturing applications. However, LSAM faces multiple design challenges, including process dependence of the material properties resulting from fiber orientation, inter- and intra-bead voids, and design constraints from the deposition process. This work seeks to address these challenges via Analytical Target Cascading (ATC) multilevel optimization algorithm. Utilizing a process-informed simulation of a finite element model of a stiffened panel, ATC optimizes the process and material properties of the part coupled with the part design. The ATC optimization algorithm is demonstrated for mass minimization of a 3D-printed rectangular stiffened plate within a 4000 × 1000 × 500 mm3 design volume, with simple-support boundary conditions along all edges, loaded in uniaxial compression, and modeled using classical lamination theory. Results indicate mass reductions exceeding 20% compared to the baseline model, while keeping manufacturing feasible.

4:00 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

Recent successes in Integrated Computational Materials Engineering (ICME) have demonstrated the potential in designing fit-for-purpose materials for a given application in a cost and time efficient manner. However, the material design process must contain a level of automation in the material decision process, implementing some optimization algorithms, to truly enable the full benefits of ICME, particularly when considering materials at multiple length/time scales. In this work, we will demonstrate how the GRC ICME schema and Python framework automates a workflow that captures, analyzes, maintains, and disseminates the digital footprint in the context of tailoring resin material at the nanoscale of a woven composite Y-joint at the macroscale for an Aurora D8 double-bubble fuselage. This digital footprint incorporates the interaction of both structural digital twins and material twins at various length scales.

4:20 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

Polymer composite structures are heavily used in aerospace, defense, transport, and energy sector due to their lightweight and high-performance behavior. The behavior of these structures highly depends on curing process as it affects evolution of material properties, residual stresses, deformation, etc. Various cure process parameters, mainly temperature cycle with respect to time, need to be optimized to get the desired characteristics for these structures. In this paper, the cure process is explicitly modeled through finite element method. Its effects are captured by modeling thermo-chemical-mechanical analysis through multiple length scales. Traditional optimization techniques are time-consuming due to the unavailability of gradients, larger simulation time and exploration space. Bayesian optimization algorithms used in this study overcome these challenges pertaining to cure process optimization. Insights from such optimization can be utilized by product designers as well as manufacturers to take timely decisions to improve the performance of these composite structures.

Artificial Intelligence /Machine Learning: Properties II

Monday PM
May 22, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: See Session Sheets

3:20 PM

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

Mechanical properties of metals and their alloys are strongly governed by their microstructure. The nanometer-sized precipitates in hardenable wrought aluminium alloys, which can be controlled by heat treatment, act as obstacles to dislocation movement within the material and are critical to the mechanical performance of the component, in this case, a radial compressor wheel of a ship's engine. Deep Learning based TEM image analysis is essential for the study to investigate the microstructural changes (precipitation coarsening) that occur as a result of aging at elevated temperatures.

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

Recent advances in data science and high-throughput materials simulations are being evaluated to accelerate advanced steel alloy development. Here we use machine learning (ML) to take advantage of the large amounts of historic data available for martensitic steels. A series of methods using varying amounts of data are used to develop predictive ML models. Our hypothesis is that the composition and processing variables are insufficient to inform a robust machine learning model, and the incorporation of CALPHAD inputs will provide the additional information required to inform the models and make a more robust framework that is generalizable to other systems. These intermediate variables are synthetic microstructures and thermodynamic properties generated using high-throughput CALPHAD simulations. We present a preliminary integrated machine learning and alloy design workflow based on steel hardness and toughness response during tempering. Model uncertainty and databasing challenges will also be discussed.

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

To reduce nuclear proliferation, low-enriched U-10Mo alloy has been identified as a promising fuel candidate for United States high-performance research reactors. During fabrication, the fuel will be encapsulated in the aluminum alloy 6061 (AA6061) cladding, to prevent fuel corrosion and fission product release. The cladding was diffusion bonded using the hot isostatic pressing (HIP), which promotes a homogeneous AA6061/AA6061 bonding interface. To reduce the high experimental cost and efficiently optimize the diffusion bonding process, a multi-fidelity Gaussian process surrogate was developed to predict the aluminum cladding bond strength. This machine learning surrogate leverages the high-fidelity experimental data with the low-fidelity numerical model to maximize the bond strength prediction accuracy. Sensitivity analysis was followed to identify the influential HIP parameters. It was found that the interface Mg2Al2O5 particles were closely related to the bond strength and the temperature was suggested as the most dominant factor in determining the bonding quality.

4:20 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

Advanced high strength steels are generally designed to meet target mechanical properties either by modifying the alloy composition or engineering the microstructure via processing. Despite the advances in computational tools available to model the process chain, exploring the vast design space is extremely challenging for achieving the target properties. Recently, generative design approaches that are used in product design are presently being envisaged for alloy design. A generative design based framework is developed for active exploration and optimization of alloy chemistry and process parameters for an integrated computational process chain consisting of casting - reheating - hot rolling - cooling (ROT+coiling) - properties in the design of hot rolled HSLA steel for desired properties through thin slab as well as conventional casting and rolling routes. The details of the novel approach, constraints, and limitations will be presented.

Materials Databases & Platforms: II

Monday PM
May 22, 2023

Room: Caribbean IV
Location: Caribe Royale

Session Chair: Raymundo Arroyave; Texas A&M University

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

The qualification and certification (Q&C) process presents a significant challenge for widespread adoption of additive manufacturing (AM) materials and processes for aerospace applications. A relational database framework will be presented as a tool for data curation of coordinated experimental and computational materials modeling research activities. A comparison of relational and hierarchical data structures in this domain will be emphasized through the evolution of a database design strategy. This framework's mission is to support the advancement of computational materials-informed Q&C by providing the necessary data infrastructure to trace reliability and reproducibility measures through unified AM materials simulation and experimental testing. FAIR (findable, accessible, interoperable, and reusable) data will be highlighted as a necessary precursor for automation of specific actions, which ultimately reduces the time and expense burden for Q&C. The discussion will be mostly limited to back-end design elements, though a few front-end user experience examples will also be shared.

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[2]; [1]Thermo-Calc Software; [2]Thermo-Calc Software Inc

Viscosity, surface tension of liquid, thermal/electrical conductivity, and their composition and temperature dependence, are all important properties for modeling the AM process together with heat and heat capacity. While the treatment of heat and fluid flow is considered as state of the art in current FEM models, material properties are treated in a highly simplified manner. During the last few years new models to predict thermophysical material properties using the CALPHAD method have been developed and by adopting a unified treatment of both process parameters and alloy dependent thermophysical properties, there is the potential for more accurate solidification simulations for AM. This presentation will describe how such an approach has been adopted to implement into Thermo-Calc a module for Additive Manufacturing. This combined approach can be thought of as an example of ICME (integrated computational materials engineering). Examples will be shown together with other ongoing/completed developments related to AM.

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

There is a need for consolidation of multi-modal datasets obtained from sensors within AM machines, build planning, and post-build imaging and analysis, going through the entire AM pipeline. We propose a database repository, built on the FAIR principles, to assist the application of machine learning tools that can harness the immense amount of data that has already been generated and set up protocols to deal with future data generation. This ranges from powder characteristics to build data to part analysis. The challenges of effectively using machine learning tools often come from a lack of sufficient and structured data. Enabling this structure throughout the AM pipeline will set a standard for future ML analysis and by knitting together disparate data sources, we can facilitate data fusion and analysis across the entire AM pipeline. We address the challenges of storage capacities, file naming conventions, and data retrieval for analysis.

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

Corrosion-Resistant Alloy Design and Lifetime Evaluations (CRADLE) platform is designed to combine first-principles data, machine learning, and data visualization for improving corrosion resistance. The platform consists of a database server, a data processing server, a machine learning (ML) server, a multi-objective optimization code, and a web-based interactive GUI. The MongoDB database can use in-house first-principles calculation results and open public access databases. The closed-loop corrosion prediction and alloy design using surface energy, work functions, and texture in a machine-learning model can be improved by users using their own data. The CRADLE framework can fuse data sets, use ML to predict higher corrosion-resistant phases, and launch first-principles calculations as needed. We will demonstrate the case of printable high entropy alloys in search of more corrosion-resistant and single-phase high-entropy alloys in the Fe-rich and low-Ni phases. The CRADLE is open access with web-based with local Docker installation.

Scientific Workflows for ICME: I (Microstructure)

Tuesday AM
May 23, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: Michael Tonks, University of Florida

8:00 AM Invited
NexusLIMS: A Laboratory Information Management System for Shared-use Electron Microscopy Facilities: *June Lau*[1]; [1]NIST

Presently, the management and the processing of research data produced by scientific instrumentation is a significant challenge. Electron microscopy researchers work with different make and model of microscopes and detectors, and with these, data produced in various (sometimes proprietary) formats. Users often implement ad hoc strategies to curate and disseminate this data. Often, data and the context under which they were acquired is irrecoverable beyond the few published images in journal articles. To capture microscopy data consistent with the FAIR data principles, we built NexusLIMS, a laboratory information management system managing microscopy output across two NIST campuses. While this example may be microscopy-specific, many of the components and concepts within are extensible to data produced by other instruments. We will show additional data infrastructure components that are co-integrated with NexusLIMS, such as central file servers, schedulers, and compute resources, and how this integration has nucleated an ecosystem for research data.

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

X-ray computed tomography (XCT) is a powerful tool for studying corrosion of commercial bond-wires. This investigation amasses large amounts of image data. Analysis of a 3D-rendered object can be computationally costly and time-consuming, while performing the task manually is impractical. The cylindrical geometry of commercial bond-wires is challenging to characterize as 3D renders, adding to the computational complexity of the analysis. Developments in computer vision tools, which leverage convolutional neural networks (CNNs) are computationally efficient and fast, making them desirable tools for automated feature extraction. In our work, we demonstrate an automated workflow for transforming a cylindrical object into a 2D representation and performing background denoising that allows for full surface view for further characterization. We integrated semantic segmentation algorithms such as DeepLab into our workflow pipeline allowing for further characterization of the surface features of the bond-wires. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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

Quantitative surface-based microscopy measurements of key and ubiquitous microstructural features (e.g., grains, fibers, internal porosity) is a foundational activity in materials engineering to establish process-to-structure-to-property relationships, as well as to provide ground truth measurements for other purposes (such as advancing nondestructive characterization methods). The need for rapid and unbiased microstructure measurements has spurred the materials community over the past three decades to develop automated microscopy methodologies to provide such information with little-or-no human intervention, which critically rely on robust data acquisition and data post-processing workflows. This contribution will present an overview of such workflows for microstructure quantification in 2D and 3D of structural materials using both reflective light and scanning electron microscope-based techniques, and highlight examples of quantitative measurements of microscale features and defects within mm-to-cm scale volumes. In addition, the contribution will discuss potential areas of improvement to further enhance digital microscopy workflows.

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

Fluoroelastomer crystallization can be easily observed using atomic force microscopy, AFM, to look at surface properties and macro-scale morphologies. In-situ measurements investigating phase-transition kinetics of fluoropolymers, under isothermal heating, generate a large dataset of time-lapsed image sequences. Interpretation of the resulting images is guided by domain-knowledge and image processing is done manually using software, which is time-consuming. In our work, we integrate automated image detection and image segmentation methods, based on convolutional neural networks in our image processing. The resulting pipeline is an end-to-end framework, which aims to automatically classify and analyze images as part of batch processing. The product of this framework can extract individual crystallites and track their growth throughout the course of the image sequence with only a few training data. Then, statistical analysis can then be incorporated opening opportunities to investigate fluoroelastomer crystallization kinetics.

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)

Certain metallic materials gain better mechanical properties through controlled heat treatments. In age-hardenable aluminum alloys, the strengthening mechanism is based on the controlled formation of nanometer sized precipitates, which hinder dislocation movement. Analysis of the microstructure and especially the precipitates by transmission electron microscopy allows identification of precipitate types and orientations. Dark-field imaging is often used to image the precipitates and quantify their relevant dimensions.The present work aims at the digital representation of this material-specific characterization method. Instead of a time-consuming, manual image analysis, a digital approach is demonstrated. The integration of an exemplary digital workflow for quantitative precipitation analysis into a data pipeline concept is presented. Here ontologies enable linking of contextual information to the resulting output data in a triplestore. Publishing digital workflow and ontologies ensures the reproducibility of the data. The semantic structure enables data sharing and reuse for other applications and purposes, demonstrating interoperability.

9:50 AM Break

Artificial Intelligence /Machine Learning: Alloys

Tuesday AM
May 23, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: Harikrishnan Rajendran; Boeing Research & Technology

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

The efficient exploration and exploitation of compositionally complex alloy spaces is extremely resource-intensive and most conventional approaches (e.g. traditional ICME and open-loop combinatorial methods) are not effective. Here, I present our recent work on the development of BIRDSHOT. BIRDSHOT incorporates the strengths of ICME and combinatorial methods while addressing all their drawbacks, as it: (i) employs novel machine learning (ML) and data-driven search algorithms to identify efficiently the feasible regions amenable to optimization; (ii) exploits correlations to fuse simulations and experiments to obtain efficient ML models for predicting PSPP relations; (iii) uses Bayesian Optimization (BO) to make globally optimal iterative decisions regarding which region in the RHEA space to explore/exploit, leveraging existing models and data; (iv) leverages the team's newly developed batch modifications to BO that enable the parallel, iterative and optimal exploration/exploitation of materials spaces; and (v) is capable of simultaneously considering multiple objectives and constraints.

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

Multi-principal element alloys (MPEAs) present a paradigm shift in materials design and consist of multiple principal elements randomly distributed on a crystal lattice resulting in an enormous phase space. On the one hand this presents opportunities to unravel novel properties whereas on the other it presents a large challenge to survey the phase space, presenting a data-science challenge. We present PREDICT (PRedict properties from Existing Database In Complex alloys Territory), a machine learning framework coupled with electronic structure methods whereby properties in MPEAs could be predicted by learning from the binary alloys database. Specifically, we demonstrate predictions of stiffness constants, Young's modulus, bulk and shear moduli, and Poisson's ratio in ternary, quaternary, and quinary MPEAs with a high-level of accuracy. A major benefit of this is that for every new composition discovered, the mechanical properties can be computed using only the existing binary alloy database, bypassing the computationally expensive calculations.

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

A descriptor-less machine learning (ML) model based only on charge density extracted from density functional theory (DFT) is developed to predict stacking fault energies (SFE) in concentrated alloys. Often, in most ML models, textbook physical descriptors such as atomic radius, valence charge and electronegativity are used which have limitations because these properties change in concentrated alloys when multiple elements are mixed to form a solid solution. We illustrate that, within the scope of DFT, the search for descriptors can be circumvented by charge density, which is the backbone of the Kohn-Sham DFT and describes the system completely. The model is based on convolutional neural networks (CNNs) as one of the promising ML techniques. The performance of our model is evaluated by predicting SFE of concentrated alloys with an RMSE and R2 of 6.18 mJ/m2 and 0.87, respectively, validating the accuracy of the proposed approach.

