3rd World Congress on AIM
ARTIFICIAL INTELLIGENCE IN MATERIALS & MANUFACTURING 2025

ICME MANUFACTURING DESIGN MATERIALS
8TH WORLD CONGRESS ON
INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING (ICME 2025)

The 7th International Congress on
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Specialty Congress 2025: All-Congress Plenary Session: Monday Plenary Session

Monday AM
June 16, 2025

Room: Plenary Room
Location: Anaheim Marriott

Session Chair: To Be Announced

8:00 AM Introductory Comments

8:10 PM Plenary
Harnessing Interoperable Digital Workflows for Materials Design: Sarath Menon[1]; Marvin Poul[1]; Markus Stricker[2]; Jan Janssen[1]; Tilmann Hickel[3]; *Joerg Neugebauer*[1]; [1]Max Planck Institute for Sustainable Materials; [2]Ruhr-Universität Bochum; [3]Max Planck Institute for Sustainable Materials / Bam Federal Institute For Materials Research And Testing

The advent of a new generation of machine learning techniques has opened up powerful and exciting opportunities to explore and exploit the vast chemical and structural configuration spaces that exist, for example, in advanced materials such as compositionally complex alloys. While Artificial Intelligence (AI) approaches applied solely to already available data sets have provided important first insights and advances, it is becoming increasingly clear that the real successes can only be achieved through an integrated approach combining active learning, computer simulations and experiments based on computer-generated input. A prerequisite for such integrated approaches is to make the very different concepts and tools used by the respective researchers interoperable and to embed and execute them in digital workflows. The presentation will provide an overview of key aspects and recent developments in this rapidly growing field, and highlight examples where such integrated interoperable digital workflows have been successfully used.

8:50 AM Question and Answer Period

Joint Sessions of AIM, ICME, & 3DMS: Fair Data I: Joint Session of AIM & ICME

Monday AM
June 16, 2025

Room: Joint Sessions Room
Location: Anaheim Marriott

Session Chair: To Be Announced

9:10 AM
Transforming Materials Science With Concepts for a Semantically Accessible Data Space: *Bernd Bayerlein*[1]; Markus Schilling[1]; Henk Birkholz[2]; Philipp von Hartrott[3]; Jörg Waitelonis[4]; Alden A. Dima[5]; June W. Lau[5]; [1]Bundesanstalt für Materialforschung und -prüfung; [2]Leibniz-Institut für Werkstofforientierte Technologien; [3]Fraunhofer-Institut für Werkstoffmechanik; [4]Leibniz-Institut für Informationsinfrastruktur; [5]National Institute of Standards and Technology

The digital transformation in materials science enables more efficient and sustainable processes. Through technological adaptations and a commitment to the FAIR principles, materials and processes are holistically addressed across entire value chains. The Platform MaterialDigital (PMD) and related initiatives are developing innovative solutions to the challenges of digitalization. The focus is on the interoperable integration of heterogeneous materials and processes data in semantically accessible data spaces. An ontological framework, based on the PMD Core Ontology and application-specific ontologies, promotes semantic interoperability of cross-domain and multi-scale (meta)data. This framework can be extended through natural language processing in a script-supported manner, as demonstrated with the Microscopy Ontology. The presentation further highlights how freely available mechanical and microstructural datasets of various aging stages of an aluminum alloy can be semantically integrated and flexibly searched. Graph-based operations enable links between processing and microstructural properties to be established, facilitating enhanced correlation analysis and pattern recognition.

9:30 AM
Towards Structured Data Spaces: Prototypical Application of Semantic Technologies as a Driver for Innovation in Materials Science: *Markus Schilling*[1]; Bernd Bayerlein[1]; Philipp von Hartrott[2]; Jörg Waitelonis[3]; Henk Birkholz[4]; Birgit Skrotzki[5]; [1]Federal Ministry of Materials Research and Testing; [2]Fraunhofer-Institut für Werkstoffmechanik (IWM); [3]FIZ – Leibniz Institute for Information Infrastructure; [4]Leibniz-Institut für Werkstofforientierte Technologien IWT; [5]Bundesanstalt für Materialforschung und -prüfung (BAM)

In the pursuit of advancing development and digitalization within materials science, ensuring quality assurance, interoperability, and adherence to FAIR principles is significant. To address these aspects, semantic technologies are employed for storage, processing, and contextualization of data, offering machine-actionable and human-readable knowledge representations crucial for data management. This presentation showcases the prototypical application of generic approaches of knowledge representation in materials science. It includes the design and documentation of graph patterns that may be compiled into rule-based semantic shapes. The development and application of the PMD Core Ontology 3.0 (PMDco 3.0) tailored for materials science is highlighted. Its integration into daily lab life is demonstrated through its functional incorporation into electronic lab notebooks (ELN). Examples of material processing and standardized mechanical testing illustrate how knowledge graph operations enhance ELN capabilities, providing a generalizable unified approach for managing diverse experimental data from different sources with automation potentials.

9:50 AM
Ontology-Based Materials Data Management for High Temperature Alloy Oxidation Data: *Madison Wenzlick*[1]; William Trehern[1]; Leebyn Chong[1]; Casey Carney[1]; Michael Gao[1]; Richard Oleksak[1]; Wissam Saidi[1]; [1]National Energy Technology Laboratory

High quality, digitally structured data is essential for creating reliable data-driven models. However, managing materials datasets presents several challenges including variable data types, formats, and relationships. Ontology-based data management is a re-emerging tool for structuring and defining materials data. In this work, an ontology was generated and applied to high temperature alloy oxidation data collected from both open-source literature as well as in-house testing. Metadata and data attributes from each study were standardized and translated into the ontology structure. The oxidation ontology further integrates with an existing mid-level materials data ontology to support the curation of additional materials information. This framework aids in encoding the complex relationships between the data in both a machine-readable and human-readable manner, enabling the ongoing interpretability of the dataset. The ontology can further be leveraged to support the flow of data from laboratory to database and provides a resource for advanced data-driven modeling and analysis.

10:10 AM

FactoryNet: A Labeled Image Dataset for the Manufacturing Environment: *Erick Braham*[1]; Andrew Bowman[1]; William Bernstein[2]; [1]UES / Air Force Research Laboratory; [2]Air Force Research Laboratory

Human labeled image datasets are essential to training and developing AI models. Most image datasets with high volumes of data contain low specificity of image classes. A public open image dataset focused on the manufacturing environment with a high volume of images in the manufacturing domain would benefit the development of visual AI for manufacturing. The FactoryNet dataset is a growing, high-quality labeled image dataset of in-context images for the manufacturing community. Initial efforts to build the dataset have utilized web scraping, factory scans, and industry collaborations. We present the first iteration of the human labeled dataset, looking at the data sanitization and design choices taken to this point. We look toward the future of this resource and how it is and will continue to be an open resource for the manufacturing community.

10:30 AM Break

10:50 AM

NFDI MatWerk Ontology: A Framework for FAIR Data Management in the Materials Science and Engineering: *Hossein Beygi Nasrabadi*[1]; E. Norouzi[1]; K. Hubaiev[1]; H. Fliegl[1]; V. Hofmann[2]; A. Azócar Guzmán[2]; S. Fathalla[2]; A. Z. Ihsan[2]; S. Sandfeld[2]; A. Gedsun[3]; J. Waitelonis[1]; H. Sack[1]; [1]FIZ Karlsruhe – Leibniz-Institute for Information Infrastructure; [2]Institute for Advanced Simulations – Materials Data Science and Informatics (IAS 9); [3]Albert-Ludwigs Universität Freiburg

The National Research Data Infrastructure (NFDI) is a German initiative established in 2020 to create a standardized and sustainable research data infrastructure across various disciplines. Within this framework, NFDI-MatWerk focuses on creating a digital infrastructure for Materials Science and Engineering (MSE) to facilitate improved data sharing and collaboration in this domain. This presentation introduces the NFDI MatWerk Ontology (MWO) version 3.0.0, a foundational framework designed to structure research data and enhance interoperability within the MSE community. MWO V3.0.0 has been mapped to the Basic Formal Ontology (BFO) to ensure comprehensive integration and compliance with top-level ontology standards. Additionally, it utilizes the NFDIcore mid-level ontology's modular approach, enriching metadata through standardized classes and properties. By serving as the backbone of a knowledge graph for MSE, MWO significantly enhances data discoverability and reusability, thereby accelerating materials development and technological innovation through optimized scientific exchange and data management.

11:10 AM

Customizing the NIMS RDE System for Optimal Data Management: *Takuya Kadohira*[1]; Jun Fujima[1]; Hideki Yoshikawa[1]; Satoshi MInamoto[1]; [1]National Institute For Materials Science

The preparation of FAIR data is crucial in AI research. While basic research on materials has successfully applied FAIR principles to simulation data, applying these principles to experimental data is challenging due to quality differences; the simulation conditions are fully known, unlike the experimental ones. The NIMS RDE system, a part of the Materials Data Platform, addresses FAIRness at data submission through input and ETL functions that are customizable for different experiments. This flexibility theoretically supports the management of experimental results as FAIR data, enhancing reproducibility and reducing redundant experiments. However, the extensive customization flexibility can be challenging, as it requires identifying how much customization is truly necessary and finding ways to minimize the effort involved in such customization. Balancing this challenge involves developing a data model that identifies essential FAIRness aspects for data utilization and provides a framework for function customization.

11:30 AM

NIMS's Data-Driven Materials Research Platform: Enhancing MLOps With Literature-Based Data Integration: *Toshihisa Anazawa*[1]; Hayato Sonokawa[1]; Hideki Yoshikawa[1]; Takuya Kadohira[1]; Satoshi Minamoto[1]; [1]National Institute for Materials Science

NIMS Materials Data Platform (MDPF) supports data-driven materials research through "DICE", a system that comprehensively handles the creation, accumulation, and utilization of materials data. MDPF is currently developing a materials development platform using MLOps by connecting systems named "RDE" (data accumulation), "pinax" (modeling), and "MInt" (execution). Simultaneously, we're training coordinators to promote data-driven materials development. While pinax can use developers' own data as well as RDE and other public databases, materials are diverse in their applications. Even when properties are reported in academic papers, they are often not databased in a reusable form.Regarding this, we propose a tool for MLOps that searches related papers, collects desired property data and process conditions from relevant papers, and aggregates them as machine learning data. This system will not only incorporate the aggregated data into pinax for MLOps but also utilize metadata extracted from papers as reference for materials developers and the coordinators.

11:50 AM

Modular and Interoperable Materials Data Science Ontology (MDS-Onto) for Knowledge Graphs and Semantic Reasoning: *Erika Barcelos*[1]; Balashanmuga Priyan Rajamohan[1]; Quynh Tran[1]; Van Tran[1]; Kai Zheng[1]; Nathaniel Hahn[1]; Hayden Caldwell[1]; Ozan Dernek[1]; Pawan Tripathi[1]; Yinghui Wu[1]; Laura Bruckman[1]; Roger French[1]; [1]Case Western Reserve University

Research data and metadata often have non-standard terms and formats. The terms and concepts are frequently subjective and adopted based on local experience and choices of research teams, and this poses major challenges for data reusability and research reproducibility. Ontologies represent a critical component toward FAIRification of data, achieving semantic interoperability and reducing barriers for data sharing, usability, analysis and modeling. In addition, they serve as the backbone of knowledge graphs, where data and results, standardized by ontologies enabling semantic reasoning and inferences. In this work we introduce the Materials Data Science Ontology(MDS-Onto), a low-level, interoperable, ontology built on a modular framework that simplifies ontology alignment by mapping MDS-Onto concepts to midlevel ontologies such as the Platform Material Digital Core Ontology (PMDco) and the Quantities, Units, Dimensions and Types (QUDT) Ontology terms. It encompasses over 20 domains in materials data science and provides a common foundation for semantic triples of the Resource Description Framework (RDF) data model. These RDF triples, or RDF statements, when stored in a graph database such as Ontotext's GraphDB, form knowledge graphs, over which people and machines can perform semantic reasoning using SPARQL queries. Knowledge graphs enable machines to reason over ing enables can span. These knowledge graphs enable machines to reason over billions of RDF statements, representing for materials data science the ability to reason over historical data and results at scale.

3rd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2025): Applied ML for Manufacturing I

Monday AM
June 16, 2025

Room: Room A
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Invited
Data Driven and High Fidelity Modeling Approaches to Advance Understanding and TRL Level of 3D Printing: *Saad Khairallah*[1]; Amit Kumar[1]; Justin Patridge[1]; Gabe Guss[1]; Eric Chin[1]; Youngsoo Choi[1]; Joseph Mckeown[1]; [1]Lawrence Livermore National Laboratory

A multi-scale ALE3D high fidelity model is developed to simulate directed energy deposition additive manufacturing. The model captures at a high fidelity the powder transport from the coaxial nozzle to the work piece as well as the effect of the carrier gas and laser ray tracing. The high cost of modeling is brought down by using deep learning and data driven reduced order modeling at different scales. The end goal is to combine modeling with a data driven (deep learning) approach for "first time right" also referred to as intelligent feedforward (IFF). We apply IFF to optimize laser power and scan speed to print complex large parts with overhang geometries, such as the Menger sponge, and obtain high density and geometric accuracy.Work Performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE- AC52-07NA27344. Lawrence Livermore National Security, LLC. Release LLNL-ABS-854766

9:30 AM
Adapting to Uncontrolled Variables in Additive Manufacturing Systems: *Andrew Fassler*[1]; Erick Braham[1]; James Hardin[2]; [1]BlueHalo/Air Force Research Laboratory; [2]Air Force Research Laboratory

In a given additive manufacturing system, there are numerous variables that can impact the product of that system. Additionally, many of these variables, such as environmental temperature or humidity, may not be directly monitored or controlled. This can cause issues in applying machine learning approaches, as the quality of the output of the additive manufacturing system may appear to diminish or drift over time with these unmonitored variables and the data collected in earlier iterations may not accurately describe the current state. We explored how to address this problem using Gaussian process regression and an informed uncertainty methodology. Machine learning models were then applied to direct ink write printing to create arched spanning structures over a 4 mm gap. Image capture and processing was used to score the prints against specific target geometries and enable closed loop experimentation and optimization to these targets.

9:50 AM
Machine Learning-Based Prediction of Temperature Fields in Synchronized Multi-Laser Powder Bed Additive Manufacturing (S-MLAM): *Hamed Attariani*[1]; Majid Dousti[1]; [1]Wright State University

Anisotropic mechanical properties, reduction in ductility, and endurance limit of the printed material with Ti6Al4V in laser powder bed additive manufacturing result from forming undesired microstructure such as columnar grains. The columnar grains formation stems from a steep temperature gradient and high cooling rate in the melt pool, which is a characteristic of this manufacturing technique. One promising approach to control the microstructure is beam shaping or using synchronized multi-beam additive manufacturing to tailor the temperature field and subsequently alter the microstructure. Here, a machine learning (ML) algorithm was employed to predict the temperature field for various synchronized multi-beam configurations such as circular, linear (horizontal and vertical), circular, and square configurations. The ML approach is promising compared to other existing computational approaches considering the wider processing window of these synchronized beams, i.e., scanning speed, laser power, number of lasers, laser configuration, and internal spacing among lasers inside a specific configuration.

10:10 AM
Data-Driven Design of Architectured Materials: Enhancing Specific Stiffness With Multi-Objective Optimization: Jinwook Yeo[1]; *Seunghwa Ryu*[1]; [1]Kaist

The development of architectured materials has revolutionized mechanical design, enabling exceptional properties through the optimization of structural geometry rather than material composition. This research focuses on three innovative approaches to designing high-specific-stiffness materials: strut-based architectures, hybrid triply periodic minimal surface (HTAM) structures, and generative AI-driven shape exploration. For strut-based architectures, multi-objective Bayesian optimization was employed to refine beam shapes, achieving a balance between stiffness and density. HTAM structures, combining multiple TPMS geometries, expanded the design space to yield configurations with superior mechanical performance. Finally, leveraging generative AI, novel architectures were explored, demonstrating unprecedented flexibility in achieving optimized designs. Finite element analysis (FEA) and experimental validation confirmed significant improvements in modulus and strength across all approaches. These methodologies underscore the transformative potential of integrating machine learning, advanced optimization techniques, and additive manufacturing to address critical challenges in aerospace, biomedical, and lightweight structural applications.

10:30 AM Break

10:50 AM
A Study Into The Generation and Usability of Synthetic Thermodynamic Data for Optimising the Manufacturing of Dual Phase Steels: *Nicola Beech*[1]; Michael Auinger[1]; [1]University of Warwick

Dual Phase (DP) steels have excellent mechanical properties but lack corrosion resistance. Consequently, they require galvanising, which directly follows annealing in a modern plant. Under annealing conditions (around 800C and up to 100% hydrogen), the alloying elements, typically 1.5-2wt% Mn and 0.5-1.0wt% Si, are prone to selectively oxidise. If non-wettable surface oxides form, such as MnO and SiO2, liquid zinc may not adhere, resulting in coating defects. Internal oxide formation is therefore preferred to keep the steel surface clean. While oxidation studies can inform in the manufacturing route of these complex steels, the thermodynamic databases they often utilise may be incomplete. To resolve this issue, the databases could be augmented using synthetic data, data generated to replicate the statistical properties of real data. This work explores the advanced machine learning techniques of synthetic thermodynamic data generation to augment oxidation data for greater insight into DP steel oxidation near critical limits.

11:10 AM

Development of a Microstructure Image Generation Technique and Machine Learning Model for Property Prediction of As-Cast Materials: *Chanwoo Park*[1]; Wonjoo Lee[1]; Howon Lee[2]; Seong-hoon Kang[2]; Jonghun Yoon[1]; [1]Hanyang University; [2]Korea Institute of Materials Science (KIMS)

This study presents a novel approach for predicting the properties of as-cast materials through the development of a microstructure image generation technique and a machine learning (ML) model. The microstructure generation is achieved using a hybrid Lattice Boltzmann Method–Cellular Automaton (LBM-CA) model, enabling realistic simulations of solidification processes and the resulting microstructural features. By generating diverse and high-resolution microstructure datasets, we constructed a comprehensive training set for ML-based property prediction. The proposed ML model employs CNNs to extract critical features from microstructure images, allowing for the accurate prediction of mechanical properties such as hardness, tensile strength, and ductility. To ensure model generalization, data augmentation techniques and transfer learning strategies were applied. The model's predictive performance was validated using experimental data from cast specimens with varying compositions and process conditions. Our approach offers significant potential for accelerating the design of cast metallic materials, reducing experimental costs, and optimizing process parameters.

11:30 AM

Leveraging Generative Models to Optimize Steel Alloys From Recycled Materials: *Santiago Muiños Landin*[1]; Chirstian Eike Precker[1]; Andrea Gregores Coto[1]; Javier Fernández Troncoso[1]; [1]AIMEN Techology Centre

This research explores the use of generative models to design new steel alloys based on compositions derived from scrap materials. Leveraging machine learning techniques like GANs and VAEs, the study aims to optimize alloy compositions for improved mechanical properties and sustainability. By integrating data from existing compositions and scrap analyses, the models predict viable alloy combinations that enhance performance, reduce reliance on raw materials, and maximize scrap reuse. Preliminary results demonstrate novel compositions with enhanced properties and cost benefits, aligning with circular economy principles. This presentation covers the methodology, model architecture, and validation of the proposed approach.improvements and cost reductions. This research presents a step towards sustainable steel production, bridging the gap between data-driven approaches and material innovation.

11:50 AM

AI-Ready Manufacturing Data for Cybersecurity: *Lily Lee*[1]; Daniel Stabile[1]; Paul Gibby[1]; Tony Reis[1]; Matt Weiss[1]; Jonathan Lee[1]; Stefan Schwindt[2]; Kathleen Finke[3]; [1]MIT Lincoln Laboratory; [2]GE Aerospace; [3]Astronautics Corporation of America

Cybersecurity in manufacturing is crucial as factories and systems become increasingly connected and digitized. However, there is a lack of datasets and machine learning algorithms specifically designed for detecting cyberattacks on manufacturing systems. To address this gap, we developed a synthetic manufacturing operations (MO) environment to generate temporal data collected from simulations. This dataset represents factory productions and quality assurance processes, with labeled events suitable for machine learning experimentation. Our team applied various machine learning techniques to demonstrate baseline results on anomaly detection, malicious event classification, and diagnostic capabilities. By open-sourcing the synthetic MO dataset and algorithm evaluations, we aim to provide a valuable tool for advancing research and developing stronger safeguards for the manufacturing sector.

3rd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2025): Development of Novel ML Methodologies I

Monday AM
June 16, 2025

Room: Room B
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Introductory Comments

9:10 AM

Physically Aligned Hierarchical Mesh-Based Network for Dynamic System Simulation: *Yeping Hu*[1]; Bo Lei[1]; Vic Castillo[1]; [1]Lawrence Livermore National Laboratory

Dynamic systems evolve through intricate interactions where local events impact global behavior, reflecting real-world interconnections. Modeling these systems requires capturing both local and long-range dynamics with accuracy and efficiency, a balance that current mesh-based Graph Neural Network (GNN) methods often struggle to achieve, especially with large datasets and complex meshes. Inspired by real-world dynamics, we introduce the Mesh-based Multi-Segment Graph Network (MMSGN), a framework designed to address these challenges through a hierarchical information exchange mechanism that aligns with physical properties. MMSGN integrates micro-level local interactions with macro-level global exchanges to accurately capture both local and global dynamics while remaining computationally efficient. Our model demonstrates superior accuracy, mesh quality, and scalability on multiple dynamic system datasets, outperforming several state-of-the-art methods and proving well-suited for large-scale, complex system simulations across diverse scenarios.

9:30 AM

Detection of Keyhole-Pore Formation in Laser Powder Bed Fusion Using Spatio-Temporal Graph Convolutional Networks: *Kristen Hernandez*[1]; Maliesha Sumudumalie[1]; Tu Pham[1]; Pawan Tripathi[1]; Sanam Gorgannejad[2]; Jean-Baptiste Forien[2]; Maria Strantza[2]; Gabriel Guss[2]; Nicholas Calta[2]; Brian Giera[2]; Laura Bruckman[1]; Aiden Martin[2]; [1]Case Western Reserve University; [2]Lawrence Livermore National Laboratory

Keyhole formation in laser powder bed fusion (L-PBF) is a dynamic process in which accurate modeling requires multiple assumptions and measurements. This inherent complexity results in inaccuracies from physics-based models and difficulty obtaining generalizable empirical models. To enhance detection in situ, low-resolution sensors are utilized alongside high-resolution imaging techniques to identify overlapping features. Accurate registration, detection, and classification of features are essential for correlating high-resolution features with low-resolution signals. Using high-speed synchrotron X-ray video imaging, we capture and extract vapor depression associated with keyhole defects, utilizing standard processing and feature extraction techniques that align with other detected signals. Extracted vapor depression geometries can be skeletonized into connected nodes with a particular set of overlapping feature components. We propose the implementation of a Spatio-Temporal Graph Convolutional Network (ST-GCN) to capture the correlations among evolving nodes in our features, thereby improving the efficiency and performance of vapor depression mapping to multisensor signals.Prepared by LLNL under Contract DE-AC52-07NA27344.

9:50 AM

Leveraging CALPHAD to Overcome Data Challenges in Machine Learning for Materials Science: *Paul Mason*[1]; Qing Chen[2]; [1]Thermo-Calc Software Inc.; [2]Thermo-Calc Software AB

Machine learning (ML) offers transformative potential in materials science by enabling data-driven discovery and optimization within complex materials systems. However, training high quality models requires access to data and meta-data which can often be sparse. This presentation will explore how CALPHAD can address key data challenges in developing ML models for materials science such as data cleaning, data quantity, feature selection, interpretability, and generalization.Through thermodynamic and kinetic simulations, CALPHAD can be used to fill data gaps, generating extensive datasets, and ensuring data consistency by identifying outliers and validating assumptions. Additionally, CALPHAD enhances feature selection by identifying key physical attributes and aids interpretability by grounding ML predictions in physics-based insights. By generating data across diverse compositions and conditions, CALPHAD also improves model generalization, enabling broader applicability. This talk highlights CALPHAD's role in supporting reliable, interpretable, and generalizable ML models while also warning of potential unreasonable uses of CALPHAD data.