9:10 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

CCAs are of interest as structural materials in molten salt reactors because current alloys certified by ASME Sec(III) Div(5) code for their mechanical properties contain high Cr that are readily corrodible in molten halides due to the thermodynamic favorability of Cr corrosion in halides at nuclear reactor operating conditions. Corrosion of compositionally complex alloys (CCAs) in molten halides is not straightforward to predict because they do not possess one obvious base element whose kinetic and thermodynamic behavior provides the basis for prediction. The lack of prediction capability presents a bottleneck to search a quasi-infinite compositional space for a particular set of alloying elements for CCAs that could be suitable for molten salt reactor structural materials. We present a generalizable Random Forest Regressor (RFR) model trained and tested on 110 experimentally tested CCAs. Shapley analysis was used to interpret the model and extract alloy design parameters for optimizing corrosion resistance.

9:50 AM Break

Linkages: Deformation I

Tuesday AM
May 23, 2023

Room: Caribbean IV
Location: Caribe Royale

Session Chair: Karthik Rajan Venkatesan; Eaton

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

A multiscale materials modelling framework is presented for simulating the microstructure and mechanical fields during selective laser melting (SLM) of a precipitate strengthened nickel-based superalloy. The approach accounts for physical phenomena associated with the additive process over a number of spatial and temporal scales including solid-liquid-vapour transitions, solidification microstructures (grains and precipitation of) and defects. A crystal plasticity model is developed for simulation of the mechanical fields and accounts for dissolution and precipitation of particles for the alloy CM247. Stress jumps acting on grain boundaries are extracted, showing the cyclic thermal loading of these boundaries to be sensitive to local texture as well as spatial gradients of the thermal fields generated by the moving heat source. Location of boundaries (relative to the passing melt pool) with high risk of resulting in cracking of a build are identified and discussed in relation to process parameters.

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

Digital twins based on full field crystal plasticity models serve as an alternative to expensive and time-consuming micro-mechanical experiments. These experiments are, however, still needed as benchmarks for the predictive quality of the modeling approaches. Here we use experimental data of additively manufactured IN625 alloy provided by the Air Fore Research Laboratory as part of a modeling challenge to study the performance of full field crystal plasticity simulations using DAMASK. In particular, we investigate how the choice of the constitutive model and the incorporation of eigenstrains influence the agreement between simulation and experiment.The challenge of initializing the simulation with a realistic field of eigenstrains when only data from a few grains is available is tackled through the use of an iterative scheme that results in an equilibrated eigenstrain field that is in agreement with the experimental data.

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

A three-dimensional microstructure of additively manufactured (AM) and post-processed Inconel-625 alloy generated as part of the AFRL's Additive Manufacturing Challenge Series is considered for the purpose of validating the modeling predictions of a crystal plasticity finite element (CPFE) solver. Far-field high-energy X-Ray diffraction microscopy (ff-HEDM) measurements of grain-average elastic strains, on a specimen loaded in tension at room temperature, are compared with predictions from a CPFE framework. The ff-HEDM measurements, obtained while the specimen was held under load-control, were made on the same microstructure considered in the CPFE framework. This one-to-one comparison enables a detailed study of the sources of discrepancy between simulation and experiment, including a thorough investigation of the sources of modeling errors. It is shown that over-constrained boundary conditions and the inability of the CPFE solver to account for stress-relaxation events (which happens during the constant-load holds) contribute to the modeling errors.

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

This work demonstrates the effective ICME workflow to understand the process-microstructure-property linkage of AM metals. Firstly, melt pool modeling will be performed to predict melt pool temperature distributions, which will be used to simulate microstructure evolution during the AM process with methods like Cellular Automata. We will then create synthetic microstructures of AM using statistical descriptions of microstructural features predicted as input. At the single grain level, we utilize a phase field solidification model coupled with a thermomechanical crystal plasticity, enabling us to assess both intra-grain/polycrystal level dislocation/stress heterogeneities introduced during solidification and residual stresses. In the final step, physics-based crystal plasticity model will be applied to the synthetic microstructures generated from the previous step, and micromechanical simulations will be performed to predict the anisotropic deformation behavior and ultimately damage of AM metals. This aims to significantly reduce time and cost required for AM development with the ICME workflow presented.

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

Nano-architectected metals can exploit the combination of resilient architecture with size-dependent enhanced properties at nanoscale to achieve exceptional mechanical performance. To obtain a mechanistic understanding of plastic deformation in these materials requires an integrated computational model which can capture the relation between dislocation microstructure characteristics and macroscopic mechanical behaviors. Recently, we develop a multi-scale model to concurrently couple dislocation dynamics (DD) modeling with finite element method (FEM). The DD simulation keeps track of dynamic motion of dislocations and compute the accompanying plastic strain, while FEM simulation solves for the stress field to satisfy equilibrium condition. By integrating these, our model could provide a unique opportunity to investigate fundamental deformation mechanism based on dislocation plasticity and corresponding macroscopic mechanical response. In this study, multi-scale simulations of meso-scale architected structures under uniaxial compression were performed. The architected structures exhibit increasing strength with decreasing unit cell size, which agrees with experimental observations.

9:50 AM Break

Artificial Intelligence /Machine Learning: Microstructure II

Tuesday AM
May 23, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: Austin E. Mann; Boeing Research & Technology

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

Microstructural features influence material properties, thus characterization of these features is essential to understanding and predicting material performance. One powerful tool for microstructural characterization is electron backscatter diffraction (EBSD). EBSD is a scanning electron microscopy (SEM) based technique that provides information about crystal structure and orientation, allowing quantification of important features such as shape, size and orientation of grains. While EBSD can provide detailed and accurate information about microstructures, this technique is time-consuming and expensive, limiting its utility for high-throughput microstructural analysis. Here, we describe deep convolutional neural networks that take backscatter electron SEM images, which are easier and faster to collect, and perform semantic segmentation to identify grains and grain boundaries, allowing for microstructural analysis typically accessible through EBSD. We demonstrate the utility and accuracy of our models by performing grain size and shape analysis for stainless steel.

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

The work seeks to create a dataset of secondary election images of Ti-6Al-4V fatigue fracture surfaces and apply transfer learned Convolution Neural Networks (CNNs) to the dataset to make connections between the fracture surfaces and the fatigue life, with the goal being fractography by computer. The images consist of the crack initiation site, short crack region, steady crack growth, and instantaneous failure region on multiple samples with varying loading conditions and fatigue lifetimes. Unsupervised learning which consists of dimensionality reduction and clustering is used to determine which subset of data, i.e., which crack growth region or magnification, provides the most physically meaningful information. Additionally, the features of those images that are deemed most important provide information that can tie the fracture surface to the fatigue life and microstructure. The images taken, the algorithms used, identified fatigue properties, and fracture characteristics will be presented.

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

Spatiotemporal studies of material degradation have rapidly improved with the high resolution imaging capabilities of X-ray computed tomography (XCT). Materials science, however, lacks the tooling to analyze the scale of data produced. As a result, analysis is limited to manually segmented features and subsets of data which is time consuming and results in large information loss. We propose leveraging computer vision and deep learning to develop automated frameworks for full-scale feature extraction and analysis. Slow strain rate tension tests were conducted with collaborators at the Diamond Light Source on field-retrieved Al-Mg plate material removed after 42-years of service exposure. A sample at 50%RH and a sample in dry air were tested to determine the effects of long-term service on stress corrosion cracking. We developed an automated deep learning pipeline that segments features of interest, quantifies their properties, and builds a complete spatiotemporal microstructural degradation profile of the dataset.

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

The quantification of the amount of absorbed light is essential for understanding laser-material interactions and melt pool dynamics in additive manufacturing process. The geometry of a vapor depression, also known as a keyhole, in melt pools formed during laser melting is closely related to laser absorptivity. This relationship has been observed by the state-of-the-art in situ high speed synchrotron x-ray visualization and integrating sphere radiometry. These two techniques create a temporally resolved dataset consisting of keyhole images and the corresponding laser absorptivity. In this work, we propose two different pipelines to predict laser absorptivity. The end-to-end approach uses deep convolutional neural networks to interpret an unprocessed x-ray image and predict the amount of light absorbed. The two-stage approach uses a fine-tuned image segmentation model to extract geometric features and predict absorption using regression. Though with different advantages and limitations, both approaches reached an MAE less than 6.9%.

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

Transmission electron microscopy (TEM) data generated in the form of bright field screenshots of microstructure can be used directly to study dislocations in great detail but is limited by the difficulty in identifying and extracting these individual defects. We attempt to automate the study of dislocations present in TEM images using a deep learning network, U-Net which can segment dislocations. Here we present a parametric model to generate synthetic training data for the supervised machine learning task of dislocation segmentation. Experimentation with different synthetic datasets which vary in dislocation microstructure as well as background for synthetic images suggest that a general synthetic data which requires very little input from real data can give better results. This study shows the importance of using synthetic training data to help studying large and real TEM data in great detail.

Applications: Alloy Design I

Tuesday AM
May 23, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: Paul Mason; Thermo-Calc Software Inc.

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

The main challenges in developing next-generation refractory alloys for ultrahigh-temperature service beyond nickel-base superalloys are balancing room temperature ductility & fracture toughness, and high temperature strength and creep resistance, while maintaining comparable oxidation resistance and densities to Ni-base superalloys. This project integrates multi-scale computational modeling with direct energy deposition additive manufacturing to rapidly design precipitation strengthened refractory high entropy alloy for use at 1300 degree Celsius and above. Specifically, high throughput phase diagram calculations and screening are carried out using CALPHAD; density functional theory calculations are performed to predict intrinsic ductility, grain boundary segregation energy, coefficient of thermal expansion and temperature-dependent elastic constants. Down-selected alloys are synthesized in small buttons of about 250g using arc melting for rapid evaluation on microstructure and mechanical properties before employing plasma arc melting and additive manufacturing for producing large ingots. Preliminary computational and experimental results of this project will be presented.

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

Body-centered cubic (bcc) refractory multicomponent alloys are of great interest due to their remarkable strength at high temperatures. Optimizing the chemical compositions of these alloys to achieve a combination of high strength, room-temperature ductility, and corrosion resistance remains challenging. With physics-informed descriptors and a simple bond-counting model, we developed regression models to predict the unstable stacking fault energy (usf) and surface energy (surf) for BCC multicomponent alloys. Then we develop hierarchical screening models to identify promising alloys from a 13-element composition space (Ti-Zr-Hf-V-Nb-Ta-Mo-W-Re-Ru-Al-Cr-Si). We rapidly screen over ~10 million quaternary alloys using our regression models to search for alloy candidates that may have enhanced strength-ductile synergies. The results combined with high-throughput thermodynamics calculations are used to discover ~1000 promising bcc refractory alloy compositions with potentially high ductility potency, the thermodynamic stability of single bcc phase at least at 800 C, and the thermodynamic capability to passive oxide films.

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

Thermal Barrier Coating (TBC) material are used to protect gas turbine blades from high temperatures. Yttria-Stabilized Zirconia (YSZ) is widely used TBC material with a maximum operational temperature of 1600 K. With the ever-increasing demands of fossil fuels and its impact to environment it is crucial to design materials that can serve at ultra-high temperatures without failure to increase the efficiency of engines. In this study we present new High Entropy Oxides (HEOs) designed on the basis of first principal calculations. Phonon calculation were performed to determine thermal expansion and conductivity of the compounds. We found that these materials possess ultra-low thermal conductivity (k) and higher stability above 1600 K. Due to increased configuration entropy and high structural distortion there is enhanced phonon scattering and hence the material possess ultra-low thermal conductivity. HEOs are compared to YSZ via an assessment of phonon dispersion, phonon lifetime, group velocity and thermal conductivity.

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

The properties of additively manufactured materials are intimately connected to the solidification process. The interfacial velocities found during additive manufacturing can lead to interfacial nonequilibrium at the moving solid-liquid interface. A thermodynamic description of moving non-equilibrium interfaces is developed that is applicable to concentrated multicomponent alloys. We find that solute drag affects both the velocity of the interface and distribution coefficients for the compositions of the two phases at the interface. This theory has been integrated with a description of dendritic growth in multicomponent alloys that incorporates CALPHAD descriptions of the Gibbs free energies and diffusion matrices with off-diagonal diffusion coefficients. This computational tool yields morphology diagrams for the solidification morphologies of complex multicomponent alloys of industrial importance during additive manufacturing. Examples of such diagrams for alloys of commercial importance, such as stainless steel 316L, will be given.

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.

High entropy alloys (HEA) are emerging as superior catalysts for diverse chemical conversions. While their vast compositional and configurational degrees of freedom offer a rich platform for catalyst discovery, elemental segregation could limit the chemical diversity at the surfaces of these alloys. Building upon our recent work (Dahale et al, Mol. Syst. Des. Eng., 2022,7, 878-888), we use a combination of machine learning based adsorption energy prediction and Bayesian optimization to identify AgAuCuPdPt HEA compositions that are both active and selective for CO_2 reduction reaction (CORR). We further show that, the reduction in the chemical diversity at the surface due to elemental segregation causes only a marginal change in the activity but a significant enhancement in the selectivity for CORR.

Scientific Workflow: II

Tuesday AM
May 23, 2023

Room: Caribbean IV
Location: Caribe Royale

Session Chair: Michael D. Uchic; Air Force Research Laboratory

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

Though lower fidelity than full-field crystal plasticity models, the computationally inexpensive viscoplastic self-consistent polycrystal plasticity model (VPSC) should excel in the high-throughput, rapid-iteration ICME paradigm. However, the text-file interface creates a steep learning curve, and lack of published automation tools for VPSC limits its potential value for ICME. The authors discuss development of a modern application programming interface (API) in MATLAB which streamlines user interaction and includes functionality for automating VPSC experiments. The MTEX toolbox—a library of MATLAB code for representing and transforming crystallographic, microstructural, and deformation data—is used as the exemplar for an easy-to-learn modern API, with a planned integration of the VPSC automation API into the MTEX toolbox for wider accessibility. To demonstrate the high-throughput capabilities, a case study will be presented that uses the VPSC automation API as part of an ICME strategy to optimize the energy efficiency of titanium alloy processing.

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

Indentation testing is a convenient and relatively cheap experiment. However, extracting the data from indentation tests requires complex post-processing, often with integrated simulations. Accordingly, the simulation of indentation has become a post-processing routine for indentation tests. Providing a highly efficient, computationally scalable, and open-source platform for indentation simulation provides invaluable machinery for materials design process. An open-source PRISMS-Indentation module is presented here as a multi-scale elasto-plastic virtual indentation framework. The module is implemented as a part of PRISMS-Plasticity software which covers length scales of continuum plasticity and crystal plasticity. The contact problem is handled using active set methods. The efficiency and scaling of the framework are then investigated by simulating a set of indentation problems at different length scales.

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

PRISMS-PF is an open-source, high-performance framework for phase-field simulations of microstructure evolution. It contains over 30 built-in applications to simulate a variety of phenomena, from microgalvanic corrosion to precipitate growth. We present an overview of the framework, including the latest developments in performance, flexibility and ease of use, with emphasis on the latest efforts to integrate PRISMS-PF with other computational frameworks of the PRISMS Center. The first of these is the ongoing work towards integration with PRISMS-Plasticity for coupled modeling of processes such as twin morphology evolution, and static and dynamic recrystallization. The second is the effort towards streamlining integration with the CASM (Cluster Approach to Statistical Mechanics) framework for automated capturing of input physical parameters required by phase-field simulations. Finally, we discuss the latest tools for metadata generation and simulation data storage and organization within the Materials Commons information repository and collaboration platform.

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

A rich, high-quality data set of metal deformation is necessary to calibrate microstructure sensitive elasto-plastic models. Profilometry-based indentation plastometry (PIP) can be used to study spatial variation in bulk plastic response; however, uncertainty in PIP tests can significantly impede accurate estimation of the variability. PIP relies on a finite element method simulation and a constitutive model of plasticity to calibrate plasticity parameters to the profile of the spherical indentation in an iterative fitting procedure. Here, the uncertainty of the PIP procedure is mitigated to enable the estimation of spatial variability of bulk plastic response at the mm length scale. 2D profile measurements taken by optical profilometry (OP) augment the 1D profiles of the standard PIP method. The uncertainty of both procedures is quantified. Whether PIP is an appropriate test for capturing the variations in plastic response is discussed.

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

We present an integrated experimental-modeling framework to quantify uncertainty during the calibration of crystal plasticity model parameters. In-situ X-ray diffraction microscopy measurements yield intergranular lattice orientations and strain tensors at designated states during R=-1 cyclic loading of a Ni-based superalloy. Intragranular fields of incompatible deformation are generated by post-processing measured strains via an anisotropic linear elastic constitutive model augmented by the theory of continuous distribution of dislocations. Complementary fields of back stress are generated via a crystal plasticity formulation with an Armstrong-Frederick-type back stress evolution law. The synthesis of simulated and measured deformation fields provides a basis for quantifying uncertainty in the parameters for evolution of back stress. Preferred reorientation of the crystallographic lattices along with these internal stresses govern the onset of plasticity and the activation of multiple slip systems which developcomplex residual stresses. The framework provides a pipeline to calibrate and quantify uncertainty in alternate material models.

Applications : Advanced Manufacturing Microstructure I

Tuesday PM
May 23, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: Adam E. Kopper; Mercury Marine

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

Additive manufacturing is a powerful method to produce an industrial part with flexible shape and superior mechanical properties. In the additive manufacturing process, a laser heating causes a melting of material, followed by a rapid cooling that results in formation of unique solidification microstructures. The multi-phase-field method is a powerful numerical simulation method to quantitatively predict the microstructure evolution during the rapid solidification in the additive manufacturing process. In this study, the rapid solidification in SUS316L stainless steel during the additive manufacturing is simulated using the non-equilibrium multi-phase-field model that is able to simulate microstructure evolutions under a strong non-equilibrium condition. The thermodynamic calculations for the multi-component SUS316L stainless steel in the multi-phase-field simulation were accelerated using aritificial neural networks. In this presentation, we present a computational framework to train the aritificial neural networks with the thermodynamic database and to implement the trained neural network into the multi-phase-field simulation.

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

Laser powder bed fusion (LPBF) for stainless steels can produce components with novel designs and material properties. However, LBPF processes introduce variance in mechanical properties and as built geometries even with identical settings on a single machine. Quantifying the uncertainties introduced by LBPF is essential for component qualification. This work presents probabilistic predictions of microstructure variability in LPBF. A high-fidelity thermal fluid model is used to predict the melt pool behavior (i.e., temperature/phase) and it's variance due to processing uncertainties. These data are used to predict microstructure size, shape and crystallographic texture using a coupled grain nucleation and kinetic Monte Carlo model for grain growth. Variability due to microstructure model parameters are also considered. This analysis will provide a tool for designers to predict a generalized margin of design for the mechanical properties of additively manufactured parts.SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

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

Process-structure simulations for metal additive manufacturing involve computing temperature fields, grain growth, and other relevant physics on a discretized domain. The discretization length scale is typically adjusted to achieve a desired convergence level for output quantities without incurring excessive computational cost. However, the same discretization may not produce acceptable error across different material systems or process parameters, requiring ad hoc adjustments for different input parameters. This work seeks to define scaling laws that relate a normalized discretization measure to errors in microstructural and crystallographic texture-based outputs across input parameter space. A case study is conducted using a computational materials framework that couples an analytical thermal model with a microstructural evolution model to simulate the laser powder bed fusion process. Normalizing length scales in the model are identified through dimensional analysis. The key outcome is a more rigorous and consistent approach for selecting a discretization length scale in process-structure simulations.

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

The ability to control microstructure in high-strength steel via additive manufacturing (AM) is of interest for many structural applications, providing a means to homogenize mechanical properties across varied part geometries and implement designed heterogeneities. The localized application of heat during AM, coupled with predictive modeling, enables the optimization of microstructure for steels showing sensitivity to AM parameters. One such steel is known as AF9628. This steel's final microstructure is mediated by the prior austenite microstructure. The current work presents a model that captures the evolution of the parent austenite grain structure in AF9628 during AM processing using a Potts/Monte Carlo method implemented in the SPPARKS software. This model is used to predict austenite grain size and morphology as a function of processing and can be used as a design tool for the control of austenitic and final microstructures.

2:40 PM Break

Applications : Advanced Manufacturing Processing II

Tuesday PM
May 23, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: Faith G. Sen; Novelis

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

Designing material systems with reproducible desirable properties remains a challenge for the fabrication of metal additive parts. The overall performance of a material can be heavily influenced by both direct and indirect stressors. In this work, spatiotemporal models were leveraged to model the spatial and temporal coherence between deposits of both single and multi-track additively manufactured stainless steel (SS 316L) samples using laser powder bed fusion (LPBF). Initially, interactions and potential additive effects between variables were established using exploratory data analysis. After, statistical modeling was used to generate insights and model the data. Network structural equation modeling (netSEM), p-values, and correlations were employed to perform variable selection followed by modeling using generalized linear models (GLM) and general additive models (GAM). These techniques successfully modeled the data which suggests that predicting pore formation for LPBF deposits is possible using statistical learning approaches, even when a limited number of points are available.

1:40 PM
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

In this paper, a previously proposed [1] constitutive equation that describes the behavior of viscoelastic materials is used to predict the behavior of PMMA (polymethyl methacrylate) under creep loading at different stresses and temperatures for varying amounts of time. The three parameters in the constitutive equation, k,, and are found by performing calculations on data from three tensile experiments and two creep experiments on a viscoelastic material. A GUI MATLAB application was written that used excel data from the experiments as input to predict the creep response for PMMA at any load, temperature, and timescale. The results of several predictions are compared against experimental data and good agreement was found.

2:00 PM
Tensile Loading Modelling of Laser-deposited AlCoCrFeNiCu High Entropy Alloy Using Comsol Multiphysics: *Modupeola Dada*[1]; Patricia Popoola[1]; [1]Tshwane University of Technology

A CAD solid model can generate near-net form, fully dense metallic objects with moderately complicated geometrical characteristics using Laser Metal Deposition technology. Results show that alloys with high entropy can reach good mechanical properties via additive manufacturing. A fine grain structure will develop because of the localized nature of the laser heating process, leading to a considerable improvement in yield strength without sacrificing ductility. However, in layers deposited by laser melting of alloyed high entropy alloy powders, significant tensile tension may develop; furthermore, high entropy alloys with dominant BCC structures may be too brittle to be examined in tension. This study investigates a straightforward and effective computational model for simulating material properties, such as the stress-strain mechanisms, using COMSOL Multiphysics for laser-deposited materials excessively brittle to be tested in tension. The first principal stresses and longitudinal strain under axial tensile loading conditions were measured using a 3D structural mechanics model.

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

Rene 80 superalloys have susceptibility to solidification cracking when manufactured with direct energy deposition. This research developed a computational framework for mapping cooling rates, thermal gradients, thermal rates, strain, strain rates, and stress components using thermomechanical simulations, microstructure prediction, and solidification crack susceptibility (by analytical RDG criteria). This work provides a practical physics-based method to evaluate the solidification cracking under a wide range of process conditions validated by experiments.

2:40 PM Break

ICME Design Tools: II

Tuesday PM
May 23, 2023

Room: Caribbean IV
Location: Caribe Royale

Session Chair: Katherine M Sebeck; US Army Combat Capabilities Development Command Ground Vehicle Systems Center

1:20 PM
The Role of Computational Materials Design in the Circular Economy of Materials: *Paul Mason*[1]; Anders Engstrom[1]; [1]Thermo-Calc Software

Growing awareness of environmental issues is influencing the entire materials and product development life-cycle. This begins with the extraction of raw materials and innovating how they are processed. Next, designing alloys that result in lower energy costs, either in terms of their processing, or through higher operating performance. Then, beginning with the end in mind, enabling materials to re-enter the economy at the end of life through improved recyclability. ICME can be applied to all stages of the materials life-cycle to develop strategies around these topics and in this presentation, several examples will be given where CALPHAD tools have been used to: Developing new higher efficiency alloys Develop more efficient manufacturing processes that result in less energy consumption or a higher yield Enable increased use of recycled materialsDevelop and optimize alternative processes for scrap melters who are dealing with ever-increasing levels of undesirable elements and impurities

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

Current efforts to modernize materials processing are hindered by a lack of fundamental, science-based understanding of the materials system (combination of feedstock material, production process, and finished part). A deeper understanding of the relationships between production process, material microstructure, and performance properties is the key to accelerating development timelines, achieving cost savings, and opening opportunities for game-changing materials systems for national security and nuclear energy. To address this challenge, an integrated methodology is being developed that brings together predictive modeling, inline monitoring, and data analytics. This methodology will enable high-fidelity in-silico experiments, efficient design of experiments, and process control which, taken together, will significantly accelerate development and qualification of materials systems. A key mechanism for integration within this effort is rigorous collection, curation, and sharing of data. This presentation will outline the methodology, highlight key advances in characterization, modeling, and ML, and demonstrate the key component of data management.

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

There has been considerable effort to develop an integrated computational materials engineering (ICME) framework. A relatively new concept of model-based material definitions has also emerged that can support a truly integrated, multi-disciplinary engineering capability. Prior literature has provided some initial background and guidance relative to establishing and utilizing a model-based materials definitions construct as part of seamless engineering workflow. This work further addresses and provides explanations of how materials and process model-based definitions are evolving and are being incorporated into workflows for interdisciplinary component design engineering optimization. Formalization of model-based material definition standards have the ability to change the way products are engineered and how software tools have the potential to change to meet this opportunity. Model-based material and process definitions have the ability to support rapid material and product certification and qualification, especially for those that are sensitive to manufacturing processing and exhibit inherent structure and mechanical property gradients.

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

Physics-based materials and process modeling has developed to a point where it is supporting the design and qualification of new components produced by additive manufacturing (AM). Focused models that describe various elements of the AM process, the evolution of microstructure and defects, and location-specific mechanical properties are key elements. Computational tools, when used as integrated modeling workflows, provide for a model-based definition framework for additive materials and processes. ICME property prediction starts with the thermal history, possibly at the scale of the individual melt pool or each layer if the local behavior is homogeneous. Examples will include spatial variation of geometry leading to variations in the local thermal history, microstructure, and properties in Ti-6Al-4V. Statistical description of microstructure provides statistically equivalent representative volume elements for predicting local mechanical properties. The alignment of model-guided testing and associated predicted properties can provide for a path to efficient and smart certification and qualification.

2:40 PM Break

Linkages: Microstructure I

Tuesday PM
May 23, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: Michael Tonks; University of Florida

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

Superalloys derive their superior high-temperature strength via interactions between ordered \947 precipitates and matrix dislocations. However, during creep deformation or cooling from service temperatures, \947/\947 interfaces (GI) often show irregularities, which can severely deteriorate the high-temperature strength of superalloys. For example, Parsa et al. (Acta Mater., 2015) reported the formation of ledges and grooves (LG) over \947 precipitates after the cooling of crept samples. Experiments fail to explain the formation of these irregularities as only the final state can be assessed. Hence, we present a coupled framework that accounts for the dynamic interaction between dislocations and moving GI and their simultaneous co-evolution. We employ an appropriate coarse-graining approach to account for the influence of the dislocations on the dynamics of GI and decoupled the glide and climb of dislocation through a time-scale separation scheme. Using this framework, we show the mechanisms resulting in the formation of LG at the GI.

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

Spherical gaussians, allowing the modeling of complex anisotropies, are used in modeling anisotropic polycrystalline grain growth (GG). Quaternions, assigned to individual grains as orientations and as misorientations for grain boundaries, conduct the ongoing mesoscale changes. A 5-D space scanning generates meaningful grain boundaries; inputted into the continuous function developed by Bulatov et al. to calculate grain boundary energy (GBE); which local minimas are used in the phase field model. The methodology involves using 2-D gaussian switches, which match the misorientation between grains with misorientations for the GBE minima. Accounting a threshold range for the minimas, the switch activates a Spherical Gaussian to set the GBE to the desired value; creating in combination a full 5-D GBE space. Multiphysics Object Oriented Simulation Environment (MOOSE), where reduced order parameters still retain individual grain identification useful for individually assigned quaternions, is used for implementation; with validation performed through bicrystal simulations of known outcomes.

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

We fabricated core-shell SU-8 nanocomposite nanopillars via vapor-phase infiltration of nanoscale amorphous aluminum oxides, into their 50 nm deep surface region and performed microstructural and nanomechanical characterization as well as analytical and atomistic modeling to gain a fundamental insight into the ultrahigh modulus of resilience exhibited by these nanocomposites, which are orders of magnitude higher than most high-strength engineering materials. The results of experimental and numerical studies show that the ultrahigh modulus of resilience of our core-shell nanocomposites results from: the low aspect ratio of amorphous aluminum oxide nano-particulates; the particulate size being comparable to or slightly larger than the free volume of the composite matrix; and the extremely thin aluminum oxide interconnecting links emanating from nano-particulates. These unique microstructural features produce the unusual combination of low Young's modulus and high yield strength, leading to the exceptionally high modulus of resilience as well as its weak dependence on strain rate.

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

High-Velocity Riveting (HVR) is a novel joining method that allows the joining of two sheets of metal through a metallurgical bond resulting from the high-speed impact with the rivet and the die. 3D finite element (FE) models were developed and used to help inform the die design and processing conditions. The model was able to simulate the joining process and inform the processing conditions. Additionally, outputs from the FE model are used as an input to a Molecular Dynamics (MD) model developed to investigate the atomistic mechanisms at nm to µm length scale that may influence the metallurgical bonding, such as inter-diffusion of atoms and local recrystallization of Aluminum at the interface. This ICME framework is suited to predict and understand the link between processing parameters and the physics of the bonding at the interface between the joined materials.

Linkages: Processing I

Tuesday PM
May 23, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: Victoria M. Miller; University of Florida

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

Single crystal sapphire can serve as substrate in electronic applications like µ-LEDs for next generation high-resolution displays. The manufacturing process includes directed solidification and cooling to room temperature, where stresses occur in the solid structure. Depending on the process parameters these stresses may lead to the generation of dislocations in one or more slip planes and cause a visible pattern in certain regions of the boule. The underlying mechanisms and the impact on the quality of the produced wafers are not yet fully understood. This work aims at the development of a material model, based on crystal plasticity theory that will be presented and applied for a simplified test case of crystal solidification and cooling. The model describes the onset and evolution of two densities corresponding to mobile and immobile dislocations and is capable to show the interconnection between the formation of dislocation patterns and remaining residual stresses after production.