10:10 AM

Machine Learning-Based Prediction of Diffusion Coefficients in Alloys: *Yanqing Su*[1]; Arjun Kulathuvayal[1]; Yi Rao[1]; [1]Utah State University

Diffusion plays a critical role in determining the microstructure and mechanical properties of alloys. Experimental determination of diffusion coefficients can be time-consuming and resource-intensive. Here, we present a comprehensive machine learning (ML) framework designed to predict diffusion coefficients across various diffusion modes in multi-component alloys (MCA) and impure metallic (IM) systems. Five ML models are respectively developed to estimate self, impurity, and chemical diffusion in MCA media, as well as self and impurity diffusion in IM media. The models are trained using statistical features derived from atomic descriptors of both the diffusing elements and the diffusion media, alongside temperature. This work highlights the potential of ML to enhance the prediction of diffusion properties in complex alloy systems, offering a powerful tool for alloy design and optimization. By significantly improving the efficiency of diffusion coefficient prediction, this approach provides a promising complement to experiments, accelerating material development for various engineering applications.

10:30 AM Break

10:50 AM

Topological Analysis of Processing to Microstructure Mappings: *Zachary Varley*[1]; Megna Shah[2]; Jeff Simmons[2]; Veera Sundararaghavan[3]; [1]Carnegie Mellon University; [2]Air Force Research Laboratory; [3]University of Michigan

The relationship between processing parameters and resultant microstructures remains a fundamental challenge in materials science. We explore a neural network approach to map between processing parameter space and microstructure morphology space, with particular emphasis on quantifying topological faithfulness in latent representations. We evaluate several complementary approaches for measuring topology preservation, combining techniques from computational topology, manifold learning, and dimensionality estimation. These metrics assess both local neighborhood structure and global topological features of the paired point clouds representing processing conditions, input data, and learned latent representations. From a materials development perspective, maintaining accurate topological relationships in the learned representations could enable more reliable navigation of processing parameter space and facilitate materials optimization. We compare the effectiveness and computational efficiency of these metrics in the context of autoencoder architectures, providing insights for developing more robust computational tools for materials design and processing-structure relationship analysis.

11:10 AM

Machine Learning of Mode Filter Grain Growth Model Characteristics: *Zhihui Tian*[1]; Lin Yang[1]; Vishal Yadav[1]; Kang Yang[1]; Amanda Krause[2]; Michael Tonks[1]; Joel Harley[1]; [1]University of Florida; [2]Carnegie Mellon University

Recent work has demonstrated a new mode filter grain growth model based on the same underlying theory as the Monte Carlo Potts model but can leverage GPU-compatible Python libraries with a relatively simple algorithm to provide computationally fast isotropic and anisotropic grain growth simulations. This study follows up on this work, exploring the interpretability of the mode filter and the ability to learn mode filter kernels, which are used to fundamentally control grain growth behavior. We show that the kernel can be used to learn inclination-dependent grain growth governed by variations in energy and mobility. We then demonstrate that this learned kernel input into the mode filter to simulated sequences of grain growth that mimics the original growth behavior. We show results from a variety of example microstructures (e.g., circle grains, hexagonal grains, polycrystals) and anisotropic scenarios (e.g., elongation from anisotropic energies and mobilities).

11:30 AM

High-Fidelity Grain Growth Modeling: Leveraging Deep Learning for Fast Computations: *Pungponhavoan Tep*[1]; Marc Bernacki[1]; [1]Centre de Mise en Forme des Matériaux (CEMEF)

Grain growth simulations are essential in materials science but are hindered by the computational intensity of traditional PDE-based methods. We introduce a machine learning framework employing a ConvLSTM network alongside a Convolutional Autoencoder to efficiently predict grain growth evolution. This model captures both spatial features and temporal dependencies while reducing data dimensionality, learning underlying patterns without explicit PDE computations. Our results demonstrate that the deep learning model reduces simulation time from approximately 30 minutes to under 10 seconds for a 2D simulation on a 1×1mm domain, without compromising prediction quality. This rapid prediction capability enables real-time analysis and offers an efficient alternative to traditional methods, potentially revolutionizing materials design and accelerating innovation in the field.

11:50 AM

Bayesian Data Assimilation in Latent Space for Phase-Field Simulation Using Variational Autoencoder: *Akinori Yamanaka*[1]; [1]Tokyo University of Agriculture And Technology

This study proposes a new Bayesian data assimilation (DA) method using the variational autoencoder (VAE) for a phase-field modeling. The proposed DA enables us to integrate the microstructure features extracted from the microstructure images using the VAE into the phase-field simulation in the latent space. In this paper, we investigate the performance of DA method by conducting numerical experiments where parameters included in the phase-field model of spinodal decomposition in a binary system and the multi-phase-field model for grain growth are estimated from the microstructure feature. The results of numerical experiments reveal that the parameters can be accurately estimated using a few latent variables that capture the noticeable microstructural change.

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): Industrial Case Studies and Success Stories

Monday AM
June 16, 2025

Room: Room E
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Invited
Toward Concurrent Product and Process Design: An Aero-Engines ICME Perspective: *Manish Kamal*[1]; Vasisht Venkatesh[1]; David Furrer[1]; Adam Pilchak[1]; [1]Pratt & Whitney

Aircraft engines are a demanding application for any material. Significant progress in Integrated Computational Materials Engineering (ICME) in the past couple of decades along with its focused application is driving rapid discovery, development and deployment of materials and process solutions in the aero-engines industry. This paper will present how Pratt & Whitney is using a holistic approach toward design and manufacturing by incorporating ICME principles. Conventional processing techniques like forging, casting and machining along with upcoming techniques like Additive Manufacturing (AM) are being simulated using a combination of commercial-off-the-shelf (COTS) tools and internal codes. These are being integrated with physics-based and machine learning based material models, as applicable, to predict microstructural features and mechanical properties. Model-based-material-definitions (MBMD) are being enabled by this integration providing location-specific properties and a concurrent product and process design approach. Examples of this approach and its application for aero-engines component manufacturing will be shared.

9:30 AM
Computational Design of High-Wear-Resistant Cemented Carbide Alloys for LPBF Processing Using ICME and Machine Learning: *Gurjot Dhaliwal*[1]; [1]Phaseshift Technologies

This study applies anIntegrated Computational Materials Engineering (ICME)framework to design a novel cemented carbide alloy forLaser Powder Bed Fusion (LPBF)additive manufacturing, targeting enhanced wear resistance for industries such as oil, gas, and mining. The approach integratesmachine learning, multi-scale simulations, and optimization techniquesto overcome challenges in incorporating more than 65% tungsten carbide (WC) while maintaining good compatibility with the LPBF process. Multi-scale simulations, includingCALPHAD, atomistic modeling,finite element analysis (FEA), andphase-field studies, were used to predict alloy behavior, optimize processing parameters, and assess microsegregation during solidification. Machine learning-driven optimization identified a low-cobalt binder composition capable of incorporating over 65% WC with a narrow solidification interval (~10K), advantageous for LPBF. Experimental validation confirmed the alloy's 3D-printability and improved wear resistance. This work demonstrates the effectiveness of ICME in designing high-performance materials for advanced manufacturing processes like LPBF.

9:50 AM
Application of ICME Tools for Addressing Fracture Toughness Issues in ERW Pipe: *Jerry Gould*[1]; Nahir Franco[2]; Olga Eliseeva[1]; [1]Edison Welding Institute; [2]Axis Pipe and Tube

ERW is a well-established technology for the manufacture of oil country tubular products. It is well understood that an artifact of ERW welding is a thin decarburized band running along the bond line. In the presence of bond line flaws, this band can act to locally reduce fracture toughness. To improve this bond line fracture toughness, in-line annealing practices have been investigated for homogenizing this bond line. Work here was done using ICME techniques. In this study, carbon diffusivity during annealing has been evaluated using computational microstructure prediction tools. Runs from the computational tools were organized using design of experiments (DOE) techniques. Data collected from the individual runs then mapped using linear functions for subsequent microstructural analysis. Carbon back-diffusion was estimated based on a Zener type analysis. These results then were used to assess degrees of homogenization associated with different decarburized bond widths as well as annealing time and temperatures.

10:10 AM
ICME Framework for Optimizing Recrystallization Behavior of Aluminum Alloys During Annealing: Abhijit Brahme[1]; *Chal Park*[2]; Jeffrey Tschirhart[2]; Aaditya Lakshmanan[2]; Sazol Das[2]; Kaan Inal[1]; [1]University of Waterloo; [2]Novelis

Rolled aluminum products have a wide range of applications including beverage packaging, automotive, aerospace, building and construction. Aluminum sheet manufacturing involves a series of complex thermal and mechanical processes. Each processing step is carefully designed to maximize throughput while achieving desired microstructural evolution for meeting product performance requirement of the final sheet product. One important processing step is annealing that induces static recrystallization of aluminum sheet, during which softer grains nucleate from heavily deformed grains with high dislocation densities. This microstructural evolution has significant influence on strength and anisotropy of the sheet product that can determine overall formability. Present study is based on a full-field cellular automata modeling framework that can be used to simulate recrystallization of aluminum alloys that can accurately simulate crystallographic texture change and recrystallization kinetics. The developed framework can be used to optimize annealing practice for different aluminum alloys.

10:30 AM Break

10:50 AM
Life Prediction of Anomalies in Aero Engine Disk Materials Using Crystal Plasticity Finite Element Method: *Yuta Kitamura*[1]; Yoshihiro Otani[1]; Giorgio Vago[1]; Shigeru Yasuda[1]; Itsuki Kawata[1]; Naoya Yamada[1]; Masayuki Tsukada[1]; [1]IHI Corporation

Titanium alloys and nickel-based alloys are widely used in aero engine disks. In these materials, it is known that anomalies such as micro texture region and dirty white spot cause a reduction in life. Since the fracture of aero engine disks can lead to serious accidents, it is crucial to understand the connection between anomalies and material fracture to be able to correctly predict the life of these disks. In this study, a crystal plasticity finite element method was used to simulate the physical phenomena occurring in materials containing anomalies. In-situ digital image correlation measurements under loading were also performed, and a fracture criterion was established based on both experiments and analyses. Therefore, a highly accurate life prediction method was developed using the crystal plasticity finite element method. Additionally, a disk-scale strength evaluation method was developed using machine learning to incorporate micro-scale information about crystal grains.

11:10 AM

Forecasting of Roll Loads During Hot Rolling Using an Artificial Neural Network Model in a Hot-Strip Mill: *Abhishek Thakur*[1]; Sanyam Totade[1]; Appa Chintha[1]; [1]Tata Steel Limited

Hot rolling is an important metallurgical process in which a hot steel slab is subjected to thickness reduction by passing through a series of rolls in a hot-strip mill. During hot rolling, the rolls at each stand experiences a tremendous amount of force which depends on the hot metal chemistry and process parameters. The forecast of these roll loads can provide a guide and help optimizing the overall hot rolling process. In this context, we developed an artificial neural network model which can predict the rolling loads for a given set of steel chemistry and process parameters. The network is trained using industrial data with compositions and process parameters used as input and roll loads predicted as output. During testing, on an average, the trained neural network model can predict 74.24% and 95.06% of rolling loads within ±5% and ±10% of the corresponding actual roll loads respectively.

11:30 AM

Advanced Integrated Model for Hot Strip Mill Processes: *AppaRao Chintha*[1]; Sai Adapa[2]; Gopala Eegala[1]; Yadvendra V[2]; [1]Tata Steel Ltd; [2]Oak Ridge National Laboratory

We present an advanced integrated model developed for the hot strip mill through a blend of physics-based and data-driven sub-models. This model spans the entire production line, from the reheating furnace to the roughing and finishing mills and includes run-out-table and coil cooling stages. It effectively simulates grain size evolution, phase transformation and precipitation, and prediction of mechanical properties. A standout feature is its dynamic heat transfer model coupled with phase transformation along the strip, which accounts for all parameters across thickness and length, with variable speed over time. This integration enables the model to predict final mechanical properties along the entire coil length rapidly, delivering results in real time post-coiling. Deployed on a Level 2 system, it enhances operational efficiency and product quality. By coupling real-time data with physical modelling, it accelerates new alloy design and process optimization, providing steel manufacturers a robust tool to meet sustainable steel design.

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): PSP Linkages: Multiscale/Multiphysics Modeling I

Monday AM
June 16, 2025

Room: Room F
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Invited

Recent Progress in Integrating Phase-Field Models With Other ICME Tools: *Katsuyo Thornton*[1]; [1]University of Michigan

Phase-field (PF) modeling is increasingly becoming a key computational technique for ICME. In this talk, we will describe the recent progress in extending and integrating the PRISMS Computational Tools, with a focus on PRISMS-PF. PRISMS-PF is an open-source, high-performance framework for PF modeling of microstructure evolution. However, it has been extended to include various physical processes, including electrochemistry to model corrosion and fluid flow to consider the effects of advective transport during solidification. It has also been integrated with PRISMS-Plasticity to model recrystallization and with CASM for parameterization. These capabilities will be highlighted with a few applications. Furthermore, the AI-enabled Microstructure Model BuildER (AMMBER), an automatic parameterization tool for PF modeling, will also be discussed. As in PRISMS, it aims at enabling a broader community to utilize PF modeling. Combined, such open-source software infrastructure will contribute to simulation-based material discovery and development within the context of MGI.

9:30 AM

Design and Optimization of a Heat Treatment for Additively Manufactured Alloy 718 in Oil and Gas Applications: *Mark Stoudt*[1]; James Zuback[1]; Carelyn Campbell[1]; Andrew Iams[1]; [1]National Institute of Standards and Technology

Alloy 718 is attractive for additive manufacturing (AM), because it exhibits good strength, corrosion resistance, and weldability. However, the AM build process generates residual stresses, and microstructural heterogeneities that promote variability in the properties and performance. The current heat treatment, designed for wrought material, is not appropriate for the solidification microstructures in AM-processed material. Thus, they often fail to meet the performance specifications for oil and gas applications. An integrated computational materials engineering (ICME) framework combining CALPHAD-based modeling tools and experimental validation was adopted to develop a heat treatment designed specifically for AM-processed Alloy 718. The microstructures and mechanical properties produced by the new protocol were virtually identical to those of wrought material in the same 825 MPa strength condition. The question is whether AM processing affected the susceptibility to environmentally assisted cracking. The rationale behind the heat treatment design, validation, and cracking susceptibility measurements will be presented and discussed.

9:50 AM

Phase-Field Simulation Framework for Modeling Martensite and Bainite Formation in Steel: *Hesham Salama*[1]; Muhammad Adil Ali[1]; Oleg Shchyglo[1]; Ingo Steinbach[1]; [1]Ruhr University Bochum

In this study, we present a combination of phase evolution, chemical diffusion, temperature evolution, and finite strain elasto-plasticity to simulate the martensitic and bainitic transformation using the phase-field software library OpenPhase[1]. It is demonstrated how the carbon concentration significantly influences the martensite start temperature and the resulting microstructure. Furthermore, the kinetics of the transformation is strongly influenced by plasticity. For bainitic transformation, it is demonstrated how the holding temperature significantly influences carbon partitioning and the resulting microstructure: higher holding temperatures allow increased carbon diffusion and partitioning, stabilizing retained austenite, which is in good agreement with experimental observations. The present study offers new insights into the microstructure formation mechanisms during martensitic and bainitic transformations in low-carbon steel and offers a consistent modeling approach to model complex phase transformation scenarios in steel and other construction materials.[1] https://openphase.rub.de/

10:10 AM

Phase-Field Modeling of Morphology Evolution of Intergranular and Intragranular Hydrides in Polycrystalline Zirconium: *Wooseob Shin*[1]; Kunok Chang[1]; [1]Kyung Hee University

Zirconium is mainly used as fuel cladding in nuclear reactors due to its advantages. However, zirconium hydrides formed inside the cladding degrade the integrity of the cladding making it brittle and prone to cracking. Therefore, understanding the hydride formation is necessary. The hydrides can be classified into two types: intergranular and intragranular. We developed a model that comprehensively considers the texture of the Zr and the crystallographic orientation of the hydride in polycrystalline Zr to show the formation of hydrides and the interaction between grain boundaries and intergranular hydrides. We considered the morphology evolution of the hydrides and grain growth simultaneously and analyzed the effect of the Zr texture on the hydride formation. In addition, we analyzed the correlation between the type of intergranular hydrides and the interacting angle which is the angle between the basal plane and grain boundary using phase-field modeling.

10:30 AM Break

10:50 AM
Predicting Three-Dimensional Microstructural Defect Evolution Under Neutron Irradiation Considering Formation Energy: *Ilhyun Cho*[1]; Kunok Chang[1]; [1]Kyung Hee University

Neutron irradiation induces atomic-level defects in materials, resulting in observable mesoscale to macroscopic defects.Phase-field methods can successfully simulate the thermodynamic and kinematic properties of materials, and are particularly advantageous for modeling the spatial and temporal evolution of microstructural inhomogeneities under irradiation. Ferritic alloys under neutron irradiation develop a range of defects, including voids and dislocation loops, which influence plasticity. The formation energy of these defects depends on the complex contributions of energies like interfacial and stacking fault energy. This study investigates the stability of voids and prismatic loops in Fe-based alloys by analyzing formation energy as a function of defect size and various environmental variables. We predicted which microstructures are preferred under specific environment and discussed the feasibility of the study using experimental results.

11:10 AM
An ICME-Based Approach to Determine the Effect of Microscale Residual Stresses on the Fatigue Strength of Solution Strengthened Ferritic Ductile Irons: *Lutz Horbach*[1]; [1]Institute for Materials Applications in Mechancial Engineering, RWTH Aachen University

Solution strengthened ferritic ductile irons (SSF-DI) are characterised by improved mechanical properties compared to conventional cast irons, with a microstructure defined by graphite nodules embedded in a ferritic matrix. Cooling to ambient temperature causes microstructural residual stresses due to thermal contraction mismatches and phase transitions. These stresses, concentrated around the graphite nodules, lead to local plastic deformation and potential crack initiation sites. Experimental determination of residual stresses is complex and numerical models are required to accurately predict them and their effect on fatigue performance in cyclically loaded components. The ICME-based approach developed in this study provides a tool for the determination of local mechanical properties of SSF-DI and contributes to an increase in efficiency in the design of structural components. The approach consists of coupling two FEM models, one to calculate residual stresses as a function of process conditions, considering phase transitions, and a subsequent model to simulate fatigue performance.

11:30 AM
PRISMS-MultiPhysics – An Open-Source Coupled Phase Field-Crystal Plasticity Framework and Its Application to Simulate Twinning in Mg Alloys: *David Montiel*[1]; Chaitali Patil[1]; Mohammadreza Yaghoobi[1]; Vaidehi Menon[1]; Brian Puchala[1]; Anton Van der Ven[2]; Liang Qi[1]; Katsuyo Thornton[1]; Veera Sundararaghavan[1]; John Allison[1]; [1]University of Michigan; [2]University of California, Santa Barbara

As one of the main deformation mechanisms in hexagonal materials, twin formation plays an important role in determining mechanical properties of magnesium and its alloys. Thus, accurately modeling twin nucleation, propagation, and growth is key to designing Mg alloys with improved performance. We introduce PRISMS-MultiPhysics (PRISMS-MP), a new open-source, high-performance framework that couples the phase-field and crystal plasticity models. We demonstrate the application of the framework to simulate nucleation and growth of twins in magnesium, including interactions between twins and grain boundaries. In addition, we discuss plans for developing an application within PRISMS-MP for dynamic recrystallization. Finally, we outline plans for parameterizing the twinning and recrystallization models with accurate thermodynamic and kinetic data obtained through integration with the PRISMS Cluster Approach to Statistical Mechanics (CASM) software.

The 7th International Congress on 3D Materials Science (3DMS 2025): Methods of Materials Simulation and Modelling in 3D & 4D I

Monday AM
June 16, 2025

Room: Room D
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Cancelled

9:30 AM
A Polycrystal Generator for Large-Scale Atomistic Calculations: *Younggak Shin*[1]; Vichhika Moul[2]; Keonwook Kang[1]; Byeongchan Lee[2]; [1]Yonsei University; [2]Kyung Hee University

Metals typically have a polycrystalline structure in which grain boundaries play a pivotal role in mechanical properties such as the yield strength, i.e. the Hall-Petch and the inverse Hall-Petch relationships. Atomistic calculations have been extensively used to understand these relationships, but now facing an unforeseen challenge: present atom-generation codes are serial codes, where the on-board memory limits the atomistic system size. In addition, reading and writing a file containing billions of atoms takes prohivitively long time in a serial I/O.Here we present a polycrystal generator called PolyPal, which is a fully parallized code with virtually perfect scalability. The software has been tested up to 10 billion atoms, which takes only minutes to generate all the positions, and write them to files. We also highlight the key features in generating different textures and alignments of microsctures to mimic the experimental specimen fabracated in various processes.

9:50 AM
Simulation of Plastic Strain Localisation in Polycrystals by 3D Discrete Dislocation Dynamics: Baptiste Joste[1]; *Riccardo Gatti*[2]; Henry Proudhon[1]; Benoit Devincre[2]; [1]Centre Des Matériaux; [2]CNRS

Understanding deformation leading to polycrystalline material failure is a major challeng in materials science. The origin of plastic strain localization and deformation propagation mechanisms remain unclear. To tackle those issues, we propose a multi-scale simulation approach using 3D Discrete Dislocation Dynamics (DDD) and the Finite Element Method (FEM) to model mesoscopic dislocation behavior. First, our results emphasize the impact of policrystalline microstructure on plastic deformation localization, revealing intragranular stress concentrations due to elastic incompatibilities. During plastic deformation, we obsereved that specific mechanisms such as cross-slip or collinear annihilation facilitate the initiation of plastic deformation within these stress concentration regions a. Furthermore, ,we implemented a local rule to model dislocation transmission, to decrease strain hardening and promotes slip localization. Our findings highlights that plastic deformation transmission is crucial to observe plastic strain localization in polycrystals.

10:10 AM

Using Discrete Harmonic Expansions and Equilibrium Conditions to Estimate Intragranular Stress Distributions in Polycrystals From Grain-Averaged Data: *Wiley Kirks*[1]; Paul Dawson[1]; Matthew Miller[1]; Kelly Nygren[1]; [1]Cornell University

High energy x-ray diffraction microscopy (HEDM/3DXRD) has allowed scientists to probe the micromechanical state of polycrystalline materials under both thermal and mechanical loading in-situ, providing "grain-averaged" elastic strain measurements of the grains within a polycrystal. However, HEDM lacks intragranular resolution, leaving polycrystalline modeling as the only way to resolve internal stress distributions. This work proposes using discrete spherical harmonic expansions over a finite element discretization of the microstructure to define the stress field - greatly decreasing the degrees of freedom compared to the original mesh. Grain-averaged HEDM data are supplemented with inter- and intra-granular equilibrium constraints to determine the expansion weights. The proposed intragranular stress recovery method is demonstrated on C103, a Nb-based refractory alloy. Refractories have become desirable to the material and aerospace communities for their high-temperature properties and resilience in extreme environments where a deeper understanding of mechanical properties is warranted for more successful application in engineering design.

10:30 AM Break

10:50 AM

Graph Neural Networks for Generalizable Machine Learning of 3D Microstructure--Property Relationships in Polycrystals: Guangyu Hu[1]; Gyu-Jang Sim[2]; Myoung-Gyu Lee[2]; *Marat Latypov*[1]; [1]University of Arizona; [2]Seoul National University

3D characterization provides unique datasets for understanding process--structure--property relationships in alloys. Graphs offer a reduced-order representation of the 3D polycrystalline microstructure that enables efficient machine learning of these relationships with graph neural networks (GNNs). In this contribution, we will present our recent advances in data-efficient training of GNNs that can generalize predictions well beyond their training sets. Specifically, we will present GNNs that predict (i) anisotropic mechanical properties of textured polycrystals in new loading directions; (ii) grain-level fatigue indicator parameters in microstructure volume elements order of magnitude larger than those used for training; and (iii) properties of polycrystals for metals and alloys not included in the training set. This contribution intends to spark 3DMS community's interest in the GNN computational platform that could significantly benefit from experimental datasets for model training and fine-tuning.

11:10 AM

Dislocation Contrast Simulations in Dark-Field X-Ray Microscopy to Identify Individual Dislocations: *Sina Borgi*[1]; Grethe Winther[1]; Henning Friis Poulsen[1]; [1]Technical University of Denmark

Exploring dislocation identification in bulk deformed crystals using dark-field X-ray microscopy (DFXM) and forward modeling. A covariance matrix of weak beam images shows how variations in dislocation properties (line direction, Burgers vector, and slip plane) affect diffraction contrast, offering insights into DFXM's sensitivity in distinguishing between different dislocations. In experimental and simulated weak beam images, dislocation distortion fields match closely, confirming DFXM's capability to identify slip planes and Burgers vectors. This is further illustrated by a dislocation undergoing double cross-slip, where the experimental and simulated Burgers vector align, reinforcing DFXM's accuracy. These advances in simulation and experimental validation establish DFXM as a powerful tool for exploring 3D dislocation dynamics. The method has potential for integration with discrete dislocation dynamics to follow dislocation networks under in situ strain, and using forward modeled images serving as a foundation for supervised machine learning in the DFXM data analysis pipeline.