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)

In the recent years the study of the nucleation due to the introduction of different shape and size nanoparticles in aluminium alloys have been studied. The critical angle needed for nucleation is going to be calculate for cubic, and pyramidal nanoparticles. Due to the complexity of the nucleation process, the wettability angle between the melted aluminium and the introduced reinforced nanoparticles was assumed to be constant. The use of this critical angle is proposed as a way of quantifying the nucleation feasibility for a specific nanoparticle geometry. Considering the theoretical calculations, a MATLAB® code has been developed to understand how the particle is going to be absorbed by the growing nucleus. In case of pyramidal particles 60o is the unique possible case of nucleating angle. For cubicand spherical nanoparticles the complete study of the available range is going to be defined in the present work.

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

Simulation of microstructure and hydrogen-induced porosity formed during solidification of aluminum-based alloys is a critical link in integrated computational materials engineering (ICME) design and manufacturing of solidification products such as castings, welds or additively manufactured components. A three-dimensional cellular automaton (CA) model has been developed to predict the formation and evolution hydrogen porosity coupled with grain growth during solidification of a ternary Al-Si-Mg alloy. The simulation results fully describe the concurrent nucleation and evolution of both solidification grain structure and hydrogen porosity, yielding the morphology of multiple grains as well as the porosity size and distribution. This model has been applied and validated in gravity and high pressure die casting, laser welding and laser powder bed fusion additive manufacturing processes. These grain structure and porosity models have been validated by X-ray micro computed tomography (micro-CT), scanning electron microscopy (SEM) and optical metallography.

4:00 PM

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

The dendrite misorientation is a typical defect in single crystal Ni-based superalloy castings. To date, there is still no explicit viewpoint on its generation mechanism. In order to trace the growth of dendrites, 30 layers of continuous slices were cut from a single crystal casting. The result shows that the growth direction of dendrite will continuously change during the solidification. A multicomponent phase-field simulation model was established to simulate the influence of solute convection on dendrite misorientation. The simulation result shows that, due to the existence of solute convection, the unstable distribution of solute can lead to the inhomogeneous driving force distribution at the tip of the dendrite, resulting in the orientation misorientation defect.

ICME Design Tools: III

Tuesday PM
May 23, 2023

Room: Caribbean IV
Location: Caribe Royale

Session Chair: James Edward Saal; Citrine Informatics

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

High-entropy alloys (HEAs) are gaining attention as structural materials due to their promising properties from cryogenic to high temperatures. The enormous composition-space design offered by the intrinsic nature of HEAs (combinatorics) can be seen as a blessing: so many new possibilities!; and a curse: how to find a needle in a haystack? To drastically reduce trials and errors, thus cost and time to market, The Alloy Optimization Software (TAOS) will be presented with HEAs optimization as a case study. In a nutshell, TAOS is an easy-to-use automated alloy optimization software that runs on stand-alone computer. TAOS is the front-end (GUI) of a sophisticated tool that can handle high-dimension alloys, unconstrained and constrained optimization of extremely complex and non-smooth functions, and leverage the CALPHAD method and databases via commercial software compatibility (Thermo-Calc through either TC-Python or TQ-Interface) and open source software integration (PyCalphad: https://pycalphad.org).

3:20 PM

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

QuesTek is both a pioneer and market leader in Integrated Computational Materials Engineering (ICME). For over two decades, QuesTek has empowered innovators by resolving materials-related challenges by applying its Materials by Design® technology. In the course of service engagements, QuesTek has designed and helped deploy dozens of novel materials, including 22 patented alloys. Dr. Sebastian will focus on case studies demonstrating how QuesTek enabled major corporations, from materials producers to materials-intensive product manufacturers, achieve critical technological development by deploying its Materials by Design® expertise and delivered success for its clients. Success stories include Apple iWatch and Tesla/SpaceX revolutionary materials. A result of 20+ years of innovation, QuesTek is developing a digital materials design platform, ICMD®, packaged as a SaaS offering. ICMD® availability should significantly impact and expand the ICME marketplace, as QuesTek's proprietary know-how will be widely available under license and subscription to materials producers, product manufacturers, federal agencies, and universities.

3:40 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

NASA and the FAA established the Computational Materials (CM) for Qualification and Certification (Q&C) steering group comprised of representatives from industry, government regulatory and research organizations, and academia with the following goals: • Inform research and development investments made by U.S. industry and the U.S. government toward maturation of CM-based approaches for Q&C of process intensive metallic materials (PIM) including additive manufacturing. • Identify key considerations and enablers required to increase airworthiness / certifying authorities' acceptance of CM methods use for Q&C of structural or flight-critical parts produced with PIM technologies. • Identify key CM technology gaps and maturation paths (in the context of Q&C applications). • Increase dialogue among stakeholder organizations. This presentation will summarize the technology and regulatory considerations that motivate this national effort, discuss progress and provide a summary and status of a multi-year roadmap that is being developed to guide technology development in this important area.

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

High strength low alloy steels achieve their enhanced properties by a combination of microalloying and controlled thermomechanical processing. An integrated microstructure based in-silico framework has been developed to enable design of hot-rolled Nb,Ti micro alloyed steels. The integrated model suite captures the precipitation kinetics of Nb,Ti (C,N) and their impact on austenite recrystallization and phase transformation of ferrite in a hot strip mill. It comprises of a cellular automata model for austenite recrystallization, phase field model for austenite to ferrite phase transformation and FEM based micromechanics model for predicting the mechanical properties of the final microstructure. A multi-component equilibrium precipitate model is utilized to compute the precipitation kinetics of (Nb,Ti) (C,N) and their influence on the evolving microstructure across the processes. A parametric study is done to evaluate the effect of chemistry and process parameters to obtain the desired mechanical properties.

Plenary Session II

Wednesday AM
May 24, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: Chuck Ward, *IMMI* Journal

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

Materials engineering encompasses synthesis of new materials, the understanding and optimization of its properties, and how it can be processed to the benefit of humankind. New material development has a growing emphasis on the useful life management of that product. Thus, any computational method which facilitates materials design, development, deployment, and product life management fits within the ICME field. Many companies use such tools without realizing that they are working within the ICME spectrum. This plenary talk covers the importance of ICME in modern manufacturing operations. Examples of the many facets of ICME utilized at Mercury Marine and Brunswick Boat Group will be presented. Additionally, insight will be provided into the significant effort involved in bringing new ICME derived materials into production.

8:40 AM Plenary
Accelerating Development of Materials with Artificial Intelligence: *James Saal*[1]; [1]Citrine Informatics

The development of novel materials and manufacturing processes can be time consuming and expensive due to the costs of experiments and the complexity of hierarchical process-structure-property-performance (PSPP) relationships that are unique across materials classes (e.g., polymers, metals, ceramics). Artificial intelligence (AI)-driven materials design is particularly useful on 1) optimization exercises that are high-dimensional, 2) problems where PSPP cause-and-effect are unknown, and 3) projects with resource constraints. While a researcher using traditional methods typically estimate which inputs are the most important to vary and develop experiments accordingly, AI can systematically create machine learning models using all input combinations and then act as a copilot for the researcher, suggesting a series of experiments to explore the design space in the most efficient manner. This talk will describe the Citrine Platform, cloud-based enterprise-level software that combines smart materials data infrastructure and AI. Citrine's experience in materials development will be illustrated with case studies.

9:20 AM Break

Linkages: Microstructure II

Wednesday AM
May 24, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: Michael D. Uchic; Air Force Research Laboratory

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

The presence of a void or secondary particle generates a stress concentration and plays a crucial role in both the mechanical response and damage evolution of metals. This work presents local stress and strain field predictions in a single crystalline matrix near a spherical void or hard inclusion. To characterize the effect of a material inhomogeneity, different modeling techniques at various length scales are utilized, such as an isotropic J2 plasticity finite element model, a coupled dislocation dynamics-finite element model, a crystal plasticity finite element model, and a phase-field fracture model. In this talk, simulation results from each model will be presented with the aim of correlating the defect microstructure characteristics and the macroscopic material behavior. In addition, results will be compared with the intention of bridging simulation length scales to obtain a better understanding of the influence of crystallographic orientation and its effect on failure predictions.

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

The engineering components of steel alloys in energy sectors are mostly operated at high-temperature and low-to-moderate stresses. Introducing precipitates by prior aging process is one of the strategies to improve the creep resistance, mainly in the dislocation glide-dominated operating condition. However, the available limited experimental observations show that the precipitates can also degrade the creep performances. Thus, understanding and quantifying the role of precipitates on the high-temperature creep behavior is critical. In this work, an advanced constitutive model within the full-field elasto-visco-plastic fast Fourier transform (EVPFFT) framework is developed to capture the effect of precipitate size and density on the creep responses of grade-91 and 347H alloys. The model calculation finds that the annihilation/depletion of dislocations, which is governed by the precipitates, during the primary-to-secondary transition modulates the creep rates. In turn, based on the rate of dislocation annihilation, increasing precipitate content can either increase or decrease the creep responses.

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

Precipitation strengthening has been proven to be a very effective method to improve the strength, especially the yield stress of alloys. In this work, uniaxial simulations were conducted on medium-entropy alloy, CrCoNi, under temperatures of 77 K and 298 K. Through precipitating Al, Fe, Cu, and Mn in the grain boundaries (GBs) of polycrystalline CoCrNi alloys, the strength and stiffness were significantly improved. Even with a low content (~0.4%) of dopant, the ultimate strength and stiffness were observed to be enhanced by 28% and 37.5%, respectively. Analysis of the deformed configurations reveals that the doped metallic ions play a role of inhibiting GBs sliding and subsequently lead to fcc to hcp phase transformation, as well as multiple inter and intra dislocations. Types of elements also exhibit an effect on the enhancement behavior due to different binding energies, which was demonstrated by the DFT calculations.

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

In developing workflows to describe the process-structure-property relationships, the first step is to calibrate the models producing the best fit to experimental data. Once this is attained, the value of ICME is the ability to vary the process variables to understand the sensitivity of the simulation to different processing conditions and chemistry variations.In this example, a Python enabled workflow is used to combine thermodynamic, kinetic and precipitation calculations to simulate the microstructure in terms of the nucleation and growth of the secondary phases which are then correlated with a simplified yield strength model to predict the precipitate, grain boundary and solid solution strengthening. Model variables are adjusted to give the best fit to experimental data and the framework is then used to adjust different processing conditions such as solution annealing temperature, aging temperature and holding time to assess the sensitivity to process variables and chemistry variation.

11:00 AM

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

A methodology to generate synthetic bimodal polycrystalline microstructures is presented. This work develops a model that couples a Generative Adversarial Network (GAN) and a classic microstructure generator to create statistically equivalent microstructures that match the surface fraction, texture, grain size, aspect ratio, and misorientation angle distributions of the EBSD data. Bimodal microstructures are composed of coarse grains and ultra-fine grains. The proposed methodology can generate bimodal microstructures obtained via rolling and annealing, severe plastic deformation, powder metallurgy, sintering, or cold-sprayed materials. This work presents the reconstruction of a cold-sprayed Al7050 alloy. Computational research is needed to understand the process-microstructure-property relationship with the goal of characterizing the fatigue life of the coatings. The generated microstructures subjected to tension along three orthogonal directions show different local and average mechanical behavior with changes in the yield stress and hardening.

Artificial Intelligence /Machine Learning: Microstructure III

Wednesday AM
May 24, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: Victoria M. Miller; University of Florida

9:40 AM

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

Engineering a microstructure morphology has been a long-lasting challenge in materials science. Historically, forward-based models, including experimental and high-fidelity models, based on trial and error, have been used to engineer a specific microstructure. In this work, we have developed a novel fused-data deep learning algorithm that is able to predict the required chemistry and processing to reach specific microstructure morphologies. FeCrCo permanent magnets are the model alloy in this work. The model input is the Fe distribution morphology and it predicts the Cr and Co concentrations and processing time and temperature for that particular morphology. The model analysis shows that shallow networks can predict chemistry well. However, deep networks are required to predict the processing time and temperature. We validated the model against a TEM micrograph and while the model is trained with synthetic data it performs reasonably well in chemistry and processing prediction for a TEM micrograph.

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

A comprehensive understanding of multiple materials phenomena requires description of three-dimensional (3D) microstructures and their significant features. Most of the experimental observations are limited to two dimensions (2D). Accessing 3D microstructural information using methods like serial sectioning is expensive and time-consuming. Frequently applied phenomenological models, like phase-field (PF) method has proven to be more realistic with the experimental observations. They directly provide information on 3D microstructures and their salient features. With the results of PF simulations, a data-driven approach is presented to estimate the 3D microstructural features from 2D (taken in the form of slices) morphological information in bainitic steels and theircorrelation with the strength of material.

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

The ability to predict as printed microstructures is essential for use in modeling mechanical performance in metal additive manufacturing. The computational expense of existing methods leads to the option of employing rapid machine learning based methods. This talk covers work using conditional generative adversarial networks (cGANs) to generate synthetic microstructures corresponding to metal additive parts made of cubic metals. A set of training data has been developed using existing methods and varying the parameters used in a laser powder bed fusion additive process (laser power, laser velocity, hatch spacing, etc.). The cGAN model is trained using 2D slices of the 3D model output that have been labeled with the printing parameters used in each simulation for conditioning. Microstructure images used for training alongside corresponding cGAN model outputs will be presented.

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

Analysing micrographs of microstructural features using transmission electron microscopy is key for predicting the performance of structural materials in nuclear reactors. Analysing micrographs is often a very tedious manual process, therefore recently many researchers have tried to automate the process by using various types of neural network, however, application of these networks still require lot of manual work. This paper compares two state-of-the-art neural networks, YOLO and U-Net to maximize the automation of tasks such as counting of microstructural features like helium bubbles and voids. To better understand the accuracies, performance and limitation of each model, we conducted robust hyperparameter validation test including suite of random splits and datasetsize-dependent and domain-targeted cross-validationtests.

11:00 AM

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

Organic molecules, known as dyes, which can absorb and emit light, are potential candidates for quantum computing owing to their unique properties, including exciton delocalization and coherence features when dyes are aggregated. Importantly, exciton delocalization and coherence can occur at ambient temperature. These novel applications are controlled by dye properties, requiring high extinction coefficient, high transition dipole moment, good aggregation ability, and high exciton exchange energy. Dye aggregate networks via deoxyribonucleic acid (DNA) templating exhibit exciton delocalization, energy transport, and fluorescence emission. DNA nanotechnology provides scaffolding upon which dyes attach in an aqueous environment. To better control the process and optimize the properties, we applied machine learning-driven multiscale modeling techniques to identify candidate dyes and reveal their dye aggregate-DNA interactions and the dye orientations. Those structural features were found to have a strong impact on the resultant performance of the DNA-templated dye aggregates. The computational results were validated with experiments.

New & Emerging

Wednesday AM
May 24, 2023

Room: Caribbean IV
Location: Caribe Royale

Session Chair: George Spanos, TMS

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

Dendrite formation remains a critical safety issue for the success of next-generation lithium-metal-anode batteries. Quantitative computational tools can enable the design of new materials and structures to suppress dendrites. We employ a fully variational and thermodynamically-consistent phase field model to quantitatively model dendrite growth on lithium metal anodes during charging. The model can consider general nonlinear reaction kinetics and correctly captures the capillary effects. We use materials parameters calculated from first-principles simulations, including the temperature-dependent anisotropic interfacial energy and the temperature- and concentration-dependent diffusivity. Moreover, we developed a method to increase the computational grid spacing and time step by two to three orders of magnitude to enable efficient and quantitative simulations with realistic system properties. We study the effects of various factors such as applied voltage and current, nucleation density, and electrode structure and propose strategies to suppress dendrite formation.

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

An electrochemical micro-scale phase-field model is developed to simulate the stripping and plating kinetics of a Na-metal anode in all-solid-state Na-ion batteries. In this model, in addition to the metallic anode and ceramic separator regions, a highly conductive but Na-poor region representing the free space is assumed to simulate the shrinking of the Na-anode during electro-stripping and its growth during plating. For a perfect anode/separator interface, we find that the growth and depletion kinetics are linear. However, the presence of multiple interfacial voids at the anode/separator interface causes deviation from this linear behaviour. Finally, we show that depletion kinetics is also proportional to the ratio of the grain boundary conductivity to that of the grain conductivity ($_{gb}/_{g}$) in the separator phase, either with or without interfacial voids.

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

Lithium-ion batteries (LIB) continue to permeate numerous sectors including electric vehicles, medical devices, and portable electronics due to their high energy densities. However, predicting the cycle life of LIBs remain challenging due to various factors including operational variability and fast charging requirements. Early cycle life prediction helps lower the cost of batteries through optimization of manufacturing processes, and thereby enhances cell life. In this context, machine learning techniques that synergistically combine physics-based data and experimental measurements hold the potential to detect underlying trends in capacity degradation. While most data-driven approaches require the utilization of high-rate tests to induce accelerated degradation, low currents pose challenges to cycle life prediction due to slower degradation onsets and longer feedback times. In this work, we develop a machine learning model to deconvolute the degradation response by feeding memory information from electrochemical signatures, enabling accurate prediction of cycle life and capacity loss in LIBs.

10:40 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.

Electrolyte plays vital role in success of a battery technology. Current generation lithium-ion batteries (LIBs) use 1M LiPF6 salt in mixture of ethylene carbonate (EC) and dimethyl carbonate as electrolytic solution. To improve thermal stability, recently concentrated electrolytes (of concentration higher than 1M) are proposed. Formation of anion rich solid-electrolyte interface layer helps battery gain better stability. However, concentrated electrolytes offer significantly lower ionic conductivity to impact power performance. Locally concentrated electrolyte (LCE) formed by using a diluent that does not solvate lithium ions and of low viscosity is shown to be promising. LCEs enable one to reap benefits of both the worlds. However, molecular mechanism responsible for improved electrolytic properties of LCEs are not well understood. We study EC + Bis(2,2,2-trifluoroethyl) ether based LCE within the molecular dynamics method, and present simulation methodology, various properties of LCEs and the insights gained from the study that help one to design novel electrolytes.

11:00 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

Battery electrolytes can have a significant influence on various macroscopic performance aspects of the battery such as internal heating, charging time and capacity fade. Since the molecular level electrolyte transport properties directly influence the system level performance, a multiscale study is necessary for optimal electrolyte selection. In this work, we conduct a multiscale comparative study of two commonly used Na ion battery electrolytes NaClO4 and NaPF6 in the non-aqueous solvent EC:DMC. Using a system level physics based model, combined with lower length-scale simulations, we compare system level performance metrics such as charging time and internal heat generation for both these electrolyte salts. Studies such as these can be very effective in identifying optimal electrolytes for next generation Na ion batteries.

Linkages: Deformation II

Wednesday PM
May 24, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: Harikrishnan Rajendran; Boeing Research & Technology

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

Industrial rolling of aluminum is a multi-step process involving numerous reductions under hot and cold temperatures with varying deformation speeds to achieve the final gauge and microstructure. This study looks at the effect of changing the temperature and strain rates for AA3104 aluminum through plane strain compression via the Gleeble Hydrawedge II. It makes use of FEA simulations to validate the strain distribution after deformation and evaluates how the resulting flow stress, developed texture, and microstructure compare to the expected industrial version. The flow stress and texture data acquired are used for calibration of an ICME model describing the microstructure and properties of the entire rolling process for AA3104 aluminum.

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

Non-grain-oriented (NO) electrical steel is widely used in electrical machines with rotating magnetic fields. The process chain consists of hot-rolling with optional batch-annealing followed by cold-rolling and final continuous annealing. Each step has a significant influence on microstructure and electromagnetic properties. A tailor-made microstructure, with specific grain-size and texture, can greatly improve magnetic properties of NO sheet material and thus the performance of rotor/stator components. For the design of such an ideal microstructure, it is necessary to quantify the influence of process-parameters on the microstructure. In the current work, texture evolutions during cold-rolling and due to recrystallization during final annealing will be evaluated based on EBSD-measurements for different conditions. Modelling approaches describing the formation of deformation and annealing texture are presented and discussed in combination with the experimental results. The through-process texture analysis provides new insights into the optimum microstructure of NO steels, leading to an improvement of electromagnetic properties.

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

Friction stir processing (FSP) is a solid-phase processing technique that provides localized modification and control of microstructures in the processed zones. Numerical models can help predict material deformation and temperature history during FSP that directly relate to microstructural refinement, densification, and homogeneity of the processed zone. This work presents a meshfree smoothed particle hydrodynamics (SPH) model for FSP of 316 L stainless steel using a thermo-elasto-plastic constitutive model and stick-slip tool-workpiece contact approach. The model's predicted material flow, temperature distribution, and stress-strain state are presented and validated with experimental data. The strain rate and temperature histories obtained from the SPH model are used for predicting Zener-Hollomon parameter and average material grain size. Numerical results on the microscale are also found to agree with experimental observations in the stir zone. This high-fidelity model is feeding results as an input to lower-length scale models and informing the process conditions.

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 - Department for Product Engineering

The use of UDIMET720 (U720) in next generation aero engines requires numerical tools to predict the microstructure evolution and final mechanical properties of closed die forged engine disks. An existing simulation tool for a different superalloy, which uses integrated computational materials engineering (ICME) to predict characteristic properties such as grain size and yield strength, is used and parametrized on the microstructural mechanisms of U720. The specific setting of a homogeneous grain size distribution through metal-physical understanding of the recrystallization processes and the formation of the necessary '-precipitate-populations is elaborated. Inhomogeneous microstructure distributions in the pre-material and their effect on the local microstructure and property evolution along the process route are taken into account. Based on specific material characterization and testing the scientifically sound and application-oriented design tool is optimized and includes all essential mechanisms of an U720 turbine disk manufacturing.

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

To reduce nuclear proliferation, low-enriched U-10Mo alloy has been identified as a promising fuel candidate for United States high-performance research reactors. During fabrication. Manufacturing the U-10Mo alloy involves a complex series of thermomechanical processing steps, including homogenization, hot rolling, annealing, cold rolling, and hot isostatic pressing. Several models/modeling methods have been developed for these individual processes. The interaction and coupling between individual processes use the concept of ICME, which aims to bridge the information passing between interacting models and investigates the impact of manufacturing processes on material microstructure evolution. Additionally, a Machine Learning (ML) model was developed and trained on both physics-based modeling and characterization data to predict the resultant microstructure after hot rolling passes and annealing. It is shown that implementing ICME leads to improved predictions, a better understanding of microstructure across multiple processes, and accelerated and more cost-effective development efforts.

3:00 PM Break

Applications: Advanced Manufacturing Microstructure II

Wednesday PM
May 24, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: Adam Kopper; Mercury Marine

1:20 PM

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]CWRU

Metal-based additive manufacturing success requires active monitoring solution for assessing quality and reliability of components. Monitors such as high speed cameras are a common and well-studied capture device for in-situ welding. The scale and time required to fabricate parts increases exponentially the number of relevant frames for feature detection, with higher resolution increases the number of feature occurrences. Techniques for automated feature extraction and quantification are required in order to perform active sensing so that errors or problems in the print process can be addressed. Laser-solid interactions present in meltpools, such as the uniformity of melt, are known predictors of build quality. Automatically determining major, minor axis, melt coordinate center, and overall area offers the first steps of using in situ measurements in real-time and obtaining characterization information to inform on print quality with minimal human intervention through the use of U-Net feature extraction and YOLO image segmentation.

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

Phase-field models offer the possibility of simulating microstructure evolution under rapid solidification conditions without having to neglect the key physical mechanisms such as nucleation, growth kinetics and solute diffusion. However, until now the phase-field simulations are mostly restricted to binary alloys owing to the complexity of obtaining thermodynamic descriptions for technical alloy compositions. In this study, we employ 3-Dimensional multi-component and multi-phase-field simulations directly coupled to thermodynamic database to obtain the bulk free energies of individual phases. In addition, thermal boundary conditions of AM are implemented in such a way that the solver allows to model both melting and solidification (with latent heat release) simultaneously. The phase filed equations are implemented in openphase studio, a C++ based software package offered by OpenPhase Solutions. Through the 3-D simulations, microstructure evolution especially the dendrite morphology, primary dendrite arm spacing and solute segregation of full alloy composition of CMSX4 is studied in detail.

2:00 PM

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

Quantifying the grain size and orientation is essential for understanding the properties of the materials, especially when increasing the creep resistance of high-temperature alloys such as Haynes 282. The grain distribution of additively manufactured metal is attributed to various factors, such as processing parameters and part geometry, making it difficult to predict the microstructure. Haynes 282 being an FCC single-phase structure, polarized light methods cannot be applied to segment out grains accurately. Therefore, it is challenging for other imaging methods to segment and analyze the orientation of the grains. In this work, we present a cost-and-time-efficient pipeline for predicting grain size and orientation distributions. This method uses a convolutional neural network (CNN) that segments out grains in SEM images and predicts a relative grain orientation, which can work as an alternative for time-consuming EBSD.

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

We present phase field (PF) simulations of the columnar to equiaxed transition (CET) occurring during solidification of Ti-Cu and Ni-Fe-Nb alloys under thermal conditions characteristic of powder fusion based additive manufacturing techniques. The PF simulations will involve direct coupling to alloy thermodynamics and a thermodynamically consistent nucleation model. The simulations are able to capture the transition from a solute-diffusion driven constitutional undercooling to thermal undercooling driven nucleation ahead of the epitaxial solidification front under AM conditions. A parametric study is presented under varying G and R conditions and alloy composition to capture the conditions under which the above transition occurs. This research was performed at the Oak Ridge National Laboratory under contract DE-AC05-00OR22725 with the United States Department of Energy (USDOE) and was supported by the High-Performance Computing for Manufacturing (HPC4Mfg) and the Exascale Computing Project (ECP) programs sponsored by the USDOE.

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

Nucleation and grain growth during metal additive manufacturing (AM) remain debatable since the nature of rapid melting and solidification induced by laser-powder interaction during AM may cause heterogeneous mixing liquid metal behaviour especially when in-situ alloying is used. Coupled thermal-chemical-fluid-microstructure modelling is developed for simulating in-situ AM to understand the chemistry-induced solidification, re-melting and microstructure development. The results indicate that thermal fluid flow and chemical mixing play an important role in rapidly solidified microstructure. The heterogeneous nucleation resulting from undercooling due to large thermal gradient and large cooling rate initiates grain nuclei forming equiaxed grains, and with the extent of thermal gradient, more anisotropic columnar grain growth occurs in AM. The keyhole serves as a strong stirrer to enhance chemical species mixing by inducing convective flow motion, which determines the local chemical composition and microstructure in in-situ alloying while melting newly fed powders and re-melting part of the previous layer.

3:00 PM Break

Linkages: Microstructure III

Wednesday PM
May 24, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: See Session Sheets

3:20 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

The embrittlement of reactor pressure vessel (RPV) steel has been a great concern of the nuclear industry. Macro-segregated areas of carbon, alloy elements and impurities occur due to uneven solidification rates at different locations during the heavy forging process. These heterogeneities can lead to significant variations in fracture toughness in the Ductile-to-Brittle Transition (DBT) region. To quantitatively assess the safety of RPV, advanced micromechanical tools combining crystal plasticity and the local approach to fracture (LAF) are developed. This multiscale approach is applied to laboratory steels with different segregation levels chemically representative of actual RPV components. Simulation results demonstrate that the current approach is capable of predicting the shift of the DBT zone and the statistical scatter of fracture toughness with the variation of alloying elements. Results give insights into factors affecting fracture properties. Comparisons to phase field damage methods and new model prospects towards more accurate predictions are also discussed.

3:40 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

Helium bubbles impact mechanical properties of nuclear materials. An Fe-Ni-Cr-H-He potential has been developed to enable molecular dynamics simulations of helium bubble nucleation and growth. This is accomplished by addressing three challenging paradoxes: (a) helium forms tightly bound dimers and clusters in the lattice but are only bound by weak van de Waals forces in the gas phase, (b) helium diffuses readily in metals yet significantly distort the lattice causing large volume expansions; (c) helium prefers tetrahedral interstitial sites to the larger octahedral sites despite strong repulsion from metal atoms. Our potential reproduces quantum mechanical results on relevant properties to bubble nucleation and growth. In addition to validation by static properties, molecular dynamics simulations establish that our potential enables the nucleation of helium bubbles from an initial random distribution of He interstitial atoms while at the same time capturing the equation of state in the pure He phase.

4:00 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

Cast iron is one of the oldest materials known to humankind. A microstructure of cast iron exhibits different morphologies of graphite that range from flake to compacted to spheroidal particles. The morphology is controlled by magnesium addition during the solidification process. Though this technology dates back several decades, the exact mechanism of shape change remains debatable. This study used a combination of industrial casting trials, analytical microscopy, and molecular dynamics simulation to understand the origin of graphite morphology in cast iron. Further, from this theoretical premise, an integrated multi-scale model of coupled heat transfer and phase transformation during the solidification of different types of cast irons was developed and validated with experimental results. Finally, constitutive models were developed for studying the microstructure-property correlations. Thus, this study provided an appropriate example of an integrated computational multi-scale modeling approach of simulating a casting, predicting solidified microstructure, and obtaining structure-property correlations.

Applications: Advanced Manufacturing Processing III

Wednesday PM
May 24, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: Austin E. Mann; Boeing Research & Technology

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

Direct energy deposition (DED) is a promising additive manufacturing process for fabricating metal matrix composite (MMC) components. Using reinforcing particles as nucleation sites, the DED process can produce fine-grained MMC parts with enhanced tensile properties. However, coexistance of interactive phenomena (e.g., Marangoni convection, recoil pressure, and multiple reflection) with extreme short period of their presence in the melt pool hinders the control of particle dispersion, which is crucial for obtaining superior mechanical properties with equiaxed grain structure. To resolve this problem, the numerical model incorporating thermo-fluid dynamics is established to predict flows in the melt pool. Also, based on the constructed simulation results and Lagrangian discrete phase model (DPM), migration patterns of particles are investigated. The obtained results showed that recoil pressure and Marangoni convection forces had a significant role in the movement of particles. The present study better explains the dispersion mechanism of supplementary particles in the melt pool.

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

In this work coupled thermal-solidification simulations of sapphire growth in single-boule furnaces with Heat Exchange Method (HEM) are presented. The heat transfer in the furnace is modelled via ANSYS Fluent® by considering: 1) heat conduction and radiation in furnace, 2) heat conduction, laminar convection and radiation in sapphire melt, and 3) heat conduction and internal radiation in sapphire crystal. The crystal growth is modelled by the enthalpy-porosity approach. The physical models used in simulations are validated with measurement data from a real furnace, which capture the crystal-melt interface position during the technological growth process. A simplified furnace geometry is considered to study the effect of different side and top heater powers on the crystal-melt interface during the growth process. A main focus is put on the possibilities for upscaling the sapphire crucible dimensions (height and width) to make the process more efficient and to be able to produce larger wafers.