11:30 AM

Dislocation Microstructure Considerations in Modeling Recrystallization: Ahmed Hamed[1]; Sreekar Rayaprolu[1]; Grethe Winther[2]; *Anter El-Azab*[1]; Khaled SharafEldin[1]; [1]Purdue University; [2]Technical University of Denmark

The sensitivity of static recrystallization kinetics to the pre-existing dislocation microstructure is a well-known empirical fact. We present a phase field model of recrystallization that takes the initial dislocation microstructure into consideration in fixing the thermodynamics and kinetic governing the growth of the recrystallized embryos. The model represents the dislocation microstructure in terms of geometrically necessary boundaries and incidental dislocation boundaries and takes as input microstructure realizations using the universal scaling laws for the spacing and the misorientation angles of these boundaries. The resulting free energy is used into an Allen-Cahn based model of recrystallization kinetics. The results show that, in agreement with experiment, the morphology of recrystallization front exhibits protrusions and retrusions, and that the deformation level and, hence, the initial microstructure play a critical role in determining the final grain structure. Building on these results, a new perspective for modeling recrystallization with a higher fidelity will be presented.

11:50 AM

The Limits of Predictability in 4D Microstructural Simulations: *Elizabeth Holm*[1]; Meizhong Lyu[1]; [1]University of Michigan

A longstanding goal of microstructural simulation is to reproduce experimentally observed outcomes in 4D (space and time). Disagreement between experiment and simulation has generally been attributed to shortcomings in the computational instantiation; however, even after several decades of improving the physical bases of computational models, a perfect match has not been achieved. In this study, we examine the sources of uncertainty in simulation and experiment using polycrystalline grain growth as an exemplar. In nominally identical molecular dynamics simulations, growth trajectories of individual grains can vary significantly due to discrete events that have cascading effects on the microstructural ensemble. Thus, microstructural events are surprisingly sensitive to atomic scale processes, which imparts an innate uncertainty in 4D simulations. While this prevents prediction of an individual grain trajectory, a range of possible trajectories can be determined for each grain; this offers a more robust, statistically-based way to compare simulation and experiment.

The 7th International Congress on 3D Materials Science (3DMS 2025): Process-Microstructure-Property Relationships in 3D

Monday AM
June 16, 2025

Room: Room C
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Cancelled

9:30 AM
Load Partitioning in Inconel 718 With Harmonic Microstructures: *Darren Pagan*[1]; Patrick Albert[1]; Kenneth Peterson[1]; Amlan Das[2]; Suchismita Sarker[2]; Douglas Wolfe[1]; [1]Pennsylvania State University; [2]Cornell High Energy Synchroton Source

Metallic alloys with microstructures with extreme bimodal grain size distributions (termed harmonic microstructures) have exhibited unique combinations of strength and ductility. The exact origin of the favorable properties is still unclear but is likely due to the partitioning of stress and plastic strain among the constituent grain distributions. Here we use a combination of in situ far-field high-energy X-ray diffraction microscopy and traditional powder diffraction to examine micromechanical evolution in harmonic Inconel 718 during tensile loading. The Inconel 718 studied has a bimodal grain size distribution with a nearly 100x variation in grain diameter and was manufactured using field-assisted sintering technology (FAST), which is able to rapidly sinter varied powder distributions to theoretical density with minimal grain growth. The load partitioning among the constitutive grain size distributions is analyzed.

9:50 AM
3D Mapping of Crack Tip Dislocation Structures in $SrTiO_3$ by Dark-Field X-Ray Microscopy: *Albert Zelenika*[1]; Can Yildirim[2]; Xufei Fang[1]; [1]Karlsruhe Institute of Technology; [2]European Synchrotron Radiation Facility

Conventionally, dislocations have not shown much relevancy for ceramic materials as they exhibit little to no plasticity at room temperature. However, recent studies of dislocations in functional ceramics are gaining interest due to their impact on functional and mechanical properties. Despite significant advances, cracks can still initiate and propagate unexpectedly, leading to catastrophic failure. To address this, we use $SrTiO_3$ as a model material, employing DFXM to visualize dislocations at relevant scales with high spatial and angular resolution. We examined samples with varying dislocation densities ($10^{12}/m^2$ - $10^{14}/m^2$), tuned with an in-house developed Brinell indentation scratching technique at room temperature, to map the spatial distribution of dislocations and strain fields in 3D. Our results reveal the 3D dislocation structure around a crack tip, providing unprecedented insights. We also compared these findings with TEM data, highlighting the complementary strengths of each method, providing valuable information for improving fracture resistance in ceramics.

10:10 AM
Three-Dimensional Twin Networks in Ti: Morphology, Connectivity, and Incompatibilities: *Duncan Greeley*[1]; Hi Vo[1]; Rodney McCabe[1]; Carlos Tomé[1]; Laurent Capolungo[1]; [1]Los Alamos National Laboratory

The mechanical response of HCP metals is mediated by the formation of 3D twin networks during deformation. Naturally, twin interactions are salient morphological features of these networks. To study the morphology of twin networks and assess the impact of twin-to-twin and twin-to-grain boundary contact on the development of mechanical incompatibilities, a 3D twin network in cryogenically compressed high-purity Ti was characterized using serial sectioned EBSD. The network structure and shear incompatibilities at twin intersections were investigated, and interface accommodation mechanisms for the incompatibilities were explored. The network displays a complex morphology centered around 'hub' twins that display over 15 intergranular and intragranular contacts. The magnitude of the induced incompatibilities depends on the 3D orientation of the twins and interfaces, and the study reveals that high incompatibilities – potential precursors to shear localization – appear to emanate from incidental contact between separate twin chains and at triple-junctions of twins.

10:30 AM Break

10:50 AM
Dislocation Migration in the Shocked Silicates Olivine and Pyroxene: *Yaozhu Li*[1]; Carsten Detlefs[1]; Can Yildirim[1]; Roberta Flemming[2]; Phil McCausland[2]; [1]ESRF; [2]Western University

Shocked silicates deform during hyper-velocity impacts, a common process in planetary evolution. Olivine and pyroxene are key rock-forming minerals, recording shock via microstructural changes. Olivine (isolated SiO tetrahedra as orthosilicates) and pyroxene (two shared oxygen atoms as single chain silicates) respond differently to shock deformation. Orthosilicates have interstitial cation bonding for stability, whereas single-chain silicates exhibit directional O-Si-O bonds that facilitate cleavage planes and directional deformation. High energy shock events trigger dislocation migration, enhanced by post-shock heating. The O-Si-O bonding in pyroxene, in particular, may allow greater ductility, accommodating deformation through bending, kinking, twisting, or fracturing along cleavage planes. Using dark-field X-ray microscopy (DFXM), we mapped 3D lattice mosaicity, revealing development of dislocation networks in low-shock meteoritic olivine indicative of shock mosaicism. We aim to further explore dislocation behavior in shocked pyroxene to confirm directional effects along its (110) plane, providing insights into shock deformation histories in planetary materials.

11:10 AM
Analysis of Growth Striations in Doped Yttrium Aluminium Garnet (YAG) Using Dark Field X-Ray Microscopy: *Antonella Gayoso Padula*[1]; [1]Technical University of Denmark

Characterizing defects in oxide materials is challenging due to the limitations of existing techniques. Methods like temperature equilibrium conductivity and impedance spectroscopy lack spatial resolution, while transmission electron microscopy (TEM) provides atomic-level mapping but is restricted to surfaces or thin sections, potentially misrepresenting bulk properties. Dark Field X-ray Microscopy (DFXM) is proposed to spatially resolve point defect distributions in bulk materials.This study focuses on dislocation-free yttrium aluminum garnet (YAG)doped with chromium, thulium, and holmium, visualizing buried chemical defects that manifest as growth striations. The striations were characterized in therms of chemical composition and orientation, with 3D models constructed to analze their behavior under an electric field. YAG, widely used in medical laser and X-ray detector scintillators, was selected as a promising candidate for studying chemical defects using DFXM. This approach holds significant potential for advancing materials with technological applications.

11:30 AM
Microstructural Characterization of Ni Foam Using EBSD and Micro-CT: *Jaehyung Cho*[1]; [1]Korea Institute of Materials Science

Based on electron backscatter diffraction (EBSD), hollow structures of Ni foam struts fabricated by electroplating on a chemically removable template were observed. Three-dimensional (3D) pore structures of Ni foams were also obtained using X-ray computed tomography (CT), and microstructural features such as porosity, pore size and strut thickness were statistically quantified. Evolution of microstructure and mechanical properties during ex situ compression of open-cell Nifoams was investigated based on X-ray CT, and experimental results were compared with predictions by the finite element method (FEM). 3D microstructures obtained by X-ray CT revealed that the stress drop started with the buckling of struts at the center of the Ni-foams.

Joint Sessions of AIM, ICME, & 3DMS: Fair Data II: Joint Session of AIM & ICME

Monday PM
June 16, 2025

Room: Joint Sessions Room
Location: Anaheim Marriott

Session Chair: To Be Announced

1:40 PM
The Materials Science and Engineering Knowledge Graph: Establishing a Centralized Metadata Index for Enhanced Data Integration: *Ebrahim Norouzi*[1]; Hossein Beygi Nasrabadi[1]; Jörg Waitelonis[1]; Harald Sack[1]; [1]FIZ-Karlsruhe

The Materials Science and Engineering Knowledge Graph (MSE-KG) [1] serves as a central repository that semantically connects metadata from diverse sources, creating a unified, searchable data space in Materials Science and Engineering. Its semantic backbone, the MatWerk Ontology (MWO) [2], extends concepts from the NFDI-core ontology [3], enabling efficient data discovery within the MSE domain. By aligning local data infrastructure with the MSE-KG, organizations can continuously feed metadata into this centralized framework, fostering cross-domain data queries and exchanges while allowing data providers to retain control. This structure enhances the visibility and accessibility of MSE resources, advancing innovation in the field. References [1] https://go.fzj.de/mse-kg [2] http://purls.helmholtz-metadaten.de/mwo/[3] https://github.com/ISE-FIZKarlsruhe/nfdicore

2:00 PM
Practical Data Management in Computational Materials for Qualification and Certification: *Andrew Kitahara*[1]; George Weber[2]; Edward Glaessgen[2]; [1]Analytical Mechanics Associates; [2]NASA Langley Research Center

Qualification and certification (Q&C) processes impose specific requirements for aviation flight hardware to prove predictability of material and part performance, reliability, and safety. Additive manufacturing (AM) methodologies such as powder bed fusion (PBF) create unique opportunities for lightweight, integrated flight hardware systems, but the Q&C requirements often negate the value of AM insertion, which is a core motivation discussed in the computational materials-informed for qualification and certification (CM4QC) roadmap. To fully integrate computational materials methods with physical AM material testing, a thorough data management platform should be developed. This presentation will present ongoing efforts to develop an infrastructure to support AM research of coupled modeling and physical testing. The goal of the data platform is to prototype and demonstrate CM4QC processes at the laboratory scale and later evolve to serve production Q&C applications. Specific points of discussion will include the schema developments, requirements-driven experimental plans, and implementation procedures.

2:20 PM
Enhancing AI Readiness Through Data Stewardship, Modular Ontologies, and FAIR Data Workflows: *Balashanmuga Priyan Rajamohan*[1]; Kai Zheng[1]; Van Tran[1]; Nathaniel Hahn[1]; Hayden Caldwell[1]; Alexander Bradley[1]; Quynh Tran[1]; Laura Bruckman[1]; Yinghui Wu[1]; Erika Barcelos[1]; Roger French[1]; [1]Sdle Research Center

The complexity of materials science data complicates collaboration and scientific progress due to inconsistent terminologies and formats. Our solution is an ecosystem for modular ontology development grounded in FAIR (Findable, Accessible, Interoperable, Reusable) principles. At its center is MDS Onto, a unified ontology harmonizing material science domains to reduce redundancy and enforce consistency. Our OntoPortal is an internal ontology repository that helps users select standardized terms when creating new ontologies. Additionally, the FAIRMaterials package enables scientists to develop domain-specific ontologies linked to the Basic Formal Ontology, supporting advanced reasoning. The package uses MDS Onto to generate data ingestion sheets that convert experimental data into FAIR-aligned Linked Data and offers an interactive web app, "Datapedia," for local datasets. This ecosystem fosters collaboration and innovation by enhancing data interoperability and establishing standardized ontology practices in materials science.

2:40 PM
X-Ray Diffraction Analysis Using TensorFlow and FAIR Data Pipelines: Finley Holt[1]; *Daniel Savage*[2]; Mohommad Mehdi[1]; Weiqi Yue[1]; Pawan Tripathi[1]; Matthew Willard[1]; Frank Ernst[1]; Roger French[1]; [1]Case Western Reserve University; [2]Los Alamos National Laboratory

X-ray diffraction generates vast, complex datasets of material behavior that demand scalable and flexible scientific analyses. The efficient management and manipulation of image and histogram data has largely been addressed in the development of the TensorFlow package for ML and AI. In this talk we will explore using our newly developed FAIRshake package, an end-to-end, modular framework that interfaces with FAIRified diffraction data using the TensorFlow Dataset API, to perform data manipulation and analysis. TensorFlow allows data transformation (e.g dark corrections, azimuthal integration, analysis) to be performed using standard TensorFlow dataset tools. The autotuning capability of TensorFlow enables excellent performance, from desktops to HPC environments, through dynamic dataset streaming and parallelization. TensorFlow datasets are shown through examples to be especially attractive for scientific analysis that can natively utilize tensor representations of data; bringing into focus the question: "How should scientific codes be interacting with FAIR data?"

3rd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2025): Applied ML for Manufacturing II

Monday PM
June 16, 2025

Room: Room A
Location: Anaheim Marriott

Session Chair: B. Garai, RV University, Bangalore, India

1:30 PM Invited
ROM-Net in Additive Manufacturing: *David Ryckelynck*[1]; [1]Mines Paris PSL University

ROM-net reduced order modeling (ROM) is applied to finite element thermo-mechanical simulation of metal additive manufacturing. This is a significant challenge due to the continuously evolving computational domain on which a local reduced basis is required to apply a ROM-net. The support of local reduced bases is closely related to the sampling of mechanical predictions. Considering the modeling of a directed energy deposition process, it is proposed to organize the training set of simulation snapshots according to an energy deposition length that represents the progress of the process. When the projection-based ROM-net is applied to the full-order model, the simulation data sequence allows the design of a local ROM depending on categories of input parameters. The similarity of data in a category is evaluated by a Grassmann distance between local reduced subspaces. The simulation of the construction of a turbine blade showed a computational speedup of about 100.

2:00 PM

3D Surrogate Modeling of Elasto-Viscoplastic FFT Simulations for Porosity-Driven Fatigue Prediction in Additive Manufacturing: *Daniel Diaz*[1]; Xingyang Li[1]; Elizabeth Holm[2]; Anthony Rollett[1]; [1]Carnegie Mellon University; [2]University of Michigan

Additive manufacturing is revolutionizing the way we manufacture products, but properties are limited by porosity produced during processing. To better understand the relationship between pore morphologies and fatigue we use an elasto-viscoplastic FFT simulation called MASSIF to calculate stress and strain field outputs and fatigue harmfulness rankings. To overcome the computational costs of simulating loading on hundreds of thousands of pores, we developed a 3D Deep Learning surrogate model that directly predicts the MASSIF stress and strain field outputs given a pore morphology. In our approach we incorporate Active Learning with Monte Carlo Dropout to train the model by selectively labeling pores from the unlabeled pool with MASSIF as the oracle labeler. This approach prioritizes labeling pore instances that the model is most uncertain of while leveraging clustering to maintain diversity in the growing training dataset. Our work opens the capability for complex physical simulation on big data.

2:20 PM

Data-Driven Prediction of Deposit Geometry in Air-Based Cold Spray Manufacturing: *Novana Hutasoit*[1]; Sujan Khadka[1]; [1]Swinburne University of Technology

Air-based cold spray additive manufacturing (CSAM) offers a cost-effective, scalable alternative to helium or nitrogen-based systems, with higher build rates than melt-based methods. However, the use of air as a propellant limits particle velocity, requiring precise tuning of process parameters to achieve high-quality deposits. CSAM systems, equipped with CNC and robotic control, allow for the adjustment of multiple parameters to optimize deposition. Despite this flexibility, no unified model predicts the combined effects of these parameters on deposit quality. This study applies machine learning techniques to develop a predictive model that incorporates key CSAM parameters to enhance cold-sprayed deposit geometry, addressing a critical challenge in the field. Additionally, the study ranks the relative importance of various process parameters, providing valuable insights into their influence on deposit quality and enabling data-driven improvements in air-based cold spray processes.

2:40 PM

Automated 3D Segmentation of Refractory Material Microstructures Using Deep Learning for Improved Corrosion Resistance: Johan Moncoutie[1]; *Lalitha Raghavan*[1]; Deniz Cetin[1]; Darren Rogers[1]; Damien Bolore[2]; Sunhwi Bang[1]; [1]Saint-Gobain Research North America; [2]Saint Gobain Research Provence

Material microstructure plays a critical role in determining the corrosion behavior of refractory materials. Traditional manual segmentation of 3D imaging data is often time-consuming, labor-intensive, and subject to inconsistencies. In this work, we introduce an automated segmentation approach using deep learning to streamline this process. A 3D U-Net convolutional neural network (CNN) architecture, specifically designed for volumetric data, is employed to segment 3D images of newly synthesized refractory materials, obtained via Focused Ion Beam Scanning Electron Microscopy (FIB-SEM). This automated approach not only saves material scientists significant time but also ensures more consistent and accurate results. Additionally, we demonstrate how linking microstructural features to macroscopic properties provides valuable insights, offering a robust tool for further material analysis and property prediction.

3:00 PM Break

3:30 PM

Active Learning for Rapid Targeted Manufacturing of Thermoelectric Thin Film Alloys: *Nathan Johnson*[1]; Aashwin Mishra[2]; Apurva Mehta[2]; Dylan Kirsch[3]; [1]Carl Zeiss Research Microscopy Solutions; [2]SLAC National Accelerator Facility; [3]National Institute of Standards and Technology

As the integration of machine learning into materials science becomes increasingly vital for the synthesis of advanced materials, this study presents an active learning (AL) strategy to hasten the creation of thin-film compositionally complex alloys (CCAs) targeting thermoelectric applications. Traditional methods for thin film synthesis are often labor-intensive and time-consuming, underscoring the necessity for more efficient yet accurate approaches. We utilized a high-throughput combinatorial sputtering technique to produce an extensive array of alloy compositions. Active machine learning guided a human researcher in efficiently determining the optimal synthesis conditions for a series of five-element alloys. Our findings reveal that the AL approach significantly surpasses conventional human-driven sampling in optimizing synthesis parameters. Additionally, we employed transfer learning to pre-train models, which further enhanced efficiency. Models initially trained on lower-dimensional alloy systems were applied to higher-dimensional systems, resulting in immediate improvements in predictive accuracy.

3:50 PM

Bayesian Calibration and Uncertainty Quantification of a Cohesive Zone Model for Metal-Oxide Interfaces: *Revanth Mattey*[1]; Jason Schulthess[1]; Alexander Swearingen[1]; James Cole[1]; [1]Idaho National Laboratory

Plate-type nuclear fuel fabricated through hot isostatic pressing (HIP) consists of a U–10Mo-based fuel foil encapsulated in an aluminum alloy cladding. Understanding the failure mechanisms of these fuel plates is crucial for safe reactor operation. A key potential failure mechanism is de-bonding between the aluminum cladding, which may be exacerbated by second phase precipitates forming along the interface during the HIP fabrication. The precipitates' shape and size, influenced by peak temperatures and cooling rates, can degrade bond strength. To model the degradation, a cohesive zone model is adopted. Calibrating interface properties with a finite element forward model and Bayesian approaches is computationally intensive. Thus, surrogate models like Gaussian Process (GP) regression are developed to predict the mechanical response which are then utilized to calibrate the fracture properties of the interface through Bayesian inversion. The total uncertainty is estimated by combining the forward propagation of parameter uncertainty and model discrepancies.

4:10 PM

Long-Term Durability of GFRP Rebars in the Alkaline Environment Under Sustained Loading Using Machine Learning and Empirical Modelling: Mudassir Iqbal[1]; Daxu Zhang[2]; *Xiao Lin Zhao*[1]; [1]The Hong Kong Polytechnic University; [2]Shanghai Jiao Tong University

Corrosion in marine environments poses a threat to the safety of engineering structures. The corrosion of steel bars induced by the penetration of chloride ions is the main reason for the deterioration of reinforced concrete structures. Novel fibre reinforced polymer (FRP) reinforced concrete structures are increasingly being developed and used in civil engineering to ensure their safety. The current American Concrete Institute (ACI) 440.1 R-15 guidelines for environmental reduction factors and long-term durability of GFRP (glass fibre reinforced polymers) rebars in harsh environments are based on limited experimental data and are deemed conservative. This study evaluated the GFRP rebars subjected to sustained loading under accelerated aging. Due to its eminent nature, tensile strength reduction of aged GFRP rebar was studied for durability evaluation using XGBoost model. Experimental data of 308 samples [1-5] were used in the investigation. The tensile strength reduction factor was studied as a function of the type of glass fibers, rebar surface, exposure type (bare / concrete embedded), the magnitude of sustained loading, type of resin, size of rebar, the volume fraction of fibers, pH of alkaline solution, temperature and duration of conditioning. The XGboost model was trained using the best hyperparameters obtained from grid tuning. The model displayed reliable results in terms of R-squared and mean absolute error for the training (0.98, 1.19 %) and test data (0.82, 3.87%), respectively. The developed model was used to study the behaviour of input variables towards tensile strength reduction using Shapely Additive explanations. The degradation of GFRP rebars is strongly influenced by key factors such as temperature, conditioning duration, solution pH, and the magnitude of sustained loading. It was observed that when the sustained load exceeded 20% of the ultimate tensile strength, the degradation process accelerated significantly. This finding is consistent with prior research, further validating the newly developed model in this study. The environmental reduction factor was determined using a machine learning approach combined with the Arrhenius relationship. Both methods were compared for accuracy. Additionally, a web-based application was developed to predict tensile strength degradation in alkaline environments. The findings and conclusions from this research contribute to a deeper understanding of the durability of GFRP rebars in challenging conditions.

4:30 PM

Harnessing AI for Precision Manufacturing of Nanofibers Membranes: *Zeeshan Khatri*[1]; [1]Mehran University of Engineering & Technology

Producing nanofibers is very challenging in terms of quality, precision, and efficiency since process parameters like voltage, flow rate, and distance are sensitive. The current paper deals with the integration of AI with the electrospinning process to bring a paradigm shift in the production of nanofibers. Through extensive data collection on critical manufacturing variables and nanofiber properties, we train a prediction model of AI for ideal parameters in the nanofibers that will have better diameter uniformity and improved mechanical strength. The laboratory confirmation proves the capability of AI to improve control of process, to reduce variability, and to minimize resources wastage. This method opens up a smarter and more efficient operation in nanofiber manufacture that offers transformative insights into areas of material science and industrial-scale applications.

3rd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2025): Development of Novel ML Methodologies II

Monday PM
June 16, 2025

Room: Room B
Location: Anaheim Marriott

Session Chair: To Be Announced

1:30 PM Introductory Comments

1:40 PM

Machine Learning-Driven Discovery of High-Hardness Multi-Principal Element Alloys With Physics Informed Priors: *Eddie Gienger*[1]; Maitreyee Sharma Priyadarshini[2]; Jarett Ren[3]; Paulette Clancy[3]; [1]Johns Hopkins Unviersity - Applied Physics Laboratory; [2]Virginia Tech; [3]Johns Hopkins University

Multi-principal element alloys (MPEAs) are known for their exceptional mechanical properties and thermal stability. However, traditional discovery methods are limited in their success given MPEAs complex compositions. Here, the previously developed Physical Analytics Pipeline (PAL 2.0), a Bayesian optimization framework employing active learning in a closed-loop setting is used to accelerate discovery. PAL 2.0 integrates Gaussian process modeling with experiments, guiding synthesis within an informed, optimized space. Through three experimental cycles, 20 novel MPEAs were synthesized. Samples in previously unexplored phase diagrams were characterized, achieving Vickers hardness values up to 1269, a 7% increase over previous benchmarks. A striking discovery is the appearance silicon and tantalum together, a combination not seen in the training dataset. The successful identification of new high-hardness alloys demonstrates PAL 2.0's potential to optimize MPEAs efficiently. This approach presents a solution for the exploration of high-dimensional material systems, underscoring the framework's adaptability for advanced materials discovery.

2:00 PM

A Coupled Thermal-Mechanical Deep Material Network: *Ashley Lenau*[1]; Dongil Shin[2]; Andreas Robertson[1]; Ricardo Lebensohn[3]; Remi Dingreville[1]; [1]Sandia National Laboratories; [2]Pohang University of Science And Technology; [3]Los Alamos National Lab

Deep material networks (DMN) are tree-like machine learning networks that train on linear homogenization relationships for a given microstructure, and then act as a representative volume element to predict non-linear material responses. Most DMNs are utilized for "single physics" problems, such as a DMN predicting the thermal or mechanical response using its predicted homogenized thermal conductivity or stiffness, respectively. However, a DMN architecture or training strategy involving multi-physics homogenization tasks is still not yet well established. Combining thermal and mechanical tasks will ultimately result in a better description of the deformation behavior of the composite for a wider variety of boundary conditions. In this study, a DMN is simultaneously trained to homogenize the stiffness and thermal conductivity of a composite. After training, the network extrapolates stress, strain, heat flux, and temperature gradient for non-linear thermomechanical relationships. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

2:20 PM

A Thermodynamically Consistent Neural Ordinary Differential Equation for Constitutive Modeling of Polycrystalline Metals: *Paul Christodoulou*[1]; Liam Mackin[1]; David Najera-Flores[1]; Rohan Patel[1]; Bradley Davidson[1]; Jarred Heigel[1]; Elliot Haag[1]; Reed Kopp[1]; [1]ATA Engineering, Inc.

It is difficult to formulate a robust constitutive model for path-dependent, nonlinear, heterogeneous materials, such as additively manufactured (AM) metals. The difficulty arising from material heterogeneity is compounded by competing material behaviors at various length scales. ATA recently developed a Neural Ordinary Differential Equation (NODE) constitutive model with multiplicative Deformation Gradient Decomposition (DGD) to enable automatic discovery of these path-dependent constitutive models from stress-strain data. DGD-NODE ensures a thermodynamically consistent set of internal state variables and state variable evolution laws to describe the elastic, plastic, and thermal components of deformation. Presented work includes training and verification of the DGD-NODE constitutive model using simulations of synthesized microstructures representative of an AM metal, and subsequent application of the constitutive model in AM process modeling simulations using the Multiphysics Object Oriented Simulation Environment (MOOSE) finite element solver.

2:40 PM

Physical-Informed Machine Learning for Silicone Formulation Development: *Qingtao Cao*[1]; Lalitha Raghavan[1]; Sheng Zhao[1]; Ying Wang[1]; [1]Saint-Gobain Research North America

The application of machine learning (ML) in formulation development has been demonstrated through various Design of Experiment (DOE) cases. However, in the early stages of development, the limited number of available formulations restricts the effectiveness of purely data-driven models, particularly when developing new formulations that extend beyond the property ranges of existing ones. To overcome this challenge, Physics-Informed ML, integrating domain knowledge from physical models with the latent patterns captured by data-driven models, shows a more robust approach. In this case study, we present a successful implementation of Physics-Informed ML, leveraging a random forest model with packing value theory to develop silicone formulations characterized by two properties traded off with each other, based on a small set of formulation available within a narrow property range. The efficacy of this hybrid approach is further highlighted through a comparative analysis, demonstrating the superior performance of Physics-Informed ML over the purely data-driven method.

3:00 PM Break

3:30 PM

Out-of-Distribution Surface Anomaly Detection Using Masked Autoencoder Vision Transformers: *Pierre Belamri*[1]; Henry Proudhon[1]; David Ryckelynck[1]; Damien Texier[2]; [1]Mines Paris - PSL University; [2]Institut Clément Ader

Automated surface-anomaly detection using machine learning has become a promising area of research with high impact on visual inspection. However, traditional supervised models rely on large, labelled datasets, making them difficult to apply in this context. Large Vision Transformers, leveraging masked image modelling, offer a solution by creating modality-agnostic latent spaces that can enhance multimodal materials characterization. We propose a self-supervised learning approach for out-of-distribution anomaly detection using EBSD orientation maps, a key modality in material science as it provides direct information on grains orientations. A Vision Transformer Masked Autoencoder is trained to reconstruct quaternions maps, learning latent representations that capture grain boundaries and orientation patterns.Our results show clear differences in Mahalanobis distances distributions for twin-free and twin-containing samples, indicating the model's ability to detect anomalies linked to sigma-3 grain boundaries and/or twin geometries. This demonstrates the potential of multimodal transformers for defect detection in polycrystalline materials.

3:50 PM

Rapid Bubble and Cavity Tracking Utilizing Machine Learning: *Kip Wheeler*[1]; Christopher Field[2]; Khalid Hattar[1]; [1]University of Tennessee; [2]Theia Scientific LLC

Bubble to cavity evolution in materials could greatly influence the mechanical stability of materials utilized in extreme environments, such as nuclear reactors. Nanoscale bubble counting is typically done by hand using transmission electron microscope (TEM) micrographs and annotation software in a non-scalable, post-acquisition workflow. Recently, machine learning (ML) models have been utilized to count and measure bubbles in a fraction of the time compared to manual annotation. A rapid neural network option is the You Only Look Once (YOLO) model. Factors that influence the model include: data volume and training time through epochs. This technique has been applied to many different materials, such as Ni, PdNi, and LiAlO3 with some degree of success. The selection of model development parameters will be explored to determine the optimal setting for time efficient ML model-based bubble counting.

4:10 PM

Prediction of Creep Life Using K-Means Clustering and Gaussian Process Regression: *Sami Ben Elhaj Salah*[1]; Edern Menou[1]; Matthieu Degeiter[2]; Armand Barbot[2]; [1]Safran; [2]ONERA

In this study, a model involving Gaussian Process Regression (GPR) is introduced to predict creep life based on chemical compositions of nickel-based superalloys, utilizing a large and heterogeneous dataset. The high variability in the data introduces significant challenges for model accuracy; thus, a clustering approach using K-means is used to split the entire dataset into more similar sets.A separate GPR model is trained to capture the specific data patterns within each cluster. These individual kernels are then combined into a global kernel, representing the cumulative predictive power across clusters. This method enables a more adaptive modeling approach, improving predictive accuracy by leveraging the local similarities within each cluster. The proposed framework provides a robust tool for predicting creep life time in order to guide novel alloy design.

4:30 PM

Multidimensional Analysis for Correlation of Mechano-Physico-Chemical Attributes With Bio-Functionality in Eight TiNbZrSnTa (TNZST) Alloys: *Carmen Torres-Sanchez*[1]; Paul Conway[1]; [1]Loughborough University

Data-enabled approaches with experiments allow exploration of the inter-play between chemical, physical and mechanical attributes of alloys with their impact on biological behaviours. Characterisation of bulk and surface properties has been performed on eight exemplar TiNbZrSnTa of different allotropes. Their or + () crystal structure dened their mechanical properties, with dual + more suitable for load-bearing applications. As these are intended for implantation, surface assessment was a primary focus. A statistical correlation was undertaken between oxide layer composition, layer thickness, surface free energy and contact angles, and behaviour of cells progressing through adhesion, attachment, proliferation, differentiation and to maturation. Pairwise Pearson coefcient correlations, visualised in a heat-map matrix, allows elucidation of inferred agnostic correlations and supported the study of primary physical and chemical attributes most affecting cell behaviour; enabling both identication of primary contributors to osteoblastogenesis and, which experimental tests reveal stronger predictors for osteogenesis in these TNZST alloys.

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): ICME for Non-Metals and Composites: Structural and Functional Applications

Monday PM
June 16, 2025

Room: Room E
Location: Anaheim Marriott

Session Chair: To Be Announced

2:20 PM
ICME Based Sustainable Biobased Flexible Packaging: *Mudra Kapoor*[1]; Amit Salvi[1]; Beena Rai[1]; [1]Tata Consultancy Services

The end-of-life challenges of multi-layer flexible plastics contribute significantly to microplastic pollution, with over 70% ending up in oceans or landfills. The difficulty in recycling these laminated films drives the need for sustainable alternatives. In response to evolving EPR regulations, a biobased packaging solutions using direct biopolymers and polymerized biomolecules from agro, food, and marine waste is developed. A Gen-AI driven ICME framework is developed to create a comprehensive database integrating material properties, functional and non-functional characteristics, and manufacturing process knowledge repositories. This approach facilitates a data-driven recommendation system for accelerated product development of biobased flexible films, evaluating performance, cost, feasibility, end-of-life impacts and overall life cycle sustainability. We illustrate this platform using Cosmetic packaging example for secondary packaging. The platform supports knowledge assisted decision-making, promoting a transition from conventional plastics to sustainable, biobased packaging materials.

2:40 PM
Molecular Dynamics Simulation of Nanoscale Heterogeneity and Fracture of Epoxies: *Xiawa Wu*[1]; [1]Penn State Behrend

Epoxies are widely used in the aerospace industry. Increasing experimental evidence shows that a nanoscale heterogeneous network influences epoxy's failure behavior. However, there is a lack of molecular dynamics (MD) investigation of the heterogeneous nanostructure of epoxies due to the spatial limitation of atomistic simulations. To fill this gap, this work develops MD models with various distributions of cross-links representing highly and sparely cross-linked epoxy regions as observed in experiments and conducts tensile deformation. The simulation results show that alternatively arranged high and low cross-linked epoxy structures predict a brittle fracture. Young's modulus and glass transition temperature show insignificant changes in heterogeneous nanostructures. The ratio of the degrees of high and low cross-links and the sizes and distributions of the heterogeneous regions are investigated. The results of this work indicate the importance of incorporating a heterogeneous network in studying the plastic and failure behavior of epoxies at the nanoscale.

3:00 PM Break

3:30 PM
Curing Process Optimization of Polymer Composite Structures Through Spatiotemporal Temperature Control: *Soban Babu Beemaraj*[1]; Arshdeep Singh[1]; Yagnik Kalariya[1]; Amit Salvi[1]; [1]Tata Consultancy Services

Composite materials offer high specific stiffness and strength; hence, they are used in high-performance applications. The manufacturing of composite parts/structures involves the application of heat to initiate curing, which governs their mechanical properties. The residual stresses, due to exothermic cure effects, developed during the manufacturing process led to premature failure. In large composite structures like wind turbine blades, spatial and temporal optimization of the temperature profile is essential to reduce temperature and cure gradients and improve the mechanical behavior. This work introduces spatiotemporal optimization of the curing process where temperature profile is optimized with respect to time and location by combining surrogate-assisted multiscale cure analysis with a Non-dominated Sorting Genetic Algorithm II (NSGA-II). The method utilizes thermo-chemical-mechanical finite element analysis to model mechanical property evolution, while surrogate model reduces computational time. The effectiveness of the proposed methodology is shown for a tapered laminated composite structure.

3:50 PM
Molecular Dynamics Study of Grain Boundaries as Defect Sinks Under Irradiation in LiAlO2 and LiAl5O8: *Ankit Roy*[1]; Weilin Jiang[1]; Giridhar Nandipati[1]; Andrew M. Casella[1]; David J. Senor[1]; Ayoub Soulami[1]; Ram Devanathan[1]; [1]Pacific Northwest National Lab

Lithium aluminate ceramics, specifically LiAlO2 and LiAl5O8, hold significant potential for applications in nuclear environments due to their superior radiation tolerance. This study utilizes molecular dynamics simulations to investigate the role of grain boundaries (GB) in radiation-induced defect evolution within these materials. The simulations reveal distinct behaviors of lithium and aluminum atoms under displacement cascades, highlighting the GBs as efficient sinks for defects. Tritium behavior in LiAlO2 is also explored, with simulations indicating rapid migration and stable configuration formation with oxygen atoms, consistent with findings from first-principles ab initio simulations. The diffusion coefficient for tritium in LiAlO2 is calculated to be 1.33×10-14 m^2/s, aligning closely with previously reported values, thereby validating the simulation framework. These findings suggest that LiAl5O8 exhibits enhanced defect healing properties compared to LiAlO2, attributed to more efficient atomic transfer between the grain and GB.

4:10 PM
Design of Rare-Earth Free Permanent Magnetic Materials With Quantum Mechanics Methods: Fe-Ni-N(B): *Md Abdul Wahed*[1]; Chang-Dong Yeo[1]; Yang-Ki Hong[2]; Shuhui Li[2]; Minyeong Choi[2]; Woo-Young Lee[3]; Haein Choi-Yim[4]; Seok Bae[5]; [1]Texas Tech University; [2]University of Alabama; [3]Yonsei University; [4]Sookmyung Women's University; [5]LG Innotek

Rare-earth (RE)-free PMs within the $(BH)_{max}$ range of 10-30 MGOe (namely Gap magnets) are receiving significant attention in scientific and technical communities to cope with the recent impetus toward green electrical power generation, EVs, and wind power. Using quantum mechanics methods, we recently designed Fe-Ni-N(B) permanent ferromagnetic materials that meet the requirements for gap magnets. We modified the lattice constant *c/a* ratio of $L1_0$ FeNi ferromagnetic materials by interstitially doping them with nitrogen (N) or boron (B), which resulted in the formation of tetragonally ordered Fe_2Ni_2N (or Fe_2Ni_2B). Then, we conducted first-principles calculations to investigate the doping effects on M_S, K_u, and T_C. It was found that 2*p* element doping significantly improved the magnetocrystalline anisotropy energy of $L1_0$-ordered FeNi. Our quantum mechanical design results show that FeNi-based alloys can be easily adjusted for their magnetocrystalline anisotropy by interstitial doping with 2*p* elements.

4:30 PM
Theory Guided Design of MoO_3/$NiMoO_4$ Heterostructures Hybridized Active Pt Co-Catalyst for Efficient Water Splitting: *Nikhil Komalla*[1]; Nelson Dzade[1]; [1]Pennsylvania State University

An excellent bifunctional catalyst based on vertically aligned MoO_3/$NiMoO_4$ heterostructured nanorod arrays hybridized with ultrafine Pt nanoparticles for hydrogen and oxygen evolution reactions (HER and OER) in industrial-grade water splitting was developed. Density functional theory (DFT) calculations revealed the formation of a metallic heterostructure with enhanced charge transfer capabilities. Additionally, strong chemical coupling between MoO_3/$NiMoO_4$ and Pt synergistically improved charge transfer and optimized Gibbs free energies of intermediate species, accelerating reaction kinetics. The synthesized Pt-MoO_3/$NiMoO_4$ catalyst demonstrated superior performance compared to conventional noble-metal catalysts like Pt/C and RuO_2 at industrial current densities (1000 mA·cm^2). It achieved low overpotentials of 38.3 mV for HER and 267.6 mV for OER at 10 mA·cm^2. When used as both cathode and anode, it exhibited exceptional performance with a cell voltage of 1.55 V and durability for over 50 hours under continuous operation. Published in Journal of Colloid and Interface Science, 670, 1227 (2024).

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): ICME: Keynote Session

Monday PM
June 16, 2025

Room: Plenary Room
Location: Anaheim Marriott

Session Chair: To Be Announced

1:30 PM Introductory Comments

1:35 PM Keynote
Shaping the Future Workforce: Navigating Digital Transformation in Engineering: *Bryce Wilcox*[1]; [1]Milwaukee Tool

The engineering landscape is undergoing a transformation due to the rise of digital tools like Integrated Computational Materials Engineering (ICME) and Artificial Intelligence (AI). To remain competitive and adapt to these changes, developing a future-ready workforce is essential. This requires a focus on reskilling and upskilling workers, closing the skills gap, and fostering continuous learning in materials science and engineering. To drive significant improvements in employee competencies, forming partnerships with academic institutions, creating specialized training programs, and revamping learning platforms will be necessary. The convergence of advanced technologies and human capital is transforming manufacturing operations and workforce dynamics, driven by trends like the Industrial Internet of Things (IIoT), advanced robotics, and predictive analytics. We will explore how these innovations impact workforce development and highlight the skills and competencies needed for success in this evolving landscape, including data analysis, programming, and interdisciplinary collaboration.

2:05 PM Question and Answer Period

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): PSP Linkages: Multiscale/Multiphysics Modeling II

Monday PM
June 16, 2025

Room: Room F
Location: Anaheim Marriott

Session Chair: To Be Announced

2:30 PM Invited
Microstructures and Properties of AlCrFeMnV, AlCrFeTiV, and AlCrMnTiV High-Entropy Alloys: *Keith Knipling*[1]; Patrick Callahan[1]; [1]Naval Research Laboratory

A series of high-entropy alloys (HEAs) containing AlCrFeMnV, AlCrFeTiV, and AlCrMnTiV have been designed using a combination of thermodynamic prediction by Thermo-Calc and by experimental observation of the microstructure and phases present in arc-melted alloys. These alloys are predominantly BCC, with some alloys forming additional minor phases. A particularly intriguing microstructure is observed in the AlCrMnTiV alloy, which contains a high number density of 50 nm ordered BCC cuboids that are coherent with the BCC matrix, resembling the well-known -' microstructures in Ni-based superalloys but in a BCC system. We will correlate the alloy microsctructures, observed using a combination of X-ray diffraction (XRD), scanning and transmission electron microscopy (SEM/TEM), and atom-probe tomography (APT), to the alloys' mechanical properties measured by Vickers microhardness and nanoindentation.

3:00 PM Break

3:30 PM
Multiscale Modeling of Microstructure Evolution of Cast Iron: From Atomistic to Macro Scales: *Ujjal Tewary*[1]; Shyamprasad Karagadde[2]; Goutam Mohapatra[1]; Satyam Sahay[1]; Indradev Samajdar[2]; [1]John Deere India Pvt. Ltd.; [2]IIT Bombay

Cast iron, an ancient material known to humans, comprises approximately 70% of modern metal castings. Its microstructure exhibits diverse graphite morphologies, encompassing flake, compacted, and spheroidal forms. This study utilized a combination of industrial casting trials, analytical microscopy, and molecular dynamics simulation to investigate the origins of graphite morphology. Based on the theoretical premise, a multiscale modeling approach was developed to simulate microstructure evolution. Molecular dynamics simulation determined the nucleation and growth kinetics for the faceted growth of graphite. These growth parameters were then integrated into a finite element-based micro-macro solidification model to simulate microstructure evolution for different graphite morphologies in cast iron. The predictions were validated by experimental results, demonstrating the effectiveness of the integrated computational multiscale modeling approach for cast iron microstructure evolution.

3:50 PM
Computation of Phase Fractions from Continuous Heating Dilatation Experiment for a Medium Mn Steel: *Kamal Kumar Gupta*[1]; Shiv Brat Singh[1]; [1]Indian Institute of Technology Kharagpur

The computation of calculation of austenite fraction and its carbon content has been performed using Newton's method that minimizes error between calculated percentage change in length and experimentally recorded percentage change in length at each temperature step up to temperature above Ac3 from dilatation data obtained on heating Fe-0.2C-5Mn-0.8Si-0.4Al medium Mn steel having initial retained austenite in martensitic micro structure for different heating rate 1,25 and 50 degree Celsius per second. The simulated change in pct. length is approximated as one third of the pct. change in volume, where volume at any temperature is proportional to sum of multiplication of mole fraction of phase and unit volume in that phase considering both mole fraction of phases and its unit volume can change with temperature.

4:10 PM
Multi-Scale Investigation of Dislocation-Precipitate-Grain Boundary Interactions in Precipitation-Hardened Al-Cu Alloys: *Anantha Lakshmi Prasanna Tatavarty*[1]; Amit Singh[1]; Sushil Mishra[1]; [1]Indian Institute of Technology Bombay

This study employs a multi-scale approach to investigate the mechanical behaviour of precipitation-hardened Al-Cu alloys, focusing on dislocation-precipitate-grain boundary interactions. Molecular statics simulations validate equilibrium configurations from prior analytical models, capturing atomic-scale effects. Molecular dynamics (MD) simulations extract critical parameters, such as dislocation mobility and drag coefficients, which inform discrete dislocation dynamics (DD) studies. DD simulations analyze mesoscale dislocation behaviour and its dependence on microstructural features. These insights are integrated into crystal plasticity finite element modelling (CPFEM) to predict macroscopic deformation responses under varying conditions. This framework bridges atomistic, mesoscale, and continuum scales, providing a comprehensive understanding of the deformation mechanisms in precipitation-hardened Al-Cu alloys.

The 7th International Congress on 3D Materials Science (3DMS 2025): 3D Data Processing, Software, and Reconstruction Algorithms I

Monday PM
June 16, 2025

Room: Room D
Location: Anaheim Marriott

Session Chair: To Be Announced

1:30 PM Invited
Reorganization of the Highly Extensible X-Ray Diffraction Library and Opportunities for Community Engagement: *Paul Shade*[1]; Kelly Nygren[1]; Patrick Avery[2]; Zack Singer[3]; Sven Gustafson[1]; Saransh Singh[4]; Chris Budrow[5]; Donald Boyce[1]; [1]Cornell University; [2]Kitware; [3]Verdant Evolution; [4]Lawrence Livermore National Laboratory; [5]Budrow Consulting LLC

For over a decade, the open-source and community-built *Highly Extensible X-ray Diffraction Toolkit* (HEXRD) has been providing a library of tools for researchers to perform high-quality data reconstructions on x-ray diffraction datasets across many modalities - with ongoing updates to improve the user interface, documentation, bug fixes, and computational efficiency. In response to the size of the current code base and growing demand to integrate more features and user-generated tools/workflows, HEXRD is being modularized into core and technique-specific utilities within the repository. In addition to making the code-base searchable and easier to navigate for the user, this structure enables code-contributors to engage with the code on the topics specific to their science/technique. This talk will cover the blueprint for the restructuring of HEXRD and phased roll-out plan. We will also cover the many ways researchers can engage with the codebase going forward - whether as a user or future contributor.

2:00 PM
Enhancing Neutron Single Crystal Visualization With NeuXtalViz: *Zachary Morgan*[1]; Zhongcan Xiao[1]; Sylwia Pawledzio[1]; Shiyun Jin[2]; Iris Ye[3]; Vickie Lynch[1]; Thomas Proffen[1]; Christina Hoffmann[1]; Xiaoping Wang[1]; [1]Oak Ridge National Laboratory; [2]Gemological Institute of America; [3]Next Generation STEM Internship Program Participant at ORNL

Advancements in single crystal neutron diffraction require tools that integrate 3D visualization with advanced data reduction to interpret complex datasets. NeuXtalViz is a 3D visualization software developed to meet this need by enhancing Mantid's platform with libraries like PyVista and scikit-learn. By consolidating wavelength-resolved tools into a single environment, NeuXtalViz supports intuitive 3D visualization and incorporates recent data reduction techniques with frameworks for structural refinement and defect modeling. This streamlined workflow improves data interpretation and builds a foundation for machine learning applications in 3D diffraction science. We discuss the technical approach, highlighting its visualization capabilities and interfaces with advanced reduction and analysis tools, and demonstrate its potential impact on the neutron scattering community. NeuXtalViz aims to address gaps in 3D data analysis, advancing future materials research in crystallography.

2:20 PM
Analysis of Extremely Large 3D Polycrystalline Aggregates: *Sean Donegan*[1]; Michael Chapman[2]; Michael Uchic[1]; [1]Air Force Research Laboratory; [2]BlueHalo

Modern 3D characterization techniques acquire extremely high-fidelity microstructural data, but are often limited to small volumes with typically only hundreds of grains. This restricts analysis of extreme microstructural events crucial for understanding phenomena like material failure. This work presents an unprecedented 3D dataset of a single-phase Ti-7Al alloy, comprising roughly 520 mm3 and containing over 1 million grains. Collected using serial sectioning and computational polarized light microscopy, this dataset enables investigation of rare microstructural features and their influence on material properties. We discuss the experimental techniques used to collect this data set, the specialized analysis approaches built to process the voluminous amount of data, and the resulting statistical features of this extremely large polycrystalline aggregate. This large-scale dataset provides new opportunities for understanding microstructure-property relationships and advancing materials design.

2:40 PM
Fouriera: Automated Spectral Methods for Multiphysics Problems via Symbolic Computing: *Bo Wang*[1]; Tae Wook Heo[1]; Kyle Pietrzyk[1]; [1]Lawrence Livermore National Laboratory

Multiphysics modeling of functional materials in the continuum scale can often be formulated into a set of partial differential equations (PDEs). Such models, along with the numerical recipes required to solve them efficiently, quickly become intractable as the model complexity grows. Despite several available software packages, most of them are based on the finite-element method, yet developing a numerical solver based on the spectral method for multiphysics problem remains a time-consuming task prone to human error.Here, we propose a method to automate the implementation of Fourier spectral methods to solve general PDEs using symbolic computing. By automating the tedious analytical work required to implement the numerical methods, Fouriera enables users to solve PDEs conveniently and interactively for multiphysics problems in an efficient manner through a graphical user interface. In this presentation, I will introduce the infrastructure of Fouriera and demonstrate its multiphysics modeling applications, such as in phase-field modeling.