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

There are a variety of manufacturing processes where plumes of metal vapor are produced as a byproduct. The composition, size, and shape of particles condensed from metal vapor may provide information in optimizing the associated manufacturing processes and conditions. Selective laser melting is a well-defined process that we use as a surrogate for manufacturing techniques that generate particles through the condensation of metal vapor. We present the development of a multiscale model for particle formation by condensation of metal vapor generated during selective laser melting. This consists of coupling (1) thermal modeling of laser-induced metal melting and volatilization, (2) fluid dynamics modeling of the metal vapor plume, and (3) phase field modeling of metal condensation. The phase field model accounts for vapor/liquid/solid phase transitions under non-isothermal conditions. This work is informed by and validated with laser melting experiments, with investigations of plume evolution and microscopy of generated particles.

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

The relationship between the local undercooling, dendrite tip velocity, and dendrite tip radius is a critical materials relationship that controls solidification-based manufacturing processes. That relationship impacts the final grain structure, crystallographic texture, and micro-segregation. However, collecting experimental data for empirically determining the relationship is extremely challenging due to the high temperatures and micrometer scales characteristic of engineering alloy solidification. This work compares various analytical relationships for relating undercooling to dendrite tip velocity for Ti-6Al-4V and characterizes the sensitivity of the formulations to the input material properties. The formulations are used alongside thermal and microstructure evolution models in a computational materials framework to simulate the powder bed fusion additive manufacturing process and characterize the impact of formulation selection on the resulting grain structure. The results of this work demonstrate the importance of the assumed relationship between undercooling and dendrite tip velocity by characterizing its impact on the simulated microstructure.

Plenary Session III

Thursday AM
May 25, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: Chuck Ward, *IMMI* Journal

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

A computational alloy design approach was used to identify a hypereutectic Al-Si-Cu alloy suitable for processing by laser powder bed fusion (LPBF). The approach was to utilize the fast-cooling rates provided by additive manufacturing to produce nm-sized Si for in-situ particle reinforcement and Cu precipitates for room temperature strengthening. Feasibility of potential compositions was determined from melt-spinning experiments to mimic rapid solidification of LPBF. The selected alloy demonstrated a large printability range with consolidation >99.97% density. Transmission electron microscopy confirmed the formation of the predicted nano-Si particles and Al2Cu precipitation. Elevated uniaxial tensile properties and fully reversed high cycle fatigue (1e7) show superior strengths compared to commercial AlSi10Mg across all test temperatures up to 300 oC. Supercharger vanes were designed for the complexity afforded by additive manufacturing with 50% mass savings. The printed vanes were tested in a supercharger assembly on a dynamometer running a COPO LSX 350 SC engine.

8:50 AM Break

ICME for Non-Metals: III

Thursday AM
May 25, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: See Session Sheets

9:00 AM Invited
Multiscale Modeling and Machine Learning-based Digital Twin for Piezocomposite Damage Sensing: *Somnath Ghosh*[1]; [1]Johns Hopkins University

This talk will discuss the development of a machine learning-enabled, multiscale-multiphysics computational platform for multifunctional piezocomposites. It will constitute a digital twin for detecting location-specific damage evolution from surface electric field sensors. The integrated platform incorporates modules involving bottom-up and top-down multiscale modeling coupled with various machine learning operations. The first module involves development of a finite deformation parametrically upscaled coupled constitutive-damage models (PUCCDM) for structural-scale electromechanical response, by hierarchical modeling of microstructures undergoing progressive damage. The PUCCDM incorporates microstructural morphology in its coefficients in the form of representative aggregated microstructural parameters (RAMPs), determined using machine learning on data generated by micromechanical analysis. The micromechanical model consists of a coupled electromechanical finite deformation phase field model for crack initiation and propagation in nonuniform piezocomposite microstructures. Finally, coupled convolutional neural and long-short term memory networks (ConvLSTM) are deployed to predict current damage for correlating sensor-based electric signals to subsurface damage indicators.

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

Characterization of the mechanical response of composite layups is often done by means of the so-called coupon testing, in which representative specimen of the layups are tested under the guidelines of ASTM standards. Recently, virtual coupon testing is being used as an alternative or preliminary step to the actual tests. In these virtual tests, finite element simulations of the layups are solved under the same conditions given by the standards, allowing a broader design space and a faster, cheaper material design. In this work, a true multiscale approach is proposed for capturing the complexity of the material behavior in virtual composite coupon testing. Finite element models of representative volume elements at the microstructural level are solved simultaneously with the solution in the coupon level for a better representation of the phenomena happening in all scales of the test. Results are compared with experimental results from the literature, showing good agreement.

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

A coupled thermo-mechanical fracture model is presented to predict the damage of \945-SiC as a representation of brittle ceramics over a wide range of temperatures (20-1400°C). Temperature-dependent damage prediction is a crucial link of ICME for ceramics in applications like thermal protection systems of hypersonic vehicles. The model, which has been implemented into MOOSE, links between material properties and performance. The model contains modules of elasticity, damage phase field, and heat conduction. Analytical approaches for determining crack length scales of simple shear and tension are presented. Validation tests are conducted for both flexural strength and fracture toughness over the specified range of temperatures. Both the flexural strength simulation results and mode I fracture toughness results agree with the experimental data. Mode II and mixed mode fracture toughness simulations results are presented with the modified G-criterion. Finally, the parallel computing capabilities of the model are considered in various scalability tests.

10:10 AM
Machine-learned Structural Descriptors for Metallic and Covalent Glassy Materials: *Thomas Hardin*[1]; [1]Sandia National Laboratories

Glassy materials, like polycrystalline metals, have a mutable internal structural state that affects stress-strain response and functional properties. The internal structural state of polycrystalline metals is well-represented by grain sizes, dislocation densities, and so forth. However, a concise set of physically real, broadly applicable structural descriptors remains enigmatic for many glasses. This gap hobbles the development of multi-scale and continuum models with engineering relevance for these materials. We report a dimensionality reduction method based on diffusion maps that parameterizes the low-dimensional manifold of local structural states found in the glass. Distributions of these machine-learned parameters constitute a computationally convenient structural description of the glass. We show how the machine-learned structural description can be linked to fracture behavior in silica glass, and to plasticity in metallic glass. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525 (SAND2022-16339 A).

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

Extensive risk reduction demonstrations and stringent requirements for efficient aero-engines cleared the way for the commercial launch of titanium aluminides. Low-pressure turbine blades (LPTBs), which usually replace cast nickel superalloys in advanced aero engines, are currently the most alluring application. Fabricating titanium aluminium matrix composites (TAMCs) with ceramic in the metal matrix offers a possible solution. While maintaining low density, TAMCs often have more advanced qualities than matrix alloys, including a high specific modulus, strength, wear resistance, and thermal stability. The isotropic characteristics, simplicity of manufacture, and low cost of particle-reinforced titanium aluminium matrix composites (PRTAMCs) make them one of the best TAMCs. The summary of current developments, issues with reproducibility, and potentially discussed and how TiAl-TiB2 LPTB development went from successful laboratory tests to successful production insertions in industrially scaled commercial jet engines. The framework and toolkits for integrated computational materials engineering modelling created by academics will be shown.

10:50 AM Break

ICME Design Tools: IV

Thursday AM
May 25, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: Paul Mason; Thermo-Calc Software Inc.

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

High strength Nickel alloys are widely used in aerospace applications to make critical components due to their excellent thermomechanical properties. The processing of manufacturing Ni ingots is an energy intensive process which starts with melting and subsequent thermomechanical processing. A typical Nickel alloy is melted 2 to 3 times (VIM/VAR/ESR), and the thermomechanical processing typically involves multiple press and radial forging reductions, reheats in furnaces, and heat treatments to achieve the required grain size and mechanical properties for aerospace and petrochemical applications. Even under controlled conditions, variation in the final product can occur including surface cracks, hidden porosity, undesired grain size, etc. leading to rework and or reprocessing. We will layout and discuss an ICME-based approach to improve the process yield, tracing the billet through its journey from melting to thermomechanical processing while utilizing continuum-modeling and thermodynamics-based models. We will elaborate on the results, challenges, and potential future steps.

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

Each year billions of aluminum beverages cans are manufactured, which means can body stock, made of AA3104, has one of the largest aluminum markets globally. Production of can body stock involves multiple key manufacturing steps, starting with large-scale DC casting, homogenization step, and a series of hot and cold rolling down to the final gauge. Since AA3104 is non heat-treatable alloy, the resulting microstructure from the final rolling steps will ultimately determine properties and performance of the can body stock. Therefore, it becomes important to develop a numerical tool that can quantitatively capture microstructure evolution during production. In this work, an ICME framework is developed to predict crystallographic texture, recrystallization, and distribution of intermetallic particles in AA3104 during hot and cold rolling processes. The framework demonstrated that it could capture evolution of microstructure of interest with sufficient accuracy as well as be used to provide suggestions to improved rolling schedules.

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

Field assisted sintering technology (FAST) is a manufacturing process for near-net shape components. The mechanical behaviour of the final part depends on the process recipe (dwell temperature, dwell time, load/pressure, heating rate, and electric current waveform), which is usually selected through user experience and extensive experimental trials. Digital threading of sensor data to physics-based computational models and vice versa promises to reduce the cost of the optimisation process and retains the know-how that can be lost when the workforce changes.The proposed digital thread implementation allows users to feed the temperature history and applied force from the FAST machine to modelling tools to add new data sets of phase transformation and macro-mechanics behaviour. The new enriched data-set will enable users to make informed decisions and optimise the process for new alloys and powder morphologies, reducing energy consumption and meeting the performance of the final part.

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

ICME requires seamless integration and exploration of material, product, and manufacturing process design spaces across multilevel. This demands the capability to co-design, that is, share ranged sets of robust design specifications among distributed material, product, and manufacturing process stakeholders through the visualization and exploration of high-dimensional material design space under uncertainty.In this paper, we present a machine learning-enhanced robust co-design exploration framework by integrating robust compromise decision support problem construct (r-cDSP) with interpretable self-organizing maps (iSOM). Using the framework, we facilitate systematic and efficient visualization, interpretation, and exploration of high-dimensional materials design space under uncertainty. The generic nature of the framework for multidisciplinary designers to a) understand the interactions and capture the dominant process mechanisms that affect materials responses and b) provide decision support for problems involving many conflicting goals under uncertainty is demonstrated using an industry-inspired steel manufacturing process chain problem.

10:30 AM

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

Given the importance of temperature in the dislocation density of crystalline materials, constitutive thermo-mechanical models provide a pathway for a more accurate description of temperature-sensitive processes. Commonly, however, the thermo-mechanical description of the material response is limited to phenomenological macroscopic models with limited interpretability. Here, thermal expansion is included in the single crystal constitutive response via an eigenstrain contribution to the deformation gradient, and a fully coupled implicit thermo-mechanical formulation is implemented into the variational framework of the crystal plasticity finite element method. Such a thermodynamically consistent model with temperature and micromechanical fields is used to investigate the response of different materials under thermal-stress boundary conditions.

10:50 AM Break

Applications: Alloy Design II

Thursday AM
May 25, 2023

Room: Caribbean IV
Location: Caribe Royale

Session Chair: Katherine M Sebeck; US Army Combat Capabilities Development Command Ground Vehicle Systems Center

9:00 AM Invited

Alloys-by-Design: Accelerating the Discovery and Deployment of Alloys to Address Future Demands for Increased Performance and Sustainability: *David Crudden*[1]; Rory Rose[1]; Farsad Forghani[1]; Shohreh Khorsand[1]; Sajjad Amirkhanlou[1]; [1]Alloyed Inc.

There is a constant demand for materials and manufacturing technologies which increase performance and efficiency in engineering applications. As many industries go through significant transformations, for example, electrification in the automotive industry, digital transformation in the manufacturing sector or decarbonization in metal processing, rapid discovery of new materials to enable this transformation is critical. Alloyed is addressing the need for rapid materials discovery using its Alloys-by-Design (ABD®) computational platform. We will present application of our platform to selected materials design problems with an emphasis on decarbonization and digital manufacture. Impact on decarbonization in metal processing is demonstrated through design of an aluminium casting alloy that does not require heat-treatment, resulting in reduced CO2 emissions and processing costs without compromise in performance. Alloy design for digital manufacturing will be discussed with reference to computational optimization of alloys for additive manufacturing. The role data-science and artificial intelligence methodologies may have in extending current capabilities to revolutionize the way we design and qualify materials in the future is also considered.

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

Different material modeling approaches are applied in the computational materials design to describe the process-structure-property relationship across the length scale. Among them, the CALPHAD (CALculation of PHAse Diagrams) approach plays an important role. Using this approach, one can predict in a very short time the distribution of phases (type, amount) which can be expected in the studied material depending on the chemical composition and manufacturing conditions, e.g. temperature. Recent developments demonstrate how to use CALPHAD for the screening of a large number of chemical compositions by performing the equilibrium and non-equilibrium (Scheil-Gulliver type) high-throughput calculations. The present work demonstrates how to extend this approach by considering the precipitation kinetics in the solid state. The focus is on the optimization of chemical composition and heat treatment parameters for additively manufactured metallic alloys. The developed tool can be however also applied to other manufacturing processes like casting or hot deformation.

9:50 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

Aluminum has been increasingly the sustainable material of choice for aerospace, automotive and beverage cans due to its high strength-to-weight ratio and infinite recyclability. Aluminum recycling is surging, and more end of automotive life aluminum scrap will be available in the market. To minimize prime aluminum use, design of new aluminum alloys which can utilize more diverse sources of scrap is needed, while simultaneously satisfying the performance requirements for desired applications. In the present work, we have coupled scrap mass flow model with a physics-informed machine-learning framework to design sustainable aluminum alloys. Microstructural features pertaining to strength, formability, and corrosion properties we estimated using CALPHAD methods and integrated into machine learning framework. The model predictions for sustainable alloy chemistries were then validated through lab trials.

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

Sixty years of academic collaboration and thirty years of commercialization by a network of small businesses have delivered a mature technology of computational materials design and accelerated qualification grounded in the CALPHAD system of fundamental databases now known as the Materials Genome. The national Materials Genome Initiative acknowledging the reality of this technology has spurred global interest and rapid adoption by US apex corporations. Designed materials with broad market impact now span a range from consumer electronics to space exploration. Ongoing design addresses the new alloys enabling new manufacturing methods such as 3D printing as well as the materials supporting affordable approaches to sustainability. The advanced design and qualification software system, ICMD®, developed at QuesTek is now prepared for commercial application.