3:00 PM Break

3:30 PM
Real Time Spot Tracking and Materials Characterization for High Energy X-Ray Diffraction Microscopy: *Daniel Banco*[1]; Wiley Kirks[2]; Sven Gustaffson[3]; Katherine Shanks[3]; Kelly Nygren[3]; Matthew Miller[3]; Eric Miller[1]; [1]Tufts University; [2]Cornell University; [3]Cornell High Energy Synchrotron Source

3D high energy X-ray diffraction microscopy (HEDM) data captured in-situ for the characterization of structural materials reveal crystal lattice spacing and orientation changes related to plasticity and fatigue. Challenges associated with large data volumes and experiment complexity result in limited interaction with data during in-situ experiments and lead to data analysis becoming a bottleneck. Here we address this issue through the development and demonstration of data analysis methods providing real-time feedback during experiments. Our sparsity-based signal processing approach tracks diffraction spots in far-field HEDM data and computes time-evolving features indicative of plasticity. The algorithm is inherently parallelizable and provides interpretable features dynamically as the spots spread, move, and overlap during an experiment. While not necessary for processing, prior ex-situ HEDM measurements and virtual diffraction simulation provided crucial guidance to the data analysis. The approach was implemented at the CHESS structural materials beamlines and validated on both simulated and experimental data.

3:50 PM
Grain-Resolved Reorientation and Orientation Gradient Development in Cyclic Loading of \945-Ti Using High Energy X-Ray Diffraction Microscopy: *Rachel Lim*[1]; Sven Gustafson[2]; Darren Pagan[3]; Anthony Rollett[4]; [1]Lawrence Livermore National Laboratory; [2]Cornell High Energy Synchrotron Source; [3]Pennsylvania State University; [4]Carnegie Mellon University

On the grain scale, materials are heterogeneous and anisotropic which can lead to development of significant grain-scale stresses in polycrystals. Increasing understanding of the effects of this heterogeneity and anisotropy requires experiments which supply three-dimensional, in situ data. High energy X-ray diffraction microscopy (HEDM) is employed to study the in situ grain-resolved evolution of Ti-7Al under during 200 tensile loading cycles below macroscopic yield. Individual grain reorientations are tracked using grain-averaged orientations from far-field HEDM, while spatially-resolved orientations reconstructed via near-field HEDM show the development of slight orientation gradients in some of the grains after the 200 cycles. A comparison between the orientation changes calculated across these two measurements shows both grains with large average reorientations and some with orientation gradient development.

4:10 PM
Characterization of Hierarchical Microstructures of TiC Reinforced Nickel Matrix Composites Using Deep-Learning Assisted 3D X-Ray Microscopy: *Kaushik Yanamandra*[1]; Hrishikesh Bale[1]; Rajarshi Banerjee[2]; [1]Carl Zeiss Microscopy; [2]University of North Texas

Metal Matrix Composites (MMCs) are increasingly important in materials science due to their exceptional properties and applications. Ni-Ti-C based MMCs, produced via laser engineered net shaping (LENS), feature unique microstructures with titanium carbide (TiC) reinforcing a nickel matrix. This study leverages high-resolution, non-destructive X-ray microscopy to analyze MMC microstructures at the sub-micron level, revealing the spatial distribution and alignment of reinforcing phases. Some TiC phases are near the detection limit of X-ray microscopy, necessitating a combination of high-resolution objectives and deep learning-based 3D reconstruction to push the resolution and contrast limit. We present results from a 3D characterization of complex MMC microstructure where in the individual matrix and reinforcing phases have been discerned across multiple scales. The findings highlight X-ray microscopy's crucial role in understanding and optimizing MMC performance, paving the way for advanced design and engineering.

The 7th International Congress on 3D Materials Science (3DMS 2025): Emerging 3D Characterization Techniques and Instrumentation I

Monday PM
June 16, 2025

Room: Room C
Location: Anaheim Marriott

Session Chair: To Be Announced

1:30 PM Invited
Advances in Scanning 3DXRD: Resolving Intra-Grain Deformation in 3D: *Nils Axel Henningsson*[1]; [1]DTU

Modern synchrotron facilities provide monochromatic X-rays with high energy and flux. The 3D X-ray Diffraction Microscope (3DXRD) has utilized these capabilities for over two decades, becoming a reliable tool for 3D characterization of polycrystalline materials. In the past eight years, a derivative technique, the scanning 3DXRD microscope, has emerged. It uses a narrow X-ray beam combined with raster scanning to capture spatial details at the sub-grain level in 3D. In scanning 3DXRD, the diffraction signal from different sub-domains within crystals is highly sensitive to the lattice deformation field. I pioneered several regression frameworks to reconstruct the intra-grain strain tensor and rotation fields from such data. In this talk, I will survey the history of scanning 3DXRD, present the state-of-the-art capabilities of the microscope, showcase its benefits and limitations, and discuss future developments in scanning 3DXRD.

2:00 PM
Observation of Thermal Fatigue-Induced Grain Rotation in Pb-Free Solder Joints by XSOL: *Jaemyung Kim*[1]; Yujiro Hayashi[1]; Hiroaki Tatsumi[2]; Hiroshi Nishikawa[2]; Makina Yabashi[1]; [1]RIKEN; [2]Osaka University

It is believed that the failure mechanism of Pb-free solder joints under thermal cycling is correlated with the rotation of -Sn grains. However, destructive measurement methods have prevented understanding the original orientation of -Sn grains before thermal cycling. While conventional X-ray-based orientation microscopies exist, they are limited to small cylindrical samples and are unsuitable for plate-like structures such as solder joints. As a result, no direct evidence of grain rotation has been available until now.To overcome this limitation, we recently developed X-ray Scanning Orientation Laminography (XSOL), which enables orientation mapping of extended plate-like specimens. We applied XSOL to conduct nondestructive analysis of a 930-m-thick plate containing solder joints. We observed that the -Sn grains in the as-soldered joints exhibited random orientations, while the c-axis of the grains tended to align parallel to the Cu substrate after thermal cycling, providing direct evidence that grain rotation occurs due to thermal fatigue.

2:20 PM

Laboratory 3D X-Ray Micro-Beam Diffraction: *Yubin Zhang*[1]; Jette Oddershede[2]; Anthony Seret[1]; Azat Slyamov[2]; Florian Bachmann[2]; Jan Kehres[1]; Carsten Gundlach[1]; Ulrik Olsen[1]; Jacob Bowen[2]; Henning Poulsen[1]; Erik Lauridsen[2]; Dorte Juul Jensen[1]; [1]Technical University of Denmark; [2]Xnovo Tech

The development of 3D non-destructive X-ray characterization techniques in home laboratories is essential for establishing 3D characterization as a new standard for materials research. Accessible instruments in universities and industry will enable many more researchers to conduct 3D characterization daily, overcoming the limitations of competitive access to synchrotron facilities. Recent efforts have focused on techniques like laboratory diffraction contrast tomography (LabDCT), which allows 3D characterization of fully recrystallized materials with grain size larger than 15 µm, offering a spatial resolution of 5 µm using commercial X-ray CT systems. To enhance the capabilities of these laboratory instruments, we have developed a new 3D laboratory X-ray micro-beam diffraction (LabµXRD) setup, utilizing newly developed Pt-coated twin paraboloidal capillary X-ray optics. The principles and proof-of-concept for LabµXRD will be detailed, along with its potential for integration with LabDCT and micro-CT for multiscale and multimodal 4D characterization of conventionally and additively manufactured materials.

2:40 PM

Deep Learning Enabled Rapid 3D X-Ray Tomography for In Situ Mechanical Characterization: *Nathan Johnson*[1]; Hrishikesh Bale[1]; Steve Kelly[1]; Newell Moser[2]; Orion Kafka[2]; [1]Carl Zeiss Research Microscopy Solutions; [2]National Institute of Standards and Technology

Laboratory X-ray characterization techniques often face limitations due to lower flux and brightness compared to synchrotron sources, leading to extended counting times for acquiring high-quality images. This issue is particularly acute for in situ experiments that require multiple datasets, sometimes stretching data collection to several days per sample. In this study, we introduce a deep learning-based reconstruction method tailored for sparse X-ray microscopy datasets. During an in situ tensile test on additively manufactured Inconel 718 dogbone specimens, we collected 1,000 two-dimensional projections over the course of an hour. Utilizing a commercial deep learning model (Zeiss DeepRecon) we achieved high-resolution 3D reconstructions using 100 projections, reducing acquisition time by 10X. The model captured up to 80% of pores and preserved the morphology of the largest pores. This reduction—from one hour to six minutes — notably enhances the efficiency of in situ experiments.

3:00 PM Break

3:30 PM

Pushing Boundaries in 3D Microstructure Mapping: The New DFXM Beamline at ESRF ID03: *Can Yildirim*[1]; Helena Isern[1]; Thomas Dufrane[1]; Marilyn Sarkis[1]; Yaozhu Li[1]; Abderrahmane Benhadjira[1]; Raquel Rodriguez-Lamas[1]; Ricardo Hino[1]; Philipp Brumund[1]; Emmanuel Papillon[1]; Thierry Brochard[1]; Damien Scortani[1]; Carsten Detlefs[1]; [1]European Synchrotron Radiation Facility

The ESRF's Dark Field X-ray Microscopy (DFXM) beamline at ID03 heralds a new era for 3D mapping of crystalline orientation and strain, advancing multi-scale imaging capabilities within embedded microstructures. Emerging from ESRF's EBSL2 Upgrade Project, ID03 offers unprecedented opportunities in high-resolution, non-destructive mapping. Relocated and upgraded from ID06-HXM, the beamline now features state-of-the-art X-ray optics for pink and monochromatic x-rays, a new goniometer, and a detection system tailored to capture subtle microstructural phenomena. Since opening to users in April 2024, the beamline's unique setup supports complex studies, from metal strain mapping to functional material assessments in semiconductors, biominerals, and energy systems. By expanding access to multi-modal, in-situ exploration, ID03 is positioned to drive innovation across materials science disciplines, meeting the needs of next-generation research in structure-property relationships.

3:50 PM

Lab-HEDM: A Laboratory-Scale Breakthrough Technique for 3D Characterization of Polycrystalline Materials: *Seunghee Oh*[1]; Yuefeng Jin[1]; Sangwon Lee[1]; Wenxi Li[1]; Ashley Bucsek[1]; [1]University of Michigan

High-energy diffraction microscopy (HEDM) is a 3D x-ray diffraction technique used to characterize the volume, position, orientation, and strain of thousands of grains concurrently, making it a powerful tool for studying the micromechanical behavior of bulk polycrystalline materials. However, HEDM remains accessible only at a few synchrotron facilities. Here, we introduce an innovative laboratory-scale version (Lab-HEDM) that employs a liquid-metal jet x-ray source. As a validation study, we benchmark the capabilities of Lab-HEDM against synchrotron-based HEDM and laboratory diffraction contrast tomography (Lab-DCT). Over 96% of grains detected by Lab-3DXRD were cross-validated with Lab-DCT and/or synchrotron-3DXRD, especially for coarse grains (> ~64 m). Results also suggest that finer grains could be resolved by employing high-efficiency detectors (e.g., photon-counting detectors). Additionally, we demonstrate how the sensitivity of Lab-3DXRD to fine grains can be improved by modifying the HEDM reconstruction procedure.

4:10 PM

Reconciling Conflicting Hydrogen Embrittlement Models Using Dark-Field X-Ray Microscopy: *Dayeeta Pal*[1]; Can Yildirim[2]; Leora Dresselhaus-Marais[1]; [1]Stanford University; [2]European Synchrotron Radiation Facility

Despite 150 years of research, the fundamental mechanisms of hydrogen (H) embrittlement are poorly understood. H atoms form a solid solution of interstitial defects in metals, altering dislocation behavior. While dislocations are essential to understand metal plasticity, it is unclear whether H enhances dislocation mobility (Hydrogen Enhanced Localized Plasticity-HELP) or reduces it (Solute Drag Theory-SDT), with no technique being able to image subsurface dislocations. Time-resolved and 3D dark-field X-ray microscopy (DFXM) has been developed to study interactions of large populations of subsurface dislocations. Since hydrogen shielding effect (HSE) is the key mechanism that explains the increased dislocation mobility in the presence of H, our work uses DFXM to generate 3D maps of dislocations, illustrating which dislocations obey the HSE mechanisms in uncharged and H-pre-charged single crystal FCC-austenitic stainless steel. We support these results with DFXM simulations and HSE models, offering the first direct measurements to reconcile conflicting H-altered mobility models.

Specialty Congress 2025: All-Congress Plenary Session: Tuesday Plenary Session

Tuesday AM
June 17, 2025

Room: Plenary Room
Location: Anaheim Marriott

Session Chair: To Be Announced

8:00 AM Introductory Comments

8:10 PM Plenary
Leveraging 3D Characterization for Model Development and Validation of Structural Alloys and Advanced Processing: *David Rowenhorst*[1]; [1]US Naval Research Laboratory

At the heart of the integrated computational materials engineering paradigm is the acknowledgement that properties and processing are fundamentally linked through proper understanding of microstructure. For most of the history of materials science, direct microstructural quantification has been determined primarily through two-dimensional observations of our materials. The advent of advanced microscopy and increased computational power and tools have led to significant advances in our ability to both quantify the true 3D microstructures, as well as model their behavior. In this presentation we will discuss how the Navy is developing new methods for characterization and modeling in 3D, both to develop new alloys that leveraged nanoscale atom probe tomography and to model microscale dislocation dynamics to provide predictions of mechanical response. Additionally, we will discuss the development and improvement of automated micro-scale serial-sectioning to collect statistically large datasets in additively manufactured (AM) 316L, and how the data from these characterizations were essential for informing and validating cellular automaton finite element models for AM structures.

8:50 AM Question and Answer Period

Joint Sessions of AIM, ICME, & 3DMS: Automated and Autonomous Research: Joint Session of AIM, ICME, and 3DMS

Tuesday AM
June 17, 2025

Room: Joint Sessions Room
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Invited
Innovations in 3D EBSD for Advanced Materials Characterization: *Andrew Polonsky*[1]; Chad Hovey[1]; James Lamb[2]; Paul Chao[1]; McLean Echlin[2]; Hojun Lim[1]; Kyle Johnson[1]; Julia Deitz[1]; Tresa Pollock[2]; [1]Sandia National Laboratories; [2]University of California Santa Barbara

Recent advancements in automation have transformed materials characterization techniques over the past decade. The capability to perform serial-sectioning within an electron microscope using ion or laser beams has facilitated the acquisition of high-fidelity 3D electron backscatter diffraction (EBSD) data, resulting in increasingly large datasets. Here we explore the application of 3D EBSD to analyze microstructures obtained through serial-sectioning with the TriBeam system, revealing insights into these materials that traditional methods cannot provide. We will address analytical considerations for non-equilibrium microstructures, such as those produced by macroscopic plastic deformation or additive manufacturing. Additionally, we will outline workflows for automated management of multi-terabyte datasets and present novel collection and analysis tools designed to minimize the reliance on specialized knowledge, thus making this advanced technique more accessible to a broader audience. Furthermore, we will discuss how these datasets can be leveraged for advanced modeling techniques to enhance our fundamental understanding of materials processing.

9:30 AM
"Advanced Calibration of GTN Damage Model for Aluminum Alloy AA6111 Using Digital Image Correlation and Bayesian Inference": *Seyed Mohammad Ali Seyed Mahmoud*[1]; Dominic Renner[1]; Ali Khosravani[2]; Surya Kalidindi[1]; [1]Georgia Institute of Technology; [2]Multiscale

This study characterizes the tensile behavior of aluminum alloy AA6111, an essential material in automotive forming processes. Predicting failure mechanisms under realistic conditions is challenging due to the complexity of deformation and damage in aluminum alloys. We present a novel approach to calibrate the Gurson-Tvergaard-Needleman (GTN) damage model by integrating tensile testing with Digital Image Correlation (DIC) for high-resolution strain field measurements. Our methodology involves a two-step Bayesian calibration: first, a Gaussian process surrogate model is trained on finite element simulations with material parameters (elastic, plastic, and GTN characteristics) and tensile response data (load-displacement curve and DIC strain field); then, inverse sampling of material parameters is conducted based on the tensile response. This Bayesian framework, combined with precise strain data, enables robust model calibration and validation, as well as uncertainty quantification of GTN parameters. The adaptable DIC-based calibration framework shows potential for broader applications across novel materials and models.

9:50 AM
Automated 3D Microstructural Characterization of a Dual-Phase Steel Using the RASSI Platform: *Michael Moschetti*[1]; Dirk Bettge[1]; [1]Federal Institute for Materials Research and Testing

The Robot-Assisted Serial-Sectioning and Imaging (RASSI) platform is an innovative 3D metallography system developed at the Federal Institute of Materials Research and Testing. It combines advanced robotics, precise sample preparation, adaptable chemical etching techniques, light optical imaging, and machine learning for image segmentation, enabling automated, high-throughput 3D microstructural characterization, and providing significant insights into complex microstructures. We demonstrate RASSI's capabilities through a study of a dual-phase steel (DP600), investigating multi-scale microstructural features and phase distributions. The result is a comprehensive dataset that can be used to enhance computational modeling and prediction of DP steel behavior under various conditions. This case study highlights how RASSI can facilitate the rapid development and optimization of advanced materials and manufacturing processes.

10:10 AM
Influence of 3D Crack Networks for High Toughness Responses in Tantalum Carbides: *Alyssa Stubbers*[1]; Gregory Thompson[1]; Chris Weinberger[2]; Sierra Durkee[1]; Evan Schwind[1]; Mireya Garcia[3]; Olivia Graeve[4]; Edgar Solano[3]; Alejandro Ramirez[3]; [1]University of Alabama; [2]Colorado State University ; [3]Instituto Politecnico National; [4]University of San Diego

The zeta-phase, -Ta4C3, is reported to have a fracture toughness above 15 MPa·m1/2, which is a factor of two to three times larger than most other ceramic materials. This fracture strength is derived from the interlocking lath structure of zeta phase precipitation in a tantalum carbide matrix. These laths provide anisotropic mitigation of crack propagation as well as a buckling response. Furthermore, a local metal-metal bond in the zeta-phase's unit cell facilitates plasticity through dislocation nucleation. The presented work addresses the 3-dimensionality of the crack pathways. Here, the carbide was subjected to microindents from which plasma-focus ion beam based serial sectioning and subsequent reconstruction renderings were undertaken to reveal the cracking network. From acquired images, three distinct crack types are cataloged: linear, bifurcating, and kinking. Finally, as serial sectioning can be a time-consuming characterization method, we have also implanted an image-based machine learning method to identify cracking features and directions between slices thereby reducing either the number of slices needed and/or the resolution required between slices.

10:30 AM Break

11:00 AM Invited
Building a Self-Driving Lab From Scratch: *Shijing Sun*[1]; [1]University of Washington

The development of autonomous laboratories marks a paradigm shift in materials research by automating experimental processes—from planning to analysis. This talk explores three approaches to laboratory autonomy to accelerate discovery. The first involves an all-in-one platform, where an AI "brain" directs workflows and real-time computer vision guides decisions. The second emphasizes modular integration, adding robotic components and using lower-fidelity proxies with human oversight for flexibility. Lastly, open-source hardware offers customizable, cost-effective automation setups, democratizing advanced tools for researchers. These approaches demonstrate how to build functional self-driving labs, transforming experimentation and accelerating materials design.

11:30 AM
FIB-SEM Serial Sectioning Tomography: Towards 24-Hour Time-to-Results: *Bartlomiej Winiarski*[1]; Patrick Barthelemy[1]; Chengge Jiao[1]; [1]Thermo Fisher Scientific

Focused Ion Beam – Scanning Electron Microscope (FIB-SEM) and Plasma FIB (PFIB)-SEM Serial Sectioning Tomography are well-established techniques for high-resolution, 3D imaging and analysis of materials at the multiscale. This method involves the sequential removal of thin layers of material, followed by imaging to reconstruct detailed 3D microstructures. Despite its potential, the time-intensive nature of the process has been a significant barrier to widespread adoption. Our research aims to optimize PFIB SST to achieve a 24-hour time-to-results. By integrating advanced automation techniques for focused beam sectioning and SEM imaging, along with streamlined and automated data processing and segmentation algorithms aided by AI, we propose a comprehensive approach to significantly reduce imaging, reconstruction times, data segmentation, and reporting. Exemplary results from a Solid Oxide Fuel Cell (SOFC) demonstrate promising improvements in both speed and accuracy, suggesting that a 24-hour turnaround is attainable.

11:50 AM
Using Novel EBSD Methods to Analyze Plastic Strain in Structural Alloys: *David Rowenhorst*[1]; [1]US Naval Research Laboratory

The microstructural characterization of materials is essential for validating and informing the models used in ICME. While there are well established workflows for understanding mean values, understanding sub-grain orientation gradients are critical for making accurate predictions in the amount of plastic strain within a material formed due to traditional thermo-mechanical processing, phase transformations, or residual stresses formed during rapid solidification. Here we will present new methods for evaluating the amount of plastic strain present in a material by applying advanced electron backscattered diffraction (EBSD) microscopy. We will show that by combining pattern denoising methods such as the NLPAR algorithm, along with new EBSD indexing methods that operate at high speeds, and high precision, one can detect grain misorientations that are below 0.2°, while collecting using typical scan conditions. As a case study, we will compare the orientation gradients in additive manufactured 316L stainless steel with newly developed CAFE-CP models.

3rd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2025): Applied ML for Manufacturing III

Tuesday AM
June 17, 2025

Room: Room A
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Introductory Comments

9:10 AM
Application of ML to Ceramics Industry: *Dominic Wadkin-Snaith*[1]; [1]Lucideon

The traditional more established Ceramics industry is energy intensive with 30% of production costs coming from energy consumption alone. Although established, additionally, the industry can suffer from uncontrolled deformation of parts under firing. Whereas nascent techniques such as 3D printing of complex and intricate parts are in their development stage and need greater optimisation before coming to commercial market. We summarise recent advances made by the application of ML techniques to data collected via process sensors to drive towards an industry 4.0 approach enabling optimisation of industrial processes within traditional ceramics sector. As well as the latest in non-destructive computer vision techniques to monitor part distortion in real time for firing profiles of interest. We will also demonstrate how ML enhancement of design of experiment has led to new direction of development in the area of ceramic 3D printing.

9:30 AM
Offline Programming for Wire-Arc DED Applications Using Machine Learning Algorithms: *Kaue Riffel*[1]; Rakhi Bawa[1]; Antonio Ramirez[1]; Justin Chan[1]; Rida Adhami[1]; Daniil Gofman[1]; [1]The Ohio State University

With the expansion of Wire-Arc DED, optimization of the deposition process is crucial for efficiency. Optimal stepover distance and printing strategy is instrumental to producing a successful build, yet existing methods use low-flexibility models or rely on human experience, resulting in costly and inefficient trial-and-error methods. This project develops an artificial intelligence to identify the optimal stepover distance from input process variables like wire feed speed and travel speed. Using non-linear regression models on experimental data of overlapping bead depositions, hundreds of synthetic data points are simulated to train a neural network. The network then identifies the best stepover distance by optimizing multiple output variables, like height difference between beads and the area of the valley of the deposition. Additional parameters, like waveform and deposition area, are also incorporated, creating a versatile tool tailored to specific applications. A graphical user interface further enhances usability for efficient DED programming.

9:50 AM

Understanding Manufacturing and Materials Design Spaces: Overcoming Expensive Data: *Erick Braham*[1]; James Hardin[2]; [1]UES / Air Force Research Laboratory; [2]Air Force Research Laboratory

Materials discovery, manufacturing optimization, and many other goals in our community have benefited using data-driven methods like machine learning, design of experiments and AI. A large driver in the implementation of these tools is to understand complex design spaces from small amounts of data. Materials and manufacturing research lends itself inherently to expensive data with costly materials, researcher time, machine time, or other limited resources. In this work we explore ways to sample intelligently to provide the most meaningful design information in the most efficient manner. By examining two case studies we can demonstrate approaches that enable little waste when exploring opaque design spaces. Firstly we examine the use of an ensemble gaussian process approach on parameterizing direct ink write 3D printing. Secondly we examine using chemical and physical properties to guide selection of formulations of compositionally complex ceramics.

10:10 AM

Correlation of ULTEM 9085 Physical, Chemical, and Mechanical Properties: *Kassandra Hernandez*[1]; Devin Roach[1]; [1]Oregon State University

ULTEM 9085 is the first Federal Aviation Administration (FAA) qualified 3D printed thermoplastic, well-known for its high strength-to-weight ratio, chemical resistance, and flame retardance. However, a large difference in mechanical properties exists between traditionally manufactured high-performance thermoplastics and 3D printed materials. This study investigated the effects of print parameters on material properties through density, surface profile, scanning electron microscopy (SEM), and void analyses across various coupon geometries and build orientations. Surface microscopy findings revealed that inter- and intra-layer bonding significantly influences density and tensile performance variations. Additionally, a machine learning (ML) model was developed to analyze tensile-tested ULTEM 9085 coupons, with 3D printing parameters as inputs and critical mechanical properties—such as strength, modulus, and yield strength—as outputs. The ML model uncovered previously unknown relationships between printing parameters and mechanical properties. Overall, this research provides essential insights for optimizing additive manufacturing processes for high-performance aerospace applications.

10:30 AM Break

10:50 AM

Machine Learning and Molecular Dynamics Simulations Aided Insights Into Condensate Ring Formation in Laser Spot Welding: *Ankit Roy*[1]; Lance R Hubbard[1]; Nicole R Overman[1]; Kevin R. Fiedler[1]; Matthew J Olszta[1]; Diana B Horangic[1]; Floyd Hilty[1]; Mitra Taheri[1]; Daniel K Schreiber[1]; [1]Pacific Northwest National Lab

Condensate formation is critical as it settles into the powder thereby altering the quality of unconsolidated powder. This study investigates the relationship between alloy composition, vapor pressure, and condensate ring thickness as seen in a two-dimensional micrograph. To study the process, laser spot welding was performed on 9 different alloys, and the inner spot weld diameter along with the condensate ring formation was studied. Leveraging machine learning models, experimental observations, and molecular dynamics simulations, we explore the fundamental factors governing condensate ring formation. The models identify laser power as a primary determinant for weld spot diameter followed by physical properties like hardness and density. Conversely, for condensate ring thickness, vapor pressure and melting point descriptors consistently emerge as paramount, as validated across all models. Molecular dynamics simulations on Ni-Cr alloys elucidate the vaporization dynamics, confirming the role of vapor pressure in governing surface vaporization.

11:10 AM

Machine Learning-Driven High-Throughput Screening for Optimal Lithium-Ion Battery Electrolyte Solvents: *Kumar Ayush*[1]; Dipesh Dubey[1]; Sriram Srinivasan[1]; Mahesh Mynam[1]; Beena Rai[1]; [1]Tata Consultancy Services

Lithium-ion batteries are essential for sustainable technologies, from electric vehicles to renewable energy integration. The design of next-generation electrolytes relies on discovering optimal liquid solvents that meet stringent performance criteria. We present a high-throughput framework employing machine learning (ML), density functional theory (DFT), and molecular dynamics (MD) for electrolytic solvent discovery, adaptable to various databases and property requirements.We screen over 118 million compounds from PubChem database by applying ML model-based filters targeting properties such as viscosity, dielectric constant, and electrochemical stability. This approach, integrating data from diverse sources, enabled the identification of a few tens of molecules. Following ML-based screening, the select candidates were validated through DFT and MD simulations, indicating strong potential for battery applications. This flexible framework exemplifies the power of ML in accelerating material discovery for batteries. In the presentation, we will discuss various datasets, ML models employed for screening, and the validation procedures conducted.

11:30 AM

Surrogate Modeling of Cluster Dynamics-Predicted Nucleation and Growth of Irradiation Defects Using Time-Series Neural Networks: *Sanjoy Mazumder*[1]; Andrea Jokisaari[1]; [1]Idaho National Laboratory

A time-series based neural network model is presented, to predict the evolution of irradiation defects in structural materials, for application in modern fast reactors. Mean-field cluster dynamics (CD) has been extensively used to investigate the kinetics of nucleation and growth of extended defects, i.e., dislocation loops and voids in materials, under specific irradiation conditions. CD is computationally expensive to predict the population of TEM-observable large defects. The interaction of irradiation defects with microstructural features like grain-boundaries and network dislocations increases the model complexity. Also, the input parameter space expands to define the unirradiated microstructure. We have performed selection of input parameters based on sensitivity analysis of the CD predictions. A long short-term memory network (LSTM) has been trained with the CD-predicted time-series data, for the chosen parameters, to capture the temporal evolution of defects. High-throughput CD simulations were performed to generate the training and validation dataset for the LSTM model.

11:50 AM

Hierarchical Bayesian Modeling for Enhanced Contamination Detection in Electron Beam Powder Bed Fusion Processes: *Temilola Gbadamosi-Adeniyi*[1]; Tim Horn[1]; [1]North Carolina State University

Contamination in Electron Beam Powder Bed Fusion (EB-PBF) critically affects material integrity and component performance. Leveraging advancements in Total Electron Emission (TEE) data, which reveal material composition, contrast, and topography, this study introduces a hierarchical Bayesian model to detect and quantify contamination across all EB-PBF layers. The model proficiently distinguishes between the presence and absence of contamination at each spatial location and layer. Incorporating a Gaussian Process (GP) captures spatial correlations, ensuring the generation of coherent contamination maps throughout the build. Preliminary results demonstrate the model's effectiveness in accurately identifying contamination-free regions, reliably detecting intentionally introduced contamination, and quantifying contamination spread in subsequent layers. Posterior predictive checks validate the model's robustness, showing strong alignment between simulated TEE signals and observed data. This hierarchical Bayesian framework offers a scalable and interpretable solution for enhancing process monitoring and quality control in additive manufacturing processes.

3rd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2025): Development of Novel ML Methodologies III

Tuesday AM
June 17, 2025

Room: Room B
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Introductory Comments

9:10 AM
The Variational Deep Materials Network: Efficient Extrapolation With Uncertainty of Homogenized Material Responses: *Andreas Robertson*[1]; Dongil Shin[2]; Remi Dingreville[1]; [1]Sandia National Laboratory; [2]POSTECH

Surrogate models are a fundamental component in any machining learning framework for materials science. They provide the necessary computational efficiency for many downstream tasks, e.g., optimization in design. Importantly, useful surrogate models must be developed to account for both uncertainty and limited data. The Deep Material Network is a physics-informed machine learning framework that can stably extrapolate to predict non-linear homogenized material responses even though it is trained on only cheap elastic data. We present our extension: the Variational DMN. The VDMN naturally accounts for aleatoric microstructural uncertainty in its prediction. Importantly, this uncertainty prediction also extrapolates, allowing the VDMN to quantify uncertainty in both linear and nonlinear material responses without the need for nonlinear data. We present the algorithmic advances necessary for these changes and then present a series of examples exploring the strengths and limitations of the VDMN as a tool for accelerated uncertainty quantification in materials science.

9:30 AM
Enhanced Resolution and Image Contrast in 3D XRM Data Using Deep Learning Based Reconstruction Methods: *Kaushik Yanamandra*[1]; Hrishikesh Bale[1]; Rajarshi Banerjee[2]; [1]Carl Zeiss Microscopy; [2]University of North Texas

Deep learning-based 3D reconstruction methods can greatly improve the achievable resolution in image quality in 3D X-ray computed tomography compared to traditional reconstruction methods by utilizing trained models that can eliminate noise and increase contrast. Furthermore, combination with scintillator-based magnification objectives this technique can push the boundaries of achievable resolution. There have been significant developments since the early versions of deep learning based reconstruction. By adopting approaches like synthetic prior in the training step, a significant improvement in image sharpness and overall image quality along with improved throughput has been achieved. Results obtained from this new method are demonstrated on a model Ni-Ti-C based Metal Matrix Composites sample, wherein the complex microstructure and alignment of reinforcing titanium carbide (TiC) phases within the nickel matrix was revealed. This approach underscores the pivotal role of incorporating advanced deep learning-based reconstruction methods in pushing the boundaries of non-destructive 3D imaging characterizing advanced materials.

9:50 AM
MatCHMaker: Machine Learning for Microstructural Analysis in Materials Characterization Modeling: *Christian Precker*[1]; Andrea Gregores Coto[1]; Satiago Muíños Landín[1]; [1]AIMEN Technology Centre

The MatCHMaker project aims to reduce time, costs, and uncertainties in developing advanced materials, supporting the Green Deal's goal of industrial decarbonization and societal well-being. This initiative leverages materials modeling and characterization to create resilient new materials and discover novel uses for existing ones. By examining the relationships between processes, microstructure, and material properties, MatCHMaker helps predict and optimize material performance. Essential techniques, like Scanning Electron Microscopy (SEM), provide critical data on microstructures, which are analyzed using machine learning methods, including Convolutional Neural Networks and Autoencoders, to automate SEM image analysis. Focused on construction, energy, and mobility, the project integrates these ML tools to forecast materials' physical properties, ultimately developing a comprehensive materials characterization tool for industrial application. In this work, we present the progress done using ML methods to predict physical properties based on microstructure data.

10:10 AM
Metallographic Image and Mask Generation Based on Denoising Deffusion Probabilistic Models for Improving Metallographic Image Segmentation: Hoang-Hai-Nam Nguyen[1]; Juwon Na[1]; *Ho Won Lee*[1]; Jaimyun Jung[1]; [1]Korea Institute of Materials Science

Microstructure segmentation is pivotal in materials science and metallurgy, providing insights essential for understanding and enhancing material properties. However, the scarcity of high-quality datasets poses significant challenges to developing robust segmentation models. To address this limitation, we leverage the capabilities of Denoising Diffusion Probabilistic Models (DDPMs), which have demonstrated superior generative performance in various engineering applications and literature, with our approach incorporating a strong attention mechanism for enhanced results. Our approach introduces an image-conditioned DDPM framework, enabling the generation of high-resolution metallographic images and corresponding segmentation masks conditioned on specific input images. By incorporating these synthetic metallographic images and masks into original dataset, we observed improvements in segmentation accuracy, highlighting the potential of image-conditioned DDPMs to bridge data gaps and enhance downstream segmentation performance. This offers a promising pathway for developing more reliable image segmentation pipelines, thereby empowering the materials science community with enhanced tools for microstructure analysis and classification.

10:30 AM Break

10:50 AM
MLOgraphy++: A Context-Enhanced U-Net Approach for Robust Grain Boundary Segmentation in Metallographic Images: Inbal Cohen[1]; Julien Robitaille[2]; Francis Quintal Lauzon[2]; Ofer Beeri[3]; Shai Avidan[1]; *Gal Oren*[4]; [1]Tel Aviv University; [2]Clemex Technologies; [3]IAEC; [4]Stanford

Our work addresses the challenge of accurately identifying grain boundaries in metallographic images, where intricate texture boundaries complicate segmentation. Current state-of-the-art models, such as the Segment Anything Model (SAM), require prompts based on prior grain knowledge, limiting their usability in texture-only segmentation tasks. Manual annotation is also time-consuming and subjective. Existing methods often rely on small, annotated patches with post-processing steps, which can lead to overfitting and reduced generalizability. We introduce MLOgraphy++, a U-Net-based approach that leverages large context windows with partial labels, eliminating the need for post-processing. MLOgraphy++ effectively handles incomplete boundaries during inference by training with contextual variation. Using the Heyn intercept method as a more representative evaluation metric, we benchmark MLOgraphy++ against the state-of-the-art MLOgraphy on the Texture Boundary in Metallography (TBM) dataset, showing it achieves comparable results while enhancing generalizability and eliminating post-processing requirements.

11:10 AM

Synthetic Microstructure Generation and Prediction Using Stable Diffusion: Hoang Cuong Phan[1]; Hoheok Kim[1]; Sehyeok Oh[1]; *Ho Won Lee*[1]; [1]Korea Institute of Materials Science

Diffusion models like Stable Diffusion XL (SDXL) excel in generating high-quality images but face challenges in adapting to specific domains with limited data, such as microstructure generation in materials science. This study presents a novel SDXL-based framework, optimized with Low-Rank Adaptation (LoRA) and DreamBooth techniques, to both generate and predict microstructure images across seen and unseen experimental parameters with minimal computational demand. By selectively fine-tuning the UNet and text encoders, with targeted modifications and optimal hyperparameters, our method accurately captures intricate microstructure characteristics. It enables controlled image generation across varied process parameters, such as temperature, annealing time, and cooling methods, thereby reducing the need for additional experimentation. Rigorous evaluations demonstrate that our approach outperforms benchmarks in both image quality and fidelity to real microstructures. This scalable strategy addresses data scarcity and costly experimentation, enabling extensive, high-quality dataset generation with predictive capabilities applicable to broader scientific domains.

11:30 AM

Transfer Learning for Ultrasonic Crystallography: Accelerating Orientation Mapping in Materials With Neural Networks: *Rikesh Patel*[1]; Wenqi Li[1]; Richard Smith[1]; Matt Clark[1]; [1]University of Nottingham

In determining the crystallographic orientation using ultrasound measurements, brute force search algorithms are used to match measured surface acoustic wave phase velocities to crystallographic orientation. This process can take hours as it is computationally intensive. We introduce a method to transfer train neural networks using calculated surface acoustic wave (SAW) phase velocities to rapidly determine crystallographic orientations. For demonstration, a model has been trained using nickel SAW phase velocities, which achieved 93.6% in validation accuracy, and applied it to classify the planes on Inconel 617 and CMX4 polycrystalline alloys. Measurements were made using the laser ultrasound technique Spatially Resolved Acoustic Spectroscopy (SRAS) and full orientation maps were achieved on 1.4Mpixels in 16 seconds, compared with the brute force searching method that requires roughly 10 hours. This method aims to be a transformative tool for materials discovery by providing near real-time microstructural insights.

11:50 AM

Texture Evolution Surrogate for Magnesium Materials: *Kyle Farmer*[1]; Elizabeth Holm[1]; [1]University of Michigan

Understanding and predicting texture evolution in materials under deformation is essential for designing materials with targeted mechanical properties. Crystal plasticity simulations offer a robust method for predicting texture changes by modeling slip system activation and strain hardening behavior at the grain scale. However, the computational demands of crystal plasticity limit its application, especially for large-scale or high-throughput analyses. In this work, we present a deep learning-based surrogate model trained on finite element method (FEM)-based crystal plasticity simulations where magnesium - an underexplored material in texture surrogate development - polycrystals are deformed following an arbitrary strain path. Our model maintains high accuracy with a significant computational speedup over FEM simulations and demonstrates excellent scalability with respect to the system size and simulation settings.

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): ICME Application to Advanced Manufacturing I

Tuesday AM
June 17, 2025

Room: Room E
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Invited

ICME Tools for In-Space Welding: *Ellis Crabtree*[1]; Andrew O'Connor[1]; Fredrick Michael[1]; Louise Littles[1]; Jeffrey Sowards[1]; [1]NASA Marshall Space Flight Center

The recent boom of the in-space economy has demonstrated need for continued development of electron beam welding (EBW) and laser beam welding (LBW) processes, which are desirable for their compactness, low mass, low power consumption, and high wall plug efficiency. Demonstrating, developing, and applying welding processes is physically difficult, and costs are high to develop and fly individual space-based trials. This drives the current approach to develop ICME physics-based models in tandem with CALPHAD techniques. In this work, a thermal model of Skylab EBW experiments is established and compared to empirical data. The model is used to show variation between Earth-based and in-space weld structure and properties through exploration of key variables that define the Low earth orbit and lunar surface space environments, namely temperature, pressure, and gravity. Finally, physical processes associated with heat and mass transport during welding are evaluated through several case studies demonstrating need for further research.

9:30 AM

An ICME Approach to Establish Causal Links Between Process Induced Microstructures and Material Properties in Austenitic Steels: *Sourabh Supanekar*[1]; Hector Basoalto[1]; [1]University of Sheffield

Integrated Computational Materials Engineering (ICME) offers a robust framework for quantifying the causal relationships between welding process parameters and resulting material properties, a critical capability for optimizing engineering performance. This study develops a multiscale, physics-based material model to predict the impact of key welding parameters—including power and velocity of heat source input —on microstructural evolution and mechanical properties in austenitic steels. By integrating cellular automaton (CA) techniques with finite element analysis (FEA), we accurately simulate process-induced microstructures and the distribution of residual stresses within the welded joints. These simulations establish causal links between welding parameters and finalproperties, allowing for precise prediction and control of material properties such as hardness, toughness, and fatigue resistance. This ICME-driven methodology highlights the potential of computational models to advance materials design and process optimization in welding, leading to enhanced reliability and performance across manufacturing applications.

9:50 AM

Material Physics Governing Rotary Friction Welding: *Miguel Espadero*[1]; Hector Basoalto[1]; Simon Bray[2]; Peter Steven[2]; [1]University of Sheffield; [2]Rolls-Royce plc

The aim of this study is to develop a physics-based constitutive framework which enables the simulation of the thermo-mechanical fields and the microstructural evolution during rotary friction welding of precipitate-strengthened nickel-based superalloys. The primary objective is to describe the micro-mechanisms governing the flow stress behaviour during the different welding phases of the inertia welding process. A dislocation slip model has been proposed which considers the dislocation-precipitate interactions in the derivation of the plastic shear strain rates. The model has successfully studied the effect of the different materials variants for the same weld, showing it is able to replicate the response observed in experiments. One of the most valuable aspects of the framework is its ability to analyse model variables as plastic strain, volume fraction or dislocation density. By doing this, a deeper understanding of the underlying mechanisms at each stage of the process can be achieved.

10:30 AM Break

10:10 AM

Particle Simulation for Powder Metallurgy Hot Isostatic Pressing: *Sam Reeve*[1]; Pablo Seleson[1]; Austin Isner[1]; Yousub Lee[1]; [1]Oak Ridge National Laboratory

We demonstrate CabanaPD, a unified simulation tool for powder-based advanced manufacturing, focusing on powder metallurgy hot isostatic pressing (PM-HIP). PM processing routes are crucial for complex component manufacturing. Simulation for powder filling and powder consolidation for PM-HIP is primarily done today with the discrete element method (DEM) and finite element method (FEM), respectively. For both, CPU-only codes, GPU codes which are not portable across hardware architectures, and/or commercial codes are used, substantially limiting the applicability for the potentially billions of particles necessary for filling and consolidation of industrially relevant components. CabanaPD, an open source peridynamics code, has recently been expanded for PM-HIP including a new DEM module for powder filling, expanded boundary conditions, models for continuum powder consolidation, and conversion from powder to continuum scales. CabanaPD builds on the Cabana and Kokkos libraries for scalability and performance portability enabling simulation from local workstations to U.S. Department of Energy leadership supercomputers.

10:50 AM

A Mechanistic Deposition Efficiency Model for Cold-Spraying Dissimilar Materials: *Christian Brandl*[1]; [1]The University of Melbourne

Cold spray (CS) composite coatings created from mixed powders can demonstrate improved strength and corrosion resistance compared to coatings made from pure metals. However, controlling the deposition performance and the resulting microstructure during the cold spray process is challenging because the complex relationship between the different material properties dictates additional process constraints.This study combines mechanistic models for particle impact velocities and critical velocities necessary for particle adhesion to predict the formation of CS layers for relevant processing parameters. The findings outline the implications for composition gradients and the optimal operating parameters. Our model enables us to identify the required processing conditions and constraints for metal matrix composite coatings within Integrated Computational Materials Engineering frameworks to optimise processing for targeted material performance.

11:10 AM

Multiscale Computational Framework for Optimization of Processing Parameters in Shear-Assisted Processing and Extrusion (ShAPE) of Nuclear Cladding Materials: *Lukasz Kuna*[1]; Lei Li[1]; Shadab Shaikh[1]; Mageshwari Komarasamy[1]; Mohan Sai Kiran Kumar Yadav Nartu[1]; Jens Darsell[1]; Isabella van Rooyen[1]; Stuart Malloy[1]; Ayoub Soulami[1]; [1]Pacific Northwest National Lab

This work aims to develop a multiscale and multiphysics computational framework to reveal insight into the process-structure-property relationship in shear-assisted processing and extrusion (ShAPE) of nuclear cladding materials for applications in challenging environments. In the developed framework, ShAPE is simulated using meshfree smoothed particle hydrodynamics (SPH) to obtain thermomechanical responses at the macroscale and utilized to inform thermodynamic simulations at the mesoscale. The temperature and strain data predicted by the SPH model serve as inputs to a mesoscale phase field and crystal plasticity (PF-CP) coupled model to simulate microstructure and texture evolutions, as well as the processed material residual properties. Ultimately, the multiscale SPH-PF-CP model will be validated with experimental data and used to establish process-structure-property relationships. The multi scale framework will inform optimization of ShAPE processing parameters to achieve desired microstructures for various types of high entropy alloys and oxide dispersion-strengthened steels.

11:30 AM

Utilizing Crystal Plasticity Surrogate Models in Finite Element Analysis of Incremental Sheet Forming: *John Weeks*[1]; Aaron Stebner[1]; [1]Georgia Institute of Technology

Incremental sheet forming (ISF) demonstrates increased design flexibility, cost-effectiveness, and expanded design spaces for small-lot productions compared to conventional forming. During ISF, targeted deformation processing enables local material properties and microstructures which may be modeled using ICME techniques such as multiscale crystal plasticity (CP) simulations. However, multiscale modeling of ISF is expensive due to changing contact definitions, large deformations, and evaluation of CP models. In this work, we use a recurrent neural network as a surrogate model for CP to enable efficient multiscale ISF simulations. We integrate a visco-plastic self-consistent CP model (VPSC8) into a finite element framework (ABAQUS/Explicit) via a VUMAT. We demonstrate an effective workflow for data generation, training, validation, and implementation for multiple materials. This approach is applied to FCC aluminum to show the advantages of ICME in modeling these processes and how this approach can be used to guide design decisions in ISF.

11:50 AM

Performance Analysis of Different Shaped Tool Electrodes During Ultrasonic Assisted Electrical Discharge Machining (UAEDM) of Inconel 718: *Shankar Singh*[1]; [1]Sant Longowal Institute of Engineering & Technology (SLIET), Longowal

Ultrasonic Assisted Electrical Discharge Machining (UAEDM) is a hybrid machining process in which small amplitude vibrations of ultrasonic frequency are imparted to either electrode, work material or dielectric fluid in conventional EDM process, for effective flushing, hence leading to improved efficiency and consistency. The present study presents UAEDM of Inconel 718 work material. During experimentation, process parameters namely copper tool electrode geometry (circular and square) vibrated at 20 KHz frequency, discharge current, servo voltage, pulse on duration, pulse off duration and tool lift time were varied to find their effect on response characteristics i.e., material removal rate, surface roughness and electrode wear rate. Experiments have been performed according to Taguchi's L18 mixed-level orthogonal array. Multiple objective optimization of performance characteristics have been done using Taguchi based Grey Relational Analysis (TGRA) technique. Furthermore, surface morphology, metallurgical characteristics (Phases, crystallite size) and microhardness of the machined surface are also studied.

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): PSP Linkages: Multiscale/Multiphysics Modeling III

Tuesday AM
June 17, 2025

Room: Room F
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Invited
Integrated Computational Materials Engineering (ICME) Impacts on Industry and New Frontiers in Digital Transformation: *Jeff Grabowski*[1]; [1]QuesTek Innovations LLC

QuesTek Innovations is both an original pioneer and current market leader in Integrated Computational Materials Engineering (ICME) technologies. Key strategic drivers such as Digital Transformation, Industry 4.0 technologies and emerging "Materials 4.0" initiatives are moving the ICME marketspace, and QuesTek is at the forefront of the dialogue. This presentation will provide an overview of ICME technologies, success stories of using ICME to design novel advanced materials and optimize legacy materials for improved performance, and the significant impacts on a wide range of industries and innovative companies such as SpaceX and Apple. QuesTek's new ICME-based software (ICMD®) and its capabilities will be reviewed, along with how early subscribers have already begun to use ICMD® on priority programs to resolve materials and manufacturing challenges and accelerate materials development. ICMD® leverages genomic datasets, physics-based mechanistic models and methodologies, proven over 25 years of services engagements.

9:30 AM
Phase-Filed Multi-Physics Modeling and Simulations for Granular/Dendritic Fragmentation: *Gensei Kobayashi*[1]; Mitsuteru Asai[2]; Shinji Sakane[1]; Tomohiro Takaki[1]; [1]Kyoto Institute of Technology; [2]Kyushu University

Granular or dendritic fragmentation that occurs in semi-solid deformation has great potential to refine the solidification microstructure. However, the detailed fragmentation mechanism in such a semi-solid state is yet to be fully understood due to the complexity of the phenomenon. To elucidate the mechanism, the numerical simulation is essential. In this study, we developed a multi-physics model and its simulation method that reproduces fragmentation in the semi-solid state. In the model, solid morphological change and grain boundary formation are represented by phase-field method, liquid flow is represented by lattice Boltzmann method, and solid deformation and motion are represented by material point method. Through some simulations, we investigated the ability of the method for expressing the fragmentation.