10:30 AM Break

Linkages: Deformation III

Thursday AM
May 25, 2023

Room: Caribbean VI & VII
Location: Caribe Royale

Session Chair: See Session Sheets

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

Micro-texture regions (MTRs), characterized as the clusters of grains with similar crystallographic orientations in the polycrystalline microstructure, play a significant role in fatigue crack nucleation and life of structures of Ti alloys. This paper develops a parametrically upscaled constitutive and crack nucleation modeling (PUCM/PUCNM) platform for predicting structural-scale fatigue crack nucleation in / Ti-6Al-4V alloys, whose polycrystalline microstructures contain MTRs. The PUCM/PUCNM platform bridges micro and macro scales through thermodynamically-consistent incorporation of representative aggregated microstructural parameters (RAMPs) in macroscopic constitutive relations. A RAMP that captures both the MTR size and contrast in the overall texture is proposed to represent MTR intensity in the microstructure. A functional form is derived using the genetic programming-based symbolic regression. The PUCM/PUCNM tool is used to simulate an engine blade under dwell loading conditions. The results exhibit the reduction of nucleation life with a higher level of MTR intensity, despite the same overall textures.

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

Fatigue remains a critical failure mechanism both of industrial and scientific interest. Fatigue testing is commonly a costly and time consuming exercise, which makes it difficult to establish microstructure to fatigue performance relationships. This is seen as an area where ICME driven "virtual fatigue testing" hybrid workflows consisting of physics- and data-driven modeling elements can support. We present a full field micromechanical approach to capture the effects of defects to fatigue performance of metallic alloys and steels. We utilize a high-throughput framework to derive a recurrent deep learning based surrogate to evaluate and act as a design tool for microstructural features improving resistance to fatigue. We demonstrate the approach on high strength steels and high entropy alloys using Bayesian workflows.

11:50 AM
A Phenomenological Model for the Relationship Between Fatigue Life and Mechanical Properties: Emiel Amsterdam[1]; *Borit Zwerink*[1]; [1]NLR

We present a phenomenological model that accurately describes the influence of the initial discontinuity distribution, the applied stress range and the main mechanical properties, such as the ultimate tensile strength and the Young's modulus, on the fatigue life of an alloy. The phenomenological model for fatigue life is constructed from a physics based fracture mechanics model that includes the effect that small cracks have on the fatigue crack growth rate. It is shown that the model is able to relate the fatigue life to i) the "effect of defect" for porosity in additively manufactured AlSi10Mg and Ti-6Al-4V, ii) the anisotropy in additively manufactured Inconel 718 and iii) the UTS of conventionally processed AA7075 with different heat treatments. The results allow for accurate screening of alloy composition and processing for the prediction of fatigue resistant alloys that can be used for optimized design of high performance engineering structures.

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

Fatigue life being an extreme value property is dictated by the local microstructure. A finite element based micromechanics approach is employed to capture the influence of microstructural features in predicting the cyclic stress-strain response of ferrite-pearlite/martensite steels. The material response is modelled through Chaboche non-linear kinematic hardening and continuum damage mechanics models. A 10% drop in peak stress is used as a criterion for estimating the number of cycles for crack initiation (safe life). The developed micromechanics model is used to evaluate the effect of microstructural parameters like grain size, phase fraction, interlamellar spacing on fatigue response. The safe life prediction model is utilized in a stochastic framework to account for variability in microstructure and phase properties. The details of the micromechanics model, safe life design methodology, stochastic framework and the effect of microstructure on fatigue response will be presented.

Applications: Advanced Manufacturing Microstructure III

Thursday AM
May 25, 2023

Room: Boca I-III
Location: Caribe Royale

Session Chair: See Session Sheets

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

Additive manufacturing (AM) of metals is to build metallic components through layer-by-layer that can make the prepared materials with unique geometries. Due to the rapid solidification and high cooling rates during AM process, the microstructure within AM metals has unique features, such as interlayer interfaces, molten pool solidification boundaries and intracrystalline substructure. It is critical to understand the relationship between the spatial heterogeneity of the microstructure and the mechanical properties of AM metals. In this work, discrete dislocation dynamics (DDD) simulations will be used to explore the effect of dislocation cells on the strength and anisotropy of the AM metals. In our DDD simulations, we will vary the dislocation cell size, dislocation density within the cell walls and loading directions to explore how these factors affect the dislocation behavior within the dislocation cells. In addition, our model will also consider the influence of solute concentrations.

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

In metal additive manufacturing (MAM), the thermal history and the grain growth associated with complex physics lead to the formation of distinguished microstructure compared with conventional manufacturing methods. A quantitative and robust process-structure (P-S) linkage for AM-processed alloys must be established to tailor the highly anisotropic as-built microstructure for obtaining desired mechanical properties. This work proposes a novel approach to model the P-S linkage for MAM with a deep-learned multimodal conditional generative model. To model the relationship between the source domain (temperature field) and the target domain (microstructure) in MAM, the training data obtained from high-fidelity thermo-fluid analysis and cellular automata (CA) based grain growth simulation is employed. The model can generate multiple inverse pole figure (IPF) maps, which can be controlled by latent space manipulation, for a given processing condition that agrees with the numerical simulation results in terms of grain morphologies and texture.

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

Recent evolutions in additive manufacturing (AM) technologies have provided significant opportunities to realize organic shape designs while concurrently achieving material properties to meet functional performance requirements. In this effort, an integrated multi-scale model has been developed to demonstrate process - microstructure - property relations. A numerical method has been established to determine local temperature gradients (TG) and cooling rates (CR) as outputs at the melt pool level. These outputs are taken as input to micro scale phase-field models to predict as-grown solidification microstructures for a range of input AM process parameters. Phase field predictions for solute distribution and evolution of ' and '' precipitates during post process after AM have also been developed. Experimental results for model calibration and property validation are discussed.

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

Interest in Additive Manufacturing has significantly increased in aerospace, automobile, and electronic industries. Complex features can be built with the specimen in single step. Similarly, post-processing such as machining and heat treatment can also be eliminated to obtain an engineered specimen with better mechanical properties. However, there are numerous challenges in studying the microstructure and mechanical properties of the deposited specimen due to the very complex heating and cooling cycle. Therefore, the heat transfer and material flow model is developed to compute the thermal cycle and correlate with the structure and mechanical properties of the specimen in the multi-layer deposition of Al-0.5Sc-0.5Si alloy. The thermal cycles, melt pool dimension, and cooling rates are computed around the vicinity of the melt pool for multi-layer deposition, and solidification morphologies are predicted using the CET solidification map. The solidification morphologies are further correlated with the microhardness in the multi-layer deposition of Al-0.5Sc-0.5Si alloy.

Applications: Advanced Manufacturing Processing IV

Thursday AM
May 25, 2023

Room: Caribbean IV
Location: Caribe Royale

Session Chair: See Session Sheets

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

In additive manufacturing (AM),to accelerate the fabrication of porosity-free parts, the optimal processing conditions of a material needs to be determined. The printability of alloys must be surveyed regarding their chemical composition and processing conditions. Since this union of the compositional and processing design spaces are intractable for experimental exploration alone, high-throughput (HTP) computational frameworks are needed to guide the search for highly printable alloys and processing parameters. In this work, various criteria for process-induced defects considered properties predicted using CALPHAD, processing parameters, and melt pool profiles obtained by thermal models. We verify the framework by constructing printability maps for the CoCrFeMnNi system. Furthermore, the framework searches for alloys in the Co-Cr-Fe-Mn-Ni HEA-constrained space to reduce the formation of macroscopic defects. This framework enables the systematic investigation of the printability of alloy spaces and can be used as a valuable tool in AM-centering alloy design.

11:30 AM

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

Novel materials with improved performance and advanced application fit property profiles such as lightweight, thermal stability, high-temperature strength, and good oxidation resistance can be designed within the framework of the vast compositional space available in high entropy alloys (HEAs). The study is to design nickel-aluminide (Ni-Al) based high-entropy alloys for lightweight, high strength, and high-temperature applications using a CALPHAD-based tool and thermodynamic physical parameters such as mixing entropy, mixing enthalpy, and valence electron concentration (VEC) to design the right match of multi principal elements. The study will establish the use of Thermo-Calc software to perform thermodynamic modelling of the phases present, phase diagrams, and transformation temperatures. The Thermo-Calc software will be used to access the necessary databases for kinetic and thermodynamic calculations for the nickel aluminide-based HEAs. The study aims to design novel HEAs based on nickel that may replace the superalloys in aero-engines.

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

The laser melting process involves rapid evolution of microstructure, phase transformation, temperature history and strain due to its high heating as well as cooling rates. In this study, high speed synchrotron X-ray diffraction technique was utilized to investigate the effect of cooling rates on phase transformation and on the evolution of temperature history, and strain in Ti-6Al-4V during in-situ laser melting process. Different cooling rates were achieved by designing multi-pass scans (back & forth) with different delay times between passes. The high temporal and spatial resolution available in the measurement enabled us to study various microscale phenomena that occur during rapid evolution of the small fusion zone. Microstructural features were probed using optical and scanning electron microscopy. Thermal history, cooling rate, and strain were estimated based on changes in the lattice spacing resulting from the thermal contraction upon solidification.

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

Processing parameters such as laser power, hatch distance, scan speed and baseplate temperature govern the final mechanical properties of an additively manufactured component. Process-structure-property (P-S-P) maps can guide in selection of process parameters to tailor the microstructure for desired properties of the component. However, the available information pertaining to microstructure evolution during non-equilibrium conditions is limited. This study is aimed at developing process-structure-property maps for selective laser melting of 18Ni-300 maraging steel using a combination of theoretical solidification models in the context of non-equilibrium solidification and prediction of grain sizes, phase fractions and estimation of microhardness from the resultant microstructure parameters. A parametric study of the effect of above-mentioned processing parameters on the final microstructure parameters will be presented. The PSP maps are then overlayed on the processing defect maps to assess the printability of the component. The potential of this in-silico approach to tailor site-specific properties will be presented.

Poster Session

Tuesday PM
May 23, 2023

Room: Caribbean V
Location: Caribe Royale

Session Chair: See Session Sheets

A Framework for Multilevel Robust Co-design of Material and Product Systems: *Mathew Baby*[1]; Anand Balu Nellippallil[1]; [1]Florida Institute of Technology

The design of products with targeted performance requires expert decision-making across the Processing-microStructure-Property-Performance levels of the materials design hierarchy. These multilevel decisions need to account for the uncertainties arising from incomplete and inaccurate information during design. Isolated decision-making across levels will not suffice in realizing targeted product performance, as it can result in design conflicts that adversely impact product performance. Hence, the interactions of multilevel decisions need to be considered. We recognize 'co-design', which involves collaborative decision-making across multilevel by considering their interactions, and 'robustness', as central to managing design conflicts and uncertainties.In this paper, we present a framework to support the multilevel, robust co-design of material and product systems. The framework facilitates systematic modeling of multilevel decisions and interactions, uncertainty management, and conflict detection and management. We illustrate the efficacy of the proposed framework using the Hot-rod rolling problem characterized by uncertain, multilevel decision-making across the Processing-microStructure-Property-Performance levels.

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

The concept of high entropy (HE) via the virtue of configurational disorder is exploited in all the classes of materials ranging from alloys, ceramics and metallic glasses. In this work we focus on 2D High Entropy MXene. MXenes are a promising class of 2D materials owing to high electronic conductivity and ease of cation intercalation making it a candidate for supercapacitors, battery material and sensors. However, there is absence of experimental or theoretical studies to evaluate thermal characteristics of these materials. In this work we study thermal properties of Ti2AlC (MAX phase), Ti2C (MXene) and (Cr0.5Nb0.5Ta0.5Ti0.5)C (HE-MXene) via first principal phonon calculation and solution of Boltzmann transport equations. The reduction in thermal conductivity is attributed to lower phonon life time and higher disorder in structure.

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

Devices like solar cells, batteries, LEDs etc. are now an integral part of our lives. Technological advancements in these devices are in vogue, either to increase their performance or to find new applications for them. These advancements often trickle down to the search for better materials or efficient processes. The space of potential materials, operations, operating conditions is vast, and selecting the right combination thereof to achieve the desired characteristics is a knowledge intensive activity. A large amount of such device fabrication knowledge is available in the form of publications, patents, company reports. We present a decision support system built on top of systematically extracted knowledge from materials science literature. The extracted knowledge is represented as knowledge graphs conforming to an ontology that can be queried to make informed decisions during device fabrication. We applied our system to the emerging class of devices-perovskite solar cells and achieved good results.

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

Many studies have extensively investigated various microstructural features to understand heterogeneous microstructure effects with mechanical responses. In this study, a representative volume element modeling approach was used to control specific microstructure features accurately beyond the experimental difficulties. In particular, the deformation behavior of the core-shell structure was clearly visualized using the finite element method with the proposed dislocation-based constitutive model considering the evolution of geometrically necessary dislocations. From these findings, we suggest that the optimal heterogeneous microstructure should be designed based on the deformation behavior with respect to the geometry, size, and shape of soft and hard domains.

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

The fossil-fuel emissions can be reduced by substituting fossil-fuel based engines with high-speed electrical motors, such as axially laminated anisotropic synchronous reluctance motor (ALASynRM). The rotor of this motor is constructed by joining Inconel and steel by using vacuum brazing with copper (Cu) filler. However, the experiments show poor wettability of Cu on IN718 during vacuum brazing. In this work Molecular Dynamics (MD) simulations are performed to study the nanoscale interfacial phenomena that occur during brazing of steel with IN600 and IN718 using Cu. The results show that IN600 coheres well with liquid Cu, whereas IN718 containing Niobium impedes the atoms diffusing from Inconel into liquid Cu. Additionally, liquid Cu atoms diffuse well into the precipitate (\947'' phase), whereas Cu atoms barely diffuse into the parent \947 phase in IN718.

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

We have developed a Monte Carlo Potts model for anisotropic grain growth in SPPARKS to study the impact of misorientation and inclination on the grain boundary (GB). The GB inclination is determined using a smoothing method. We compare the grain growth behavior for three different GB energy functions: 1) energy is only a function of misorientation; 2) energy is only a function of inclination; 3) energy is fully dependent on five degrees of freedom, three from misorientation, two from inclination. In addition, we also compare the growth for different initial grain structures: 2D bicrystal with a circular grain, 2D tricrystal with a triple junction, 2D polycrystal, 3D bicrystal with a spherical grain, 3D tetracrystal with a quadruple junction, and 3D polycrystal.

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

Fatigue is amongst the major physical processes associated with crystalline materials that lead to premature failure. Understanding how fatigue cracks initiate in crystalline materials is very challenging because the microstructural features around these cracks evolve continuously with cyclic loading. A phase-field model for heterogeneous microstructures is developed to study the evolution of phase, stress, and plastic strains in metallic material systems under cyclic loads. A small strain plasticity model based on the principles of continuum mechanics is integrated into the phase field model. Local momentum balance is solved on a staggered grid using the finite difference method to compute displacement fields. For calculations of plastic strains, a Prandtl-Reuss-type model consisting of an associated flow rule in combination with the von Mises yield criterion and a linear isotropic hardening approximation is implemented. Evolution of the stresses, plastic strains are obtained by establishing the consistency condition using a two-step return mapping algorithm.

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

Assessing the durability of photovoltaic (PV) module backsheet is critical to increasing module lifetime. Laboratory-based accelerated testing is inefficient in assessing large-scale failures of commercial polymeric materials. Additionally, there is growing concern that standard condition tests do not reflect non-uniformities in field exposure, and that certain modules experience more severe degradation due to their location. Anisotropy in field exposures is installation-dependent and reflects different levels of exposure to irradiance due to mounting geometry, ground surface albedo, and climatic zone. Bificial_Radiance, describes the amount of reflected irradiance on the backsheet using measured racking parameters. In our work, site specific weather data are gathered for the entire length of exposure for the modules. We then determined the total full-spectrum dose for the incident irradiance on the backsheet. The simulation results are integrated with historical field survey data to better understand outdoor exposures and allow us to better correlate with indoor accelerated tests.