9:50 AM
Semi-Solid Deformation Simulations for Prediction of Segregation Band Using Multi-Phase-Field Lattice Boltzmann Model: *Namito Yamanaka*[1]; Shinji Sakane[1]; Tomohiro Takaki[1]; [1]Kyoto Institute of Technology

During metal casting, semi-solid materials deform under external forces, leading to solidification defects. In particular, external shear forces induce shear band formation through grain contact and rearrangement, directly affecting the formation of segregation band, thus accurate prediction and control of this phenomenon are desired. In this study, we developed the evaluation method for semi-solid simple shear deformation using the multi-phase-field lattice Boltzmann model to clarify where and how shear band is formed. Through the simulations with this method, we examined the effects of solid fraction, deformation rate, and grain morphology, which significantly impact shear band formation. The simulations also offered detailed insights into the size, position, and formation mechanism of shear band.

10:10 AM
Benchmarking Massively Parallel Phase-Field Codes for Alloy Solidification: *Jiefu Tian*[1]; David Montiel[2]; Kaihua Ji[3]; Trevor Lyons[1]; Jason Landini[2]; Katsuyo Thornton[2]; Alain Karma[1]; [1]Northeastern University; [2]University of Michigan; [3]Lawrence Livermore National Laboratory

Phase-field (PF) modeling is a powerful method for simulating solidification microstructures in processes ranging from casting to additive manufacturing. Massively parallel PF simulations must be conducted on high-performance computing platforms to access experimentally relevant length and time scales. However, direct comparisons of high-performance PF codes are rare, except for those based on simplified benchmarking problems. This study benchmarks two state-of-the-art PF codes through direct quantitative comparison of their predictions for 3D convection-free directional solidification of a binary alloy for which microgravity experimental benchmark data is available: GPU-PF, a CUDA-based finite difference code utilizing GPUs, and PRISMS-PF, an MPI-based open-source finite element code with adaptive meshing. The comparison shows that both codes produce essentially identical microstructures but differ in their performance and convergence as a function of mesh size. This comparison highlights each tool's unique strengths and reinforces their value in advancing PF modeling for alloy design within an ICME framework.

10:30 AM Break

10:50 AM
Fractal Structure Development and Simulation in Spinodal Phase Change: *Rahul Basu*[1]; [1]UGC, JNTU

The study of spinodal decomposition, has attracted significant attention. A novel approach to simulating fractal-like structures arising from spinodal phase changes is developed. The intricate patterns formed during phase separation and dependencies on initial conditions and material properties are investigated. Utilizing advanced computational techniques, a phase-field model captures the dynamics of spinodal decomposition in multi-component systems. Simulations reveal that the resulting fractal structures exhibit self-similarity and scale invariance, suggesting underlying universal behaviors govern formation. The time dependencies and radii of of these fractal microstructures are compared with traditional microstructures. Both 2D (thin film) and 3D (bulk) simulations are attempted. Our findings demonstrate that the fractal characteristics mimic the intricate patters obtained in Spinodal transformations. These can significantly enhance material performance, offering pathways for the design of advanced materials with tailored properties. This sets the stage for future explorations in the synthesis and application of fractal materials in various technological domains.

11:10 AM
Convolution Tensor Decomposition Method for Efficient High-Resolution Solutions to the Allen-Cahn Equation: *Ye Lu*[1]; [1]University of Maryland Baltimore County

The Allen-Cahn equation is widely used to characterize phase separation or the motion of anti-phase boundaries in materials, under the framework of phase field modeling. Its solution is known to be time-consuming when high-resolution meshes and large time scale integration are involved. To overcome this challenge, we propose a convolution tensor decomposition based model reduction method [1] for efficiently solving the Allen-Cahn equation. Numerical examples using both 2D and 3D Allen-Cahn type problems will be presented for demonstrating the performance of the method. The proposed computational framework opens numerous opportunities for simulating complex microstructure formation in materials on large-volume high-resolution meshes at a deeply reduced computational cost. Reference:[1] Lu, Ye, Chaoqian Yuan, and Han Guo. "Convolution tensor decomposition for efficient high-resolution solutions to the Allen–Cahn equation." Computer Methods in Applied Mechanics and Engineering (2025).

11:30 AM

Phase Field Simulation of Segregation in Single Crystal Ni-Based Superalloys and Its Influence on Creep Properties: *Sean Böhm*[1]; Andre Borsatto Baldissera[1]; [1]Univerity of Bayreuth

Ni-based superalloys exhibit inhomogeneous microstructures dependent from the manufacturing route, thus resulting in inhomogeneous properties such as tensile strength and creep strength. Hence, combined FEM and phase-field simulation models are developed. The simulation models allow to determine the influence of casting parameters and subsequent heat treatment parameters on local microstructures of Ni-based superalloys. The combined simulation models are calibrated on the Ni-based superalloy CMSX4. CMSX4 contains gammaprimeforming elements Al, Ti and Ta, which segregate in the interdendritic regions, and slow diffusing elements Re or W, which segregate in the dendrites. The segregations influence the solid solution hardening and gammaprime precipitate structure, resulting in local differences in crystal properties. The combined simulation models predict local i.e. position dependent creep properties as well as global creep properties. The combined simulation models thus establish a link between process and heat treatment parameters and creep properties.

11:50 AM

Overview of "NASA Biological and Physical Sciences (BPS) Reduced Gravity and Microgravity Integrated Computational Materials Engineering (ICME) Study Final Report": *Louise Littles*[1]; [1]NASA MSFC

NASA's push for advanced materials and processes in space and terrestrially, as captured in the latest National Academy of Sciences Decadal Survey on Biological and Physical Sciences Research in Space has underscored the need for BPS engagement with the ICME community. BPS and its predecessors have sponsored extensive flight and ground experiments yielding benchmark datasets including thermophysical properties and solidification. An overview is provided of a recent report highlighting critical research areas such as meso-scale bridging to grain-structure and coupling of fluid flow and solidification where benchmark materials science experiments conducted in the quiescent and microgravity environment are case studies. Rapid improvements in compute power and diversity are enabling linked simulations from micro- through mesoscale. A variety of accomplishments and findings resulted from this confluence of academia, industry, and government experts. The recommendations of the report provide a path to pursue ICME as an evolution of BPS projects.

The 7th International Congress on 3D Materials Science (3DMS 2025): 3D Data Processing, Software, and Reconstruction Algorithms II

Tuesday AM
June 17, 2025

Room: Room D
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Invited

A Polycrystalline X-Ray Virtual Diffractometer for Direct Comparisons to Experimental Data: *Sven Gustafson*[1]; Paul Dawson[2]; Matthew Miller[2]; Kelly Nygren[1]; [1]Cornell High Energy Synchrotron Source; [2]Cornell University

Micromechanical modeling routinely simulates spatially resolved fields for polycrystals with thousands of grains undergoing continuous in-situ deformation; however, current experimental techniques cannot probe such fields within all grains with the spatial, angular, and temporal resolution to facilitate direct comparison. Current reconstructions only extract grain averaged information even though experimental detector images from far-field high energy diffraction microscopy contain relevant spatially resolved information and the technique operates with sufficient temporal resolution. To facilitate an experiment to model comparison, a finite element based virtual diffractometer is presented here to produce realistic diffraction images from model generated microstructures, a spatially resolved x-ray beam, and a pixelated detector. The functionality of the virtual diffractometer is demonstrated with experimental to virtual detector image comparisons for an ideal crystal. The evolution of detector image data from an in-situ mechanical test is then compared with a virtual diffraction simulation of the corresponding model generated microstructure.

9:30 AM

Advancing 3D Grain Mapping Accessibility for the Materials Science Community: Insights into Recent Developments of Data Acquisition, Reconstruction and Analysis: *Jun Sun*[1]; Florian Bachmann[1]; Mario Heinig[1]; Frank Niessen[1]; Jette Oddershede[1]; Erik Lauridsen[1]; [1]Xnovo Technology

Mapping the 3D-spatial crystallographic orientation of polycrystalline materials holds tremendous value for 3D materials science and related phenomena, as the properties and performance of materials are intricately linked to their 3D microstructural morphology. 3D non-destructive crystallographic imaging techniques emerged at synchrotron light sources in the early 2000s, and substantial efforts have been made over the past decades to establish and optimise X-ray diffraction contrast tomography (DCT) into the laboratory setup, with the mission to achieve wide accessibility for materials scientists to non-destructive 3D grain mapping techniques.In this talk, we will present the recent developments of lab-based 3D grain mapping responding to the needs of the 3D materials science community, including: 1) advanced diffraction data acquisition allowing characterisation of large, representative sample volumes, 2) reconstructing multiple crystalline phases allowing a wider coverage of sample systems, and 3) challenges and approaches in processing and analysis of 3D grain maps.

9:50 AM

Comparative Analysis of Reconstruction Methods for Lab-Scale X-Ray Computed Tomography of 3D Defects in Semiconductor Packages: Eshan Ganju[1]; Yaw Obeng[2]; William Harris[3]; Charles Bouman[1]; Gregery Buzzard[1]; *Nikhilesh Chawla*[1]; [1]Purdue University; [2]NIST; [3]Zeiss

Rapid co-design of semiconductor packages necessitates an efficient and non-destructive metrology to detect defects. Lab-scale X-ray Computed Tomography systems, while valuable, face challenges such as long scan times due to limited x-ray flux and imaging artifacts arising from density variations and reconstruction methods. This study critically evaluates three distinct reconstruction techniques for lab-scale XCT data: Filtered Back Projection (FBP), Model-Based Iterative Reconstruction (MBIR), and Deep Learning (DL) approaches. FBP serves as the baseline for comparison. MBIR leverages physical models and noise statistics to enhance image quality and potentially reduce scan times. DL methods, trained on extensive datasets, offer a data-driven approach to reconstruction. Reconstruction performance was assessed through quantitative metrics, scan and reconstruction time, and signal-to-noise ratio. The advantages and limitations of each method are discussed in detail, supplemented by visual assessments of exemplars in semiconductor packages, to provide insights into their suitability for high-fidelity lab-scale XCT semiconductor packaging applications.

10:10 AM
Optimizing CT Image Quality With Deep Learning for Enhanced 3D Materials Science Applications: *Parisa Asadi*[1]; Adrian Sarapata[1]; Andriy Andreyev[1]; [1]Zeiss

X-ray computed tomography (CT) is fundamental to non-destructive 3D imaging, though image quality is often hampered by noise. This study examines the benefits of FAST Mode image acquisition (ability to scan in 20 seconds) for rapid sample inspection and DeepRecon Pro 3D-image reconstruction, a deep learning-based noise reduction method adaptable to various imaging conditions. Using a U-Net architecture, DeepRecon Pro processes projection images or volumes to produce noise-suppressed, high-fidelity reconstructions, outperforming traditional techniques like FDK and non-local means (NLM). The latest DeepRecon version integrates synthetic priors and a two-stage training process, introducing noise-matching models that further enhance accuracy. Quantitative metrics, including mean square error (MSE) and structural similarity index (SSIM), highlight DeepRecon's effectiveness across diverse noise intensities and projection counts. These advancements support faster, more accurate CT imaging for critical 3D materials science applications where precision and efficiency are paramount.

10:30 AM Break

10:50 AM
PolyProc: A Computational Package for Processing 3D/4D PolyCrystalline Microstructure Data: *Varun Srinivas Venkatesh*[1]; Marcel Chlupsa[1]; Ashwin Shahani[1]; [1]University of Michigan

Direct imaging of three-dimensional microstructures with X-ray diffraction techniques yields valuable insights into the crystallographic features that influence material properties and performance. Incorporating a temporal dimension allows for direct observations of the microstructural evolution. As these techniques and datasets become more widely available, the demand for processing inherently noisy, multi-dimensional, and multimodal data has increased. To address this demand, we present recent updates to the *PolyProc* package, a suite of algorithms that parse the full breadth of microstructure, including the grains, interfaces, and triple junctions, as well as time-resolved statistics. We introduce several new capabilities, including the quantification of grain boundary curvatures and velocities; grain boundary character and normal distributions; and grain boundary and triple junction percolation analyses. Finally, we present a novel algorithm that utilizes grain neighborhood information to track the same grains in time. Altogether, these advancements streamline the analysis and visualization of 3D/4D microstructural data.

11:10 AM
Informed Unsupervised Machine Learning Analysis of Dislocation Microstructure From High-Resolution Differential Aperture X-Ray Structural Microscopy Data: *Khaled SharafEldin*[1]; Bryan Miller[2]; Wenjun Liu[3]; Jon Tischler[3]; Benjamin Anglin[2]; Anter El-Azab[1]; [1]Purdue University; [2]Naval Nuclear Laboratory; [3]Advanced Photon Source, Argonne National Laboratory

This study leverages high-resolution Differential-Aperture X-Ray Structural Microscopy (DAXM) to probe the local microstructure and strain at sub-micron resolution in deformed 304 steel at 2% strain. We developed a machine learning technique to understand the multimodal statistical nature of the lattice rotation lattice rotation and deviatoric elastic strain. The multi-peak nature of the rotation distribution measured over a disoriented grain not aligned with the loading axis of a polycrystalline specimen was fit to a collection of multi-variate Cauchy distributions, which were then mapped back to form a contiguous regions of the crystal rotated near the average values of each distribution, representing the coarsest grain subdivision scale. The dislocation density tensor was also extracted, and its norm was laid over the rotation field to confirm the subgrain boundaries. This study highlights the potential of integrating advanced X-ray microscopy techniques with data-driven analysis methods to uncover detailed microstructure scales in deformed crystals.

11:30 AM
Real-Time 3D Visualization of Eutectic Solidification Dynamics Using Limited Angle Tomography: *Soumyadeep Dasgupta*[1]; Paul Chao[2]; Xianghui Xiao[3]; Ashwin Shahani[1]; [1]University of Michigan; [2]Sandia National Laboratory; [3]Brookhaven National Laboratory

Multi-phase 3D structure from eutectic solidification brings versatile properties to alloys. By studying solidification in real-time, we gain insights into interfacial dynamics, enabling improved control and design of advanced materials. Synchrotron X-ray nanotomography provides a 3D perspective of microstructural evolution at the nanoscale; however, its temporal resolution is constrained by factors, e.g., the microscope hardware capabilities, sample shape etc. To achieve sub-10s temporal resolution, we employ Limited Angle Tomography (LAT). Using LAT, we investigate the directional solidification of a near-eutectic Al-AlNi alloy as a proof-of-concept. A novel composite reconstruction approach termed 'pseudo-4D imaging' mitigates artifacts inherent to LAT, allowing us to visualize the solidification process in 3D space and time. This technique relies upon data fusion of real-time radiographs with postmortem 3D reconstruction of the fully-solidified specimen. The approach holds promise not only for solidification science but also for the 3D characterization of other time-sensitive phenomena within constrained viewing windows.

The 7th International Congress on 3D Materials Science (3DMS 2025): Time Resolved 3D Characterization I

Tuesday AM
June 17, 2025

Room: Room C
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Invited
Capturing Grain Boundary Migration in Polycrystals: *Amanda Krause*[1]; [1]Carnegie Mellon University

Curvature is considered the common local driving force for grain boundary motion in all polycrystals. However, models and simulations derived from curvature-based motion cannot predict irregular, albeit commonly observed, grain growth behavior. This talk will highlight how 3D x-ray diffraction microscopy methods provide new insights for enabling microstructural design. 3D x-ray diffraction microscopy methods are non-destructive and map the full microstructure, providing an opportunity to observe grain growth in real 3D polycrystals. In this talk, experimental observations of growth in strontium titanate, alumina, and nickel will be compared to Monte Carlo Potts simulations to interrogate the role of curvature and grain boundary energy in microstructure evolution. Then, potential descriptors for abnormal grain growth, in which a few grains maintain a growth advantage, in recrystallized pure nickel will be evaluated. The outstanding challenges and opportunities for using 3D x-ray diffraction microscopy to elucidate microstructural evolution will be discussed.

9:30 AM

On the Thermal Aging of the Nanoporous Structure of Sintered Ag on a Cu Substrate: *Xavier Milhet*[1]; Jerome Colin[2]; Kokouvi Happy N'Touaglo[1]; Adine Nait Ali[1]; Loic Signor[2]; [1]Pprime Institute Cnrs Ensma; [2]Institut Pprime Cnrs Université de Poitiers

As power modules are a complex assembly of different materials, all of them having different coefficients of thermal expansion, a fine evaluation of the evolution of the materials and interfaces is necessary. In this work, time resolved evolution (4D) of the nanoporous microstructure of sintered Ag (s-Ag) and sintered Ag on Cu (s-Ag/Cu) during thermal aging was monitored at high temperature using in-situ X-ray nanotomography. For both types of specimen, the density of S-Ag remains constant, the evolution is driven by the bigger pores and the pore growth follows the Ostwald ripening mechanism. Faster kinetics of growth is observed for s-Ag/Cu before deviating from Ostwald ripening after a critical time. Furthermore, complex evolutions in small pores clusters can be observed in both type of specimens. Those behaviors are discussed based on diffusion mechanisms in relation with a competition between local stresses relaxation and surface energy during diffusion.

9:50 AM

Polycrystalline Effects on Early Strain Heterogeneity Leading to Fracture for an Aluminium Alloy Under Plane Strain Tension: 3D Correlative X-Ray Tomography and Crystal Plasticity Simulations: Maryse Gille[1]; Thilo Morgeneyer[1]; Jette Oddershede[2]; Romain Quey[3]; *Henry Proudhon*[1]; [1]Mines Paris-PSL; [2]Xnovo Technology ApS; [3]Mines Saint-Etienne

The internal strain heterogeneity leading to fracture is studied in an aluminium alloy under plane strain tension, which is a common failure state in stamping processes. The polycrystalline effects are investigated using multimodal X-ray lab tomography 3D data acquired on a miniaturized plane strain tensile specimen. The real microstructure in the center of the undeformed specimen is obtained non-destructively using lab-based diffraction contrast tomography. Crystal plasticity finite element (CP-FE) simulations are performed on the meshed microstructure. Besides, digital image correlation is performed in the material bulk using intermetallic particles visible in absorption contrast tomography data acquired during an in situ tensile test performed in 12 increments up to fracture. Strong correlations are found between the CP-FE predictions based on the meshed real grain structure and the measured strain fields. The early strain heterogeneity in form of spatially stable slanted bands as precursor of final fracture is attributed to polycrystalline effects.

10:10 AM

Tracking the Dynamics of Strain-Energy-Driven Grain Growth in 3D: *Marcel Chlupsa*[1]; Zach Croft[1]; Katsuyo Thornton[1]; Ashwin Shahani[1]; [1]University of Michigan

Understanding microstructural dynamics under non-isothermal annealing is crucial for the manufacture of shape memory alloys (SMAs). This study examines how stored strain energy influences grain growth in a model CuAlMn SMA. Using synchrotron high-energy X-ray diffraction microscopy (HEDM), we map grains and precipitates in 3D over time, analyzing strain, grain boundary curvatures, and the relation between the two. We quenched the sample at three time-points in the heat treatment to acquire data. To complement these experiments, corresponding phase-field simulations address spatiotemporal gaps in the HEDM data. Departures from experimental observations, e.g., more compact grains, serve to highlight unique features associated with strain-energy-driven growth. Our combined experiments and simulations reveal significant variations in grain sizes, shapes, strains, and boundary curvatures over the course of the non-isothermal anneal. This work underscores the complexities of microstructural dynamics driven by stored strain energy, which are not fully captured by conventional theories or metallographic analysis.

10:30 AM Break

10:50 AM

Tracking the Emergence and Persistence of Abnormal Grain Growth in the Commercial Aluminum Alloy AA5252 Using 3D X-Ray Microscopy: *Helmuth-André Schulz-Harder*[1]; Jules Dake[1]; Wolfgang Ludwig[2]; Haixing Fang[2]; Pierre-Olivier Autran[2]; Karolína Gutbrod[1]; Carl Krill[1]; [1]Institute of Functional Nanosystems, Ulm University; [2]The European Synchrotron (ESRF)

Although abnormal grain growth (AGG) has far-reaching consequences for a wide range of industrial applications and has been investigated for decades, its origin is still not fully understood. One major obstacle is the lack of time-resolved 3D data regarding this phenomenon. To tackle this problem, we acquired time series of 3D maps of a commercial aluminum alloy AA5252 using synchrotron-based diffraction contrast tomography (DCT). The reconstructed grain maps reveal the presence of extreme abnormal grains, the evolution of which can be followed over time and even traced back to the point where they may have emerged. To gain more insight into the role of second-phase particles on the growth of abnormal grains, additional phase-contrast tomography (PCT) measurements were performed. Combining these two data sheds new light on the locations at which abnormal grains emerged and how they were able to maintain a persistent growth advantage.

11:10 AM

Intragranular Evolution of Slip System Strength and Activity in Titanium Using Point-Focused High-Energy Diffraction Microscopy: *Wenxi Li*[1]; Hemant Sharma[2]; Peter Kenesei[2]; Jun-Sang Park[2]; Sidharth Ravi[3]; Orcun Koray Celebi[3]; Daegun You[3]; Tolga Berkay Celebi[3]; Huseyin Sehitoglu[3]; Ashley Bucsek[1]; [1]University of Michigan; [2]Argonne National Laboratory; [3]University of Illinois at Urbana-Champaign

In-situ point-focused high-energy diffraction microscopy is used to non-destructively capture the deformation behavior of a millimeter-scale grain network in bulk commercially pure titanium with subgrain-scale spatial resolution. The intragranular crystallographic orientation, elastic strain, and slip system activity are tracked as the material is loaded in tension beyond the macroscopic yield point. The results are used to measure intragranular critical resolved shear stress values for prismatic and basal slip systems, which closely align with room-temperature values predicted by density functional theory. The local elastic strain and plastic shear strain maps are also used to investigate the heterogeneous nature of local plastic deformation. Analysis of the principal stress directions reveal that grain boundaries act as barriers to slip, leading to localized stress concentrations and driving stress redistribution. This study provides new insights into intragranular stress states, slip system activity, and grain–grain interactions, advancing the understanding of crystal plasticity in polycrystalline materials.

11:30 AM

Quantifying Ductile Fracture Mechanisms in AA2198-T851 Through Void Tracking of In-Situ Laminography Experiments: *Thomas Tancogne-Dejean*[1]; Christian Roth[1]; Thilo Morgeneyer[2]; Dirk Mohr[1]; [1]ETH Zurich; [2]MINES ParisTech, PSL University, Centre des Matériaux

Synchrotron laminography has proven to be an effective method for examining the nucleation, growth, and coalescence of voids at the material level. Here, monotonic experiments are conducted on AA2198-T8 using a laminography stage on a synchrotron X-ray line. The specimens tested include a "smiley" shear geometry, tensile specimens with notch and circular cut-outs, as well as a compact tension geometry, effectively spanning stress states from low (=0) to high (>>1) triaxialities. Multiple scans of the entire gage section with resolution of approximately 1μm^3 allow capturing the meso-structural evolution within the material in 3D up to fracture. Additional macroscopic experiments are used to identify parameters for a non-quadratic plasticity model with isotropic hardening. A novel two-step void tracking algorithm, leveraging finite element displacement fields and heuristics, is introduced to provide deeper insight into void nucleation, growth, and coalescence. It allows for the first time a quantitative analysis of respective void populations.

11:50 AM
Micromechanical Behavior of Fe-36Ni Invar Alloy at Cryogenic Conditions Characterized Using High Energy X-Ray Diffraction Microscopy: *Raghul Asok Kumar*[1]; Dhruv Anjaria[2]; Kenneth Peterson[1]; Reilly Knox[1]; Katherine Shanks[3]; Jean-Charles Stinville[2]; Darren Pagan[1]; [1]Penn State University; [2]University of Illinois Urbana-Champaign; [3]Cornell High Energy Synchrotron Source

Fe-36Ni Invar alloy is known to have enhanced ductility and tensile strength at cryogenic conditions and hence the alloy finds potential energy storage applications. However, in cryogenic conditions, the crystal-scale origins of these mechanical properties have not been probed for the want of appropriate characterization tools. Recent advancements in synchrotron testing capabilities enable the characterization of microstructure along with the mechanical behavior of individual crystals in polycrystalline metallic materials at low temperatures resembling service conditions. With the help of these advancements, here we track the evolution of grain-averaged lattice orientations and stress during in-situ mechanical loading of Fe-36Ni Invar alloy at 80K. These results are then compared with the material's micromechanical response at room temperature.