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

Atomic force microscopy (AFM) provides valuable insights into the crystallization of fluoroelastomers, which impacts performance in applications. Time-lapsed acquisition of AFM image sequences provides quantitative information on crystallization kinetics. However, corresponding datasets are large. Open-source software and tools are routinely used for data processing, but it can be time-consuming and challenging to process thousands of images. In this work, we integrate automated feature detection and segmentation algorithms, leveraging evaluation by convolutional neural networks. End-to-end frameworks, such as UNet image segmentation, allows for batch processing such as generating binarized masks which can be used to obtain image properties. This can help in quantifying the projected area fraction of the crystalline phase in each image. It can also track individual crystallites as a function of time when combined with an open-source software for AFM-image processing, which serves as the "ground truth" for comparison.

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

In this study, we assess the variation in temperature at selected subsurface depths between the surface of the earth extending to approximately 300m. It is a common rule of thumb that a 10 degree Celsius change in temperature doubles the degradation and failure rates of systems deployed. Thus, understanding temperature distribution both laterally and vertically in the subsurface is an important factor in understanding substructure materials degradation. We produced maps depicting subsurface temperature variation at selected shallow depths across the continental United States; respectively, 100m, 200m, and 300m using (ordinary) kriging. Additionally, Nevada, Michigan, and Ohio were selected for more detailed temperature mapping evaluation including a comparison of three different geostatistical methods; Ordinary Kriging, Fixed Rank Kriging, and Conditional Simulation. Results from all methods employed and at all depths analyzed confirmed heterogeneous temperature patterns across the United States and within the individual states.

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

Multi-domain tracking method improves object tracking by sharing domain information whilst learning private information. In that context, each video sequence as a specific domain serves for a domain-specific layer. We observe an finding that target features from different domains are highly confused with each other. To this end, we propose a domain interaction training paradigm called domain contrast to boost discriminative features by effectively using amounts of instances from all the domains in two novel aspects: 1) a memory-saving training algorithm is proposed to solve the "out-of-the-memory" problem, and 2) a composite class-balanced loss is explored to tackle a imbalanced problem, which not only involves the usual class imbalance problem but also accounts for the case of the totally mere negative instances. Experiments on multiple tracking benchmarks show that our mechanism consistently achieves the tracking performance gain of both base multi-domain tracker and its real-time variant.

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

High-entropy alloys are emerging as a novel class of catalysts for chemical conversions like electrolysis for hydrogen production, CO_2 electrochemical reduction, fuel cells etc. AuAgCuPdPt equimolar HEA was recently shown to be an active catalyst for CO_2 reduction. In this work, we have used EAM molecular dynamics potential based Hybrid Monte Carlo/Molecular Dynamics (MC/MD) simulations to study surface segregation in AuAgCuPdPt FCC HEA. Simulations were carried out for spherical nanoparticles, cubical nanoparticles, and slabs of various crystallographic surface orientations to obtain detailed structural and concentration profiles normal to the surfaces. In all cases, Ag atoms were found to preferentially segregate to the surface while the subsurface layer mainly consisted of Au atoms. Hardly any Pt atoms were found on the surface layers. Detailed neighborhood analysis of surface sites revealed that the percentage of chemically unique sites were larger for elements with lower concentration at the surface.

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

The microstructure and tensile deformation of a number of sintered TiB2-reinforced near-titanium aluminide matrix composites have been studied. When TiB2 was added to the microstructures via spark plasma sintering processing at values of 0.5 and 3.0 vol pct, it was contrasted with unreinforced TiAl. For every composition and reinforcement variety, the effects of temperature and time have been examined. Within the studied composites, a range of TiB2 sizes was measured. TiB2's elastic moduli, tensile strengths at ambient temperature, and overall strain-hardening response all rise as the volume fraction of TiB2 increases. According to the findings, both indirect and direct sources contribute to the strengthening and flow behaviour of these composite materials. Strengthening contributions are indirectly derived from the microstructural changes within the matrix of the composite.

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

Corrosion has a wide impact on society, causing catastrophically damage to structural engineered components. High-entropy alloys are emerging materials for superior corrosion performance. However, experimental search for corrosion-resistant materials is time consuming and expensive. Machine learning models trained on first-principles data holds the promise in acceleration of materials design and discovery by predicting materials properties at a low computational cost. In this work, we use first-principles calculations to identify thermodynamic and kinetic metrics for corrosion behaviors of metals. Based on those metrics, we then employ a data-driven approach to guide the autonomous discovery of high-entropy alloys for corrosion protection. Limitations and improvements of the proposed methods will be discussed.

Microstructure-based Modelling Approach to Determine Hydrogen Diffusion and Trapping in Steels: Maribel Arribas[1]; Ana Rosa Carrillo[1]; *Ane Jimenez*[1]; Jean Baptiste Jorcin[1]; [1]Tecnalia Research & Innovation

In this work, a hydrogen diffusion and trapping model has been coupled with electrochemical permeation measurements to characterize de diffusion and trapping parameters associated with a pipeline steel. The obtention of hydrogen trapping parameters is not straightforward, especially for complicated microstructures with multiple trapping sites, and generally the existing models consider a high number of fitting parameters. In the present model, the number of fitting parameters has been reduced by defining new microstructure-based functions which give a physical meaning to parameters which have been typically treated as fitting parameters. As a result, a better estimation of the hydrogen diffusion and trapping parameters is obtained, providing an improved modelling framework for the definition of the appropriate microstructure features that result in a better performance of the pipeline steels in contact with hydrogen.

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

The heat treatment process is a necessary part after solidification in single crystal superalloy. The microstructure after heat treatment affects the service performance significantly. However, heat treatment experiments are time-consuming and costly. To investigate the microstructure evolution in Ni-based superalloys during heat treatment, a multicomponent multiphase-field model is established for the heat treatment process in Ni-based single crystal superalloys. The Thermo-Calc database is used to calculate kinetic and thermodynamic parameters in multicomponent superalloy. The microstructure evolution will be discussed according to the simulation results and the effect of cooling rate and heat treatment time will also be explored. Finally, the design of heat treatment process will be considered.

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)

The MaterialDigital (PMD) platform has been funded by the German Federal Ministry of Education and Research (BMBF) by 2019. The platform aims to digitalize materials and processes including the provision of infrastructures to represent complete material lifecycles, considering the FAIR principles (discoverable, accessible, interoperable, reusable). The PMD-funded KupferDigital project is developing a data ecosystem for digital materials research. The fundament of the data ecosystem is ontology-based digital representations of copper materials. In the current research, we present the methodology and toolchains for the development of domain-level ontologies for materials testing that address the requirements of materials testing standards. The collection of the required terminology from the testing standard, the semantic representation of the process graphs, the conversion of the ontology files, their integration with the upper-level ontologies, and the data mapping processes were presented for the Brinell hardness testing use case. The data integration process was successfully validated by the SPARQL query of the mapped datasets.

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

It is crucial to ensure the effectiveness and efficiency of semiconductor devices when they work in harsh environments. In this work we are developing a new novel simulation tool that predicts the impact of ionizing radiation on the performance of a semiconductor device. The approach will couple TCAD capability to predict device performance with detailed radiation models to predict charge carrier and lattice defect production. The tool is implemented using the open-source Multiphysics Object-Oriented Simulation Environment (MOOSE). We determine the performance of the devices by calculating local carrier concentration and local current density vs. DS voltage dynamically over time. The results show the relationship of performance degradation rate and irradiation. The final tool will be open source, have robust quality assurance practices, and be able to be referenced in designing more radiation hard devices.

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

In this work, we examine the effects of crystallographic orientation and temperature on the mechanical performance of a single crystalline face-centered cubic (FCC) CoCrNi MEA. Uniaxial tensile loadings were applied on the MEA plates oriented along the [100], [110], [111], and [112] directions at 77 K and 298 K. Our simulation results reveal a strong orientation and temperature effect on the stiffness, strength, and ductility of the MEA. The [111]-oriented plate exhibited the highest elastic modulus, yield stress, and modulus of toughness, demonstrating a strong strain-hardening response; while the [100]-oriented plate produced the lowest corresponding values among the tested cases. At 77K, deformation twinning was the dominant deformation mechanism in the [100] and [110]-oriented MEA plates, and for the [111] and [112]-oriented MEA plates, dislocation slip was dominant. At 298K, dislocation slip was the dominant deformation mechanism in all orientations.

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

The threat of corrosion to metals is a costly and dangerous problem. It is known that corrosion-resistant alloys form passive oxide films that shield the metal from the environment, but a stronger understanding of passive film formation is necessary to continue designing and modifying functional corrosion-resistant alloys. A theory of passivation based on the percolation of metal-oxygen-metal mer units has been developed for binary alloys, but Monte Carlo simulations based on this theory have assumed a regular solution model. Thus, short-range order (SRO) is not included, leading to discrepancies with experiment. In this work, we address SRO by training cluster expansion models on density functional theory calculations. Our models quickly predict the energies of mesoscale structures in the Cu-Rh system, enabling fast and accurate Monte Carlo simulations of configuration ensembles. We provide a kinetic analysis of the initial stages of passivation and compare our results with experimental observations.

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

The occurrence of hot cracking in the additive manufacturing process involves a variety of factors from different aspects. This leaves the effort trying to quantify hot cracking phenomena often lacking generality. Thus, unifying models that take account of processing parameters, thermodynamics, and mechanical properties remain a big gap in modeling the hot cracking phenomenon. Our current study intends to evaluate variables in different aspects but related to the hot cracking phenomenon. The topmost relevant variables will be identified and correlated with the occurrence of hot cracking through machine learning algorithms. To this end, synchrotron-based high-speed techniques together with a melt pool simulation model will be used to generate the training data. The end goal is to build up a unifying model that can predict hot cracking susceptibility based on information at different scales and aspects.

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

This paper explore ICME workflow that enables the virtual design of radiation resistant materials. Carbides, solute clusters, and dislocation loops are a critical microstructure/material features of reactor pressure vessel steel. Irradiation generates these defects, which contribute to reduction of ductility and the ductile-to-brittle transformation of metals used in fission or future fusion power plants. In this paper, authors' consider the fracture in unirradiated and irradiated microstructures of reactor pressure vessel steel. Finite-element simulation results are compared with peridynamic theory's results to address key features like defect size effect. Several cases of intragranular and intergranular fractures are presented.

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

There is a great interest in material science to predict the microstructure of the product that underwent specific processing conditions. Usually, such information is obtained from trial-and-error experiments. Machine Learning can generate the computationally expensive simulation results almost instantly, without knowing the governing laws. Deep learning algorithms, especially generative adversarial networks (GANs), have demonstrated outstanding performances in synthesizing highly realistic images. Deep neural networks are hungry for data and need thousands to millions of data for training. In this work, the StyleGANv2-ADA model was explored to generate synthetic microstructural images using few hundreds to thousands of images. Quantitative metrics like Frechet Inception Distance were used to assess the performance of the model. Quantitative Morphometric Analysis (QMA) was also performed to compare the distribution of microstructural features of real and synthetic images. StyleGAN like models will be crucial in establishing structure-process linkage in limited datasets (<1500 images) typical of metallurgical studies.

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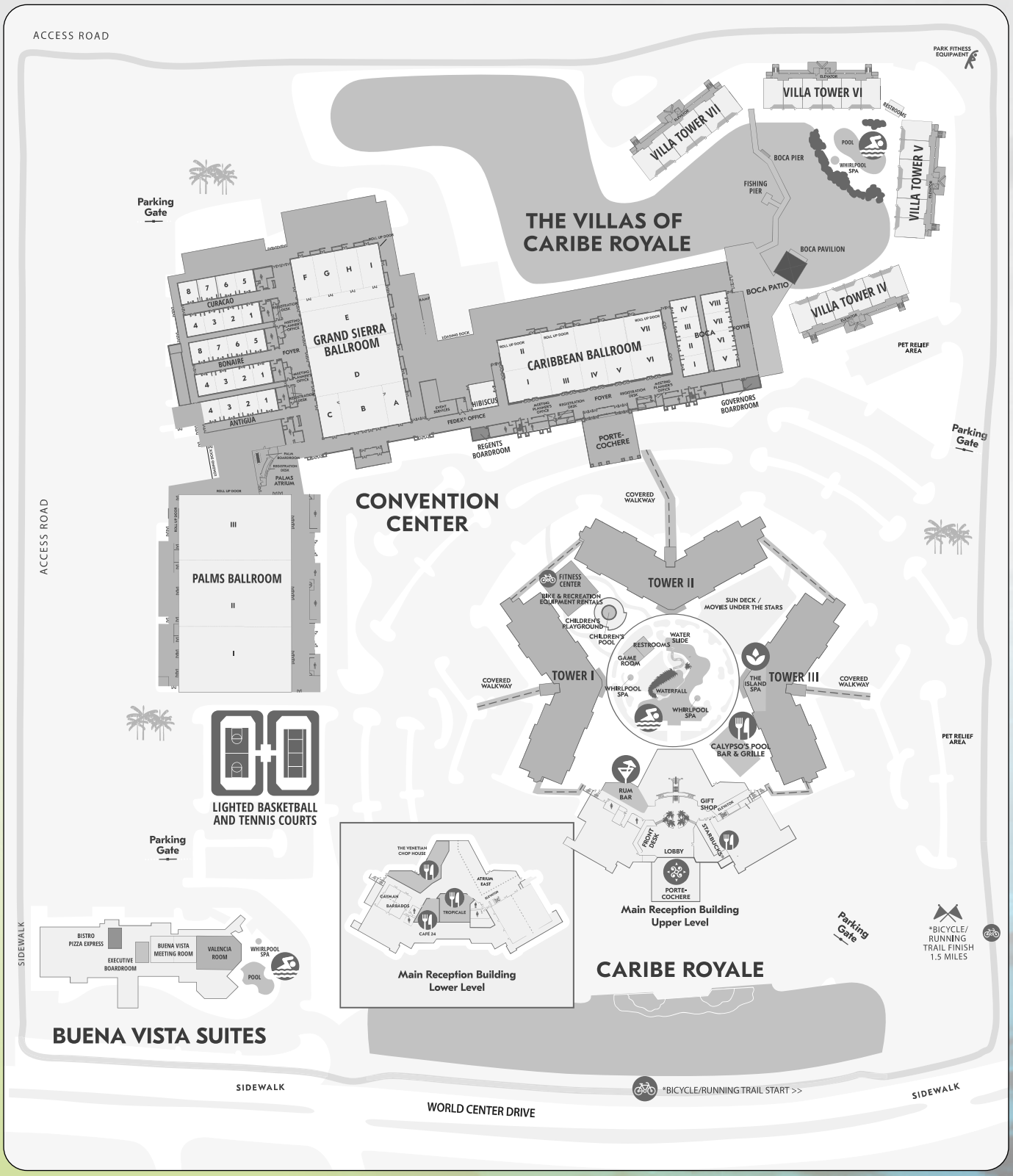

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