Joint Sessions of AIM, ICME, & 3DMS: Digital Twins for Manufacturing: Joint Session of AIM & ICME

Tuesday PM
June 17, 2025

Room: Joint Sessions Room
Location: Anaheim Marriott

Session Chair: To Be Announced

1:30 PM Invited
Toward Sentient Manufacturing: *Christopher Spadaccini*[1]; [1]Lawrence Livermore National Laboratory

By integrating manufacturing process simulation, computationally driven design approaches, in-situ diagnostics, non-destructive evaluation, rapid characterization, data analytics and machine learning, and digital twins, we may be able to reduce fabrication timescales and costs, while improving quality and repeatability of components. Individually, each of these areas are helping to advance manufacturing and materials deployment but together could be even more powerful. Ultimately, we envision component design through manufacturing to be part of a sentient ecosystem where autonomous, on-the-fly process adaptation and even design changes are possible during the manufacturing process itself. Each area that contributes to this vision can be individually explored; however, the true power of the concept will be in the integration. Integrating these elements of the ecosystem to create a more aware, or sentient, materials and manufacturing enterprise, would allow for fabrication corrections and design changes on-the-fly, radically advancing the state of the art.

2:00 PM
Digital Twins for Accelerated Materials Innovation: *Surya Kalidindi*[1]; [1]Georgia Institute of Technology

This presentation will expound the challenges involved in the generation of digital twins (DT) as valuable tools for supporting innovation and providing informed decision support for the optimization of material properties and/or performance of advanced heterogeneous material systems. This presentation will describe the foundational AI/ML (artificial intelligence/machine learning) concepts and frameworks needed to formulate and continuously update the DT of a selected material system. The central challenge comes from the need to establish reliable models for predicting the effective (macroscale) functional response of the heterogeneous material system, which is expected to exhibit highly complex, stochastic, nonlinear behavior. This task demands a rigorous statistical treatment and fusion of insights extracted from inherently incomplete, uncertain, and disparate data used in calibrating the multiscale material model. This presentation will illustrate with examples how a suitably designed Bayesian framework combined with emergent AI/ML toolsets can uniquely address this challenge.

2:20 PM
Manufacturing and Control of Fiber Reinforced Polymer Composites Through FMEA-Based Digital Twin: Arshdeep Singh[1]; *Soban Babu Beemaraj*[1]; Sooriyan Senguttuvan[1]; Amit Salvi[1]; [1]Tata Consultancy Services

Manufacturing high-quality polymer composite parts without rejection is critical, especially for aerospace and wind energy structures requiring precise temperature control. This paper presents a Failure Mode and Effect Analysis (FMEA) framework for composite manufacturing, implemented through a digital twin that monitors and controls the process. Using this digital twin, multiple process deviations and potential failure scenarios in composite manufacturing are modeled, and optimal corrective actions are computed to create the FMEA table. This digitally generated FMEA table is then used to detect anomalies in the physical manufacturing process. To simulate this process, a multi-scale cure kinetics model is developed to capture the part's thermo-chemical-mechanical state. Additionally, the Joule heating effect is modeled for resistive heating elements embedded in a PID-controlled molding tool. Demonstrated on a tapered laminated composite with multiple heating zones, this approach enhances quality control and ensures more efficient composite manufacturing.

2:40 PM
Harnessing Deep Learning Conditional Diffusion Models for Microscopy Modality Transfer of Light Optical Microscopy to Electron Backscattering Microscopy Diffraction Misorientations: *Nicholas Amano*[1]; Bo Lei[2]; Elizabeth Holm[1]; Dominik Britz[3]; Martin Müller[3]; [1]University of Michigan; [2]Lawrence Livermore National Laboratory; [3]Steinbeis-Forschungzentrum Material Engineering Center Saarland

Analyzing microstructures is essential in metallurgical science and manufacturing, prompting significant investment in the preparation and imaging of structured materials. In this research, we present a deep learning method that employs conditional diffusion models to generate the electron backscattered diffraction microscopy (EBSD) misorientation maps of quenched and tempered steel images from light optical microscopy (LOM) data. By leveraging the cost effective and relatively easy to produce LOM micrographs to generate high quality EBSD misorientation maps, we hope to accelerate the characterization step during steel manufacturing. This work is supported by a unique dataset of synchronized LOM and EBSD misorientation micrographs taken from the same sample locations and scales. We showcase diffusion models applicability to materials science imaging by reproducing EBSD misorientations from LOM images of highly complex multiphase steel. Our results indicate that diffusion models produce plausible and internally consistent EBSD misorientation mappings, but their absolute values are somewhat unreliable.

3:00 PM Break

3:30 PM
Modelling Physical-to-Virtual Feedback Flow of Digital Twins for Induction Furnace: *Maruthi Annamaraju*[1]; Surya R. Kalidindi[1]; [1]Georgia Institute of Technology

Digital Twins readily find applications in the manufacturing domain providing efficient real-time control through continuous updates using representative numerical models and sensor-based measurements of the manufacturing process. The focus of our work lies on modelling the physical-to-virtual feedback flow for a Digital Twin representing an Induction Furnace involved in an induction furnace/ultrasonic atomizer system used in processing metal powders by homogenizing and atomizing a binary molten metal system.Our framework involves (1) Numerical modelling; and (2) Gaussian Process-based emulators. The numerical model employs finite element solvers to compute electromagnetically driven non-isothermal molten metal flow and a phase-field model for the homogenization of the binary molten metal system. To calibrate the Digital Twin, we learn the discrepancy between the numerical model and sensor-based measurements using Gaussian Process-based emulators enhancing the predictive capability of the DT. Additionally, we show improvements in the estimates of model parameters calibrated using inverse modelling.

3:50 PM
Harnessing Multi-Modal Metrology Data for Predictive Modeling in Laser Powder Directed Energy Deposition: *Michael Juhasz*[1]; Eric Chin[1]; Youngsoo Choi[1]; Joseph McKeown[1]; Saad Khairallah[1]; [1]Lawrence Livermore National Laboratory

In this presentation, we utilize extensive multi-modal on-machine metrology data from Laser Powder Directed Energy Deposition (LP-DED) to create a robust surrogate model for the 3D printing process. By employing Dynamic Mode Decomposition with Control (DMDc), we capture the intricate physics within this dataset. Our physics-based model focuses on key thermodynamic parameters, enabling accurate predictions of critical outcomes. It integrates 21 process parameters, including laser power and scan rate, to predict outputs like melt pool temperature and size. The model also incorporates uncertainty quantification, providing reliable bounds on predictions and enhancing confidence in results. We validate the model by applying it to a new part and monitoring the printing process, finding that its predictions closely align with actual measurements. Prepared by LLNL under Contract DE-AC52-07NA27344.

4:10 PM
Generalized Graph Foundation Models as Versatile Data-Driven Digital Twins for Complex Technological Systems: *Pawan Tripathi*[1]; Benjamin Pierce[1]; Hein Aung[1]; Tommy Ciardi[1]; Kristen Hernandez[1]; Raymond Wieser[1]; Yangxin Fan[1]; Weiqi Yue[1]; Erika Barcelos[1]; Jayvic Jimenez[2]; Brian Giera[2]; Robert Gao[1]; Mengjie Li[3]; Kristopher Davis[3]; Laura Bruckman[1]; Roger French[1]; [1]Case Western Reserve University; [2]Lawrence Livermore National Laboratory; [3]University of Central Florida

Generalized graph foundation models offer a flexible approach to constructing data-driven digital twins (ddDTs) for complex technological systems. Unlike traditional, physics-based digital twins that require idealized models built from first principles, ddDTs leverage real-world data streams to provide adaptable and modular representations of system behavior. By using spatiotemporal graph neural networks (st-GNNs) as a foundation, ddDTs capture dynamic interactions and performance characteristics, allowing for accurate monitoring and prediction across a range of applications. This work introduces a unified pipeline to develop graph-based foundation models for diverse systems, including solar photovoltaic fleets, direct ink write additive manufacturing, and laser powder bed fusion. The proposed approach avoids the constraints of physics-based assumptions, enabling a single ddDT architecture to address various performance issues and operational questions without extensive reconfiguration. These foundation models streamline digital twin implementation, supporting efficient, data-driven decision-making in technologically complex environments.

3rd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2025): Applied ML for Manufacturing IV

Tuesday PM
June 17, 2025

Room: Room A
Location: Anaheim Marriott

Session Chair: To Be Announced

1:30 PM Invited
Modern Methods for Understanding the Electrochemical Stability of Inorganic Materials: *Joseph Montoya*[1]; [1]Toyota Research Institute

Electrochemical stability is a critical property of the materials we must develop in order to advance technologies that can help mitigate climate change, but deriving actionable insights from either machine learning or atomistic simulation can be challenging. In this talk, I will discuss recent progress in Toyota Research Institute's (TRI) efforts to predict electrochemical stability and to identify causes of electrochemical instability. I will survey topics ranging theory to practice, including (1) DFT-derived Pourbaix diagrams, how they've been made more efficient and more accurate, and can be extended to include effects of concentration and structure (2) design of catalysis experiments for variable electrolyte identities and concentrations and (3) modes of evaluating electrochemical performance stability from battery cycling data.

2:00 PM
Causality and Saliency in Unimodal and Multimodal Datasets: *Brad Boyce*[1]; [1]Sandia National Laboratories

Developing interpretable/explainable machine learned (ML) models will enhance our trust in the algorithms, expose their shortcomings, and guide us towards enhanced solutions. We will draw from five recent case studies on ML derived relationships in process-structure-property data. These five studies will illustrate distinct strategies towards interpreting ML models. The studies span two manufacturing methods: physical vapor deposition and laser powder bed fusion, and numerous data sources including both experimental data and synthetic data from simulations. Causality is interpreted through embedded physical models, saliency maps in image data, and through unsupervised clustering in mutli-modal datasets. Also, traditional forensic materials science, though laborious, provides a pathway to unravel cause-and-effect in high-performing materials identified by high-throughput exploration. Sandia is a multiprogram laboratory managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

2:20 PM
Advancing Data-Driven Uncertainties and Predictions of the Stress Strain Response of Polycrystalline Alloys: *Jing Luo*[1]; Yejun Gu[2]; Jaafar El-Awady[1]; [1]Johns Hopkins University; [2]Institute of High-Performance Computing, A*STAR, Fusionopolis

Autonomous materials design requires reliable constitutive models to predict mechanical behavior efficiently and accurately. However, predicting the stress-strain response of polycrystalline metals remains challenging due to the complex interplay of microstructural features at multiple length-scales. Here, we present a physics-informed machine learning framework for predicting stress-strain curves of polycrystals by leveraging extensive experimental datasets from literature. Our approach is distinguished by incorporating the evolution of dislocation density as a key state variable governing plastic deformation, enabling physically meaningful predictions. Through Bayesian inference and uncertainty propagation methods, we develop a rigorous framework for quantifying uncertainties in the predicted mechanical response of polycrystals. Our models demonstrate robust extrapolation capabilities when applied to multi-principal element alloys through the integration of physics-based solution enhancement. Additionally, we analyze the fundamental differences in deformation mechanisms between face-centered cubic and body-centered cubic polycrystals, highlighting how crystal structure, deformation modes, and experimental data quality influence the model predictions.

2:40 PM

Transfer Learning for Nanomaterial Classification: Lavanya M[1]; *Baishali Garai*[1]; Yashmeet Baid[1]; Shabbeer Basha[1]; Sristi L[1]; [1]RV University

Nanomaterials play crucial role in manufacturing by enhancing product properties and enabling new functionalities in industries like aerospace and automotive. They create stronger, lighter materials and improve surface properties such as scratch resistance, waterproofing, and anti-corrosion. Nanomaterials can be classified into various categories, each with unique properties suited to specific industries. There is vast amount of unstructured data available in scientific literature about properties of nanomaterials but extracting meaningful data from them is challenging for researchers. Images, particularly from scanning electron microscopes (SEM), are critical in identifying nanomaterials. This work employs transfer learning to classify nanomaterials using SEM image dataset and does a comparative study among two pretrained models: ResNet50, and VGG16. Each model was trained on SEM images, and their performance was evaluated for nanomaterial classification. Among them, VGG16 demonstrated best performance, highlighting its effectiveness in accurately identifying nanomaterials from SEM images.

3:00 PM Break

3:30 PM

Innovative AI Method for Predicting Grain Size Distribution During Grain Growth Mechanism: *Eliane Younes*[1]; [1]Mines Paris

Grain growth (GG) significantly affects the mechanical properties of materials, making its prediction important in materials science. Traditional methods, such as ToRealMotion (TRM), Monte-Carlo Potts, Cellular Automaton, Vertex, Phase Field, and Level-Set methods, are effective but computationally demanding. This has led to growing interest in more efficient approaches, like machine learning, particularly deep neural networks. Deep learning, especially LSTMs, is well-suited for capturing sequential changes in evolving microstructures and modeling complex patterns over time. Building on this, we developed an LSTM-based model designed for isotropic grain growth. A large database of validated simulations of normal grain growth in an idealized system was created, using diverse parameters to ensure a versatile predictive model. The trained model showed strong agreement with analytical predictions across various test cases. By fine-tuning parameters and training duration, we identified the dataset requirements for accurate and efficient grain growth predictions, improving computational tools in materials science.

3:50 PM

Strength in Uncertainty: Federated Learning for Accelerated Innovation: *Joel Strickland*[1]; Bogdan Nenchev[1]; [1]Intellegens

This work presents a federated learning framework that enables B2B collaboration by aligning machine learning models trained on diverse datasets without the need to merge sensitive data. Using a shared calibration set, the framework standardizes uncertainties across models predicting critical material properties, such as strength, toughness, and hardness. It selects the prediction with the highest confidence for each output, allowing businesses to leverage the strengths of all models simultaneously, even when models have differing inputs and outputs. This approach accelerates innovation by enabling faster, more accurate predictions while eliminating the need for data centralization, reducing costs, and shortening time-to-market. Effective uncertainty management minimizes risks and improves decision-making, crucial in industries where safety and performance are paramount. With robust privacy protections, companies across sectors like automotive, aerospace, and manufacturing can confidently adopt decentralized models, optimize processes, gain a competitive edge, and drive innovation without compromising data security.

4:10 PM

Machine Learning Applications in Manufacturing Operations Environment: *Lily Lee*[1]; [1]MIT Lincoln Laboratory

Placeholder submission. Pending approval from sponsor to submit abstractWe will present a manufacturing data set to evaluate machine learning algorithms for potential application in manufacturing process and baseline results from a select sample of machine learning techniques.

4:30 PM

Microstructure Statistics and Interpretable Property Prediction in Multifunctional Electrodes Using Random Forests: *William Huddleston*[1]; Hugh Smith[2]; Alp Sehirlioglu[2]; [1]HX5, LLC; [2]Case Western Reserve University

A machine learning image analysis pipeline was developed to quantify microstructural features and enable interpretable property prediction. Processing-microstructure-property relationships were surveyed for battery anode composites using quantified particle counts, relative particle distances, and shape statistics from skeletonization. Extracted features quantified changes in the spatial distribution and coalescence of particles as a function of composition and sintering conditions, enabling deconvolution of percolation from particle coarsening. Random forest regression models were trained to predict electronic conductivity from either feature averages or principal component scores calculated from feature distributions, providing prediction with 0.95 and 0.974 adjusted-R_2, respectively. Model structures were analyzed to determine the relative influence of each feature, revealing that particle size, skeleton complexity, and edge-to-edge spacing were most important. The data-driven analysis pipeline leveraged dimensionality reduction to enable property prediction with high accuracy and enhanced interpretability, showing potential for knowledge discovery in high-throughput experimentation and ground-truth microstructural data for multiscale simulations.

4:50 PM

Optimizing Deep Learning Training for Scientific Imaging of Fiber-Reinforced Composites: *Aly Badran*[1]; Benjamin Provenchure[2]; Mike Marsh[2]; Jonathan Kroll[3] [1]GE Aerospace; [2]Comet Tech; [3]University of Texas at Austin

Deep learning models have revolutionized scientific imaging by enhancing pixel-wise labeling accuracy. However, U-Net and related architectures often face implementation challenges due to insufficient training optimization studies. This topic explores U-Net training using x-ray CT images of fiber reinforced composites, analyzing the impact of training data volume, and data augmentation. We employ seven-fold replications to address training process variability. Variance in training and the complexity of images are explored. Increased training data volume significantly improves model accuracy and speed, reducing variance among replicates. Notably, data augmentation substantially enhances performance, especially with limited ground truth data. High data augmentation coefficients are recommended for scientific imaging semantic segmentation models. Future work on quantifying image complexity will guide minimum required training data volumes for specific tasks in scientific imaging.

3rd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2025): Development of Novel ML Methodologies IV

Tuesday PM
June 17, 2025

Room: Room B
Location: Anaheim Marriott

Session Chair: To Be Announced

1:30 PM Introductory Comments

1:40 PM
Strongly Physics-Constrained Neural Networks for Mechanical Superresolution: *Vivek Oommen*[1]; Andreas Robertson[2]; George Karniadakis[1]; Remi Dingreville[2]; [1]Brown University; [2]Sandia National Laboratories

Neural operators facilitate the efficient estimation of the solution fields to partial differential equations. However, these methods are restricted by the availability of sufficient data for training. This problem is especially pronounced in crystal mechanics applications because at high resolutions the computational cost of running simulations becomes overwhelming. We propose a framework for multi-resolution training of neural operators in crystal mechanics, where the training is only supervised with low-resolution datasets generated from acceptably cheap simulations. To fill in the missing information, we introduce a new variant of neural operators: Structure- Preserving UNets. These networks are strongly physics-constrained: the deformation compatibility and stress equilibrium PDEs are directly incorporated into the architecture. In this talk, we present the novel architecture that makes physically consistent and computationally efficient predictions at high resolution. To understand the proposed framework's strengths and weaknesses, we compare it against traditional softly constrained physics-informed neural networks.

2:00 PM
Beyond Bespoke Models: Foundational Vision Transformers for Microstructure Representation and Machine Learning of Microstructure-Property Relationships in Alloys: *Sheila Whitman*[1]; Aditya Jain[1]; Marat Latypov[1]; [1]University of Arizona

Machine learning is rapidly emerging as a powerful approach to establishing microstructure–property relationships in structural materials. Most existing machine learning efforts focus on the development of task-specific models for each individual class of materials and individual properties. To go beyond bespoke models, we propose utilizing foundational vision models for the extraction of task-agnostic microstructure features and subsequent lightweight machine learning. We demonstrate our approach on two case studies: stiffness of synthetic two-phase microstructures learned from simulation data and Vickers hardness of superalloys learned from experimental data. Our results show the potential of foundational vision models for robust microstructure representation and efficient machine learning of microstructure–property relationships without the need for expensive task-specific training or fine-tuning. We further explore the extension of this approach to include additional alloy information (composition, processing) besides the microstructure for multimodal representation and learning of alloy properties.

2:20 PM
Generative Priors for Regularizing Ill-Posed Problems: Applications to 3D Polycrystalline RVE's: *Michael Buzzy*[1]; Surya Kalidindi[1]; [1]Georgia Institute of Technology

Many problems in Materials Science are ill-posed, meaning that, given a task there may be one, many, or no possible solutions. Classic examples of ill-posed problems include materials design and microstructure reconstruction, where a user may be interested in obtaining a microstructure which corresponds to a desired property or structural descriptor. When solving inverse problems, the existence (or lack thereof) of multiple solutions presents a persistent problem in high dimensional spaces, where the set of possible solutions becomes incredibly vast and difficult to enumerate. New algorithms utilizing generative priors provide a promising avenue for regularizing these high dimensional ill-posed problems. This talk will discuss the theory and benefits of generative priors, as well as demonstrate their practicality by solving materials design and microstructure reconstruction problems relating to 3D Polycrystalline RVE's.

2:40 PM
Physics-Informed Generative AI for Predicting Material Deformation: Latent Diffusion Modeling From Undeformed Microstructures: *Kavindu Wijesinghe*[1]; Ashwin Ajit[1]; Janith Wanni[2]; Steven Arnold[3]; Ajit Achuthan[1]; [1]Clarkson University; [2]University of Wisconsin Madison; [3]NASA Glenn Research Center

This research introduces a physics-informed generative AI framework that utilizes Latent Diffusion Models (LDMs) to predict microstructural deformation in materials by leveraging undeformed optical microscopy images alongside embedded crystallographic data. Conditioning the LDM with experimentally derived insights, our approach achieves high-fidelity predictions of critical deformation processes up to higher strain levels, capturing phenomena such as slip band evolution and grain boundary migration under uniaxial tensile loading. Through fine-tuning on high-resolution stainless steel 316L datasets, generated via in-situ tensile testing with panoramic imaging, this work integrates physics-informed machine learning with experimentally validated material deformation modeling. By synthesizing time-sequenced data that reflects both evolving and emergent microscopic features, this method offers a scalable, resource-efficient alternative for alloy design and testing, advancing toward next-generation materials withtailored mechanical properties and providing rapid, predictive insights into material behavior under complex loading conditions.

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): ICME Application to Advanced Manufacturing II

Tuesday PM
June 17, 2025

Room: Room F
Location: Anaheim Marriott

Session Chair: To Be Announced

1:30 PM Invited
Leveraging Laser Parameters and Layer Remelting to Tailor Microstructure in Laser Powder Bed Fusion: *Nicole Aragon*[1]; Theron Rodgers[1]; Daniel Moser[1]; [1]Sandia National Laboratories

Additive manufacturing (AM) processes, such as laser powder bed fusion (LPBF), provide unique opportunities to create freeform and complex parts. However, AM processing conditions significantly influence the as-solidified microstructure. In addition, AM processes introduce additional complexities such as remelting due to subsequent laser passes. We present a three-dimensional model that simulates solidification, solid-state evolution phenomena, and texture evolution using Monte Carlo methods. The simulations couple microstructure evolution with an analytical Green's function-based thermal model to create a fully integrated microstructural prediction tool. The developed tool is used to study LPBF of 316L stainless steel. In this work, several process conditions are considered along with additional layer remelting strategies using low and high energy densities to evaluate the effect on grain morphology and texture. The simulation results are validated with experiments performed at equivalent process parameters. Results show that grain size and texture strength increase with total energy density.Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

2:00 PM

A Framework for Efficient Part-Scale Microstructure Prediction in Laser Powder Bed Ti-6Al-4V Using Combined Physics-Based Modeling and Machine Learning Surrogate Methods: *Anthony Spangenberger*[1]; Bonnie Whitney[1]; Diana Lados[1]; [1]Worcester Polytechnic Institute

Microstructure formation in additive manufacturing (AM) spans lengths from centimeter-scale components to micrometer-scale grain sizes, making their simultaneous resolution in computational simulations intractable with current high-fidelity physics-based methods. These models are needed to simulate microstructure sensitivity to process parameters, as the basis for subsequent property prediction models, and to mitigate process defects and anisotropy. A three-part modeling framework for laser powder bed Ti-6Al-4V is proposed to address this deficit: (i) coupled continuum heat transfer and kinetic Monte Carlo simulation of grain morphology and texture at the part-scale, (ii) phase field (PF) modeling of the /' solid-state transformation at the subgrain-scale, and (iii) a scale-bridging surrogate of the PF model for transient /' phase fraction and width predictions. Model calibration and validation are supported by in-situ synchrotron heat treatment studies and electron backscatter diffraction data that inform transformation kinetics and grain morphological/textural variations across a wide range of processing parameters.

2:20 PM

Leveraging Cross-Disciplinary Physics for Enhanced Additive Manufacturing Modeling: *Masoud Anahid*[1]; Sergei Burlatsky[1]; Manish Kamal[2]; David Furrer[2]; [1]RTX Technology Research Center; [2]Pratt & Whitney

Integrated multi-scale and multi-physics modeling is key for enhancing Additive Manufacturing (AM) process understanding and developing relevant controls for manufacturing. This presentation provides an approach where general principles governing physical phenomena and traditionally confined to non-AM domains can be leveraged successfully for AM process modeling. Through illustrative examples, this presentation will demonstrate how fundamental models from thermodynamics, fluid dynamics, and material science can be integrated into modeling AM processes. For instance, the study of melt pool dynamics, commonly used in coating, welding, and casting, can be adapted to enhance the understanding and control of melt pools in AM. Similarly, knowledge of dislocation dynamics and plasticity, crucial for analyzing dwell fatigue and thermo-mechanical fatigue, can be leveraged to develop predictive models for estimating the fatigue life of AM components. Development of integrated physics-based models is traditionally resource-intensive, however, the examples shown here demonstrate that cross-disciplinary physics can be leveraged for AM.

2:40 PM

Process-Structure-Property Modelling for Tailored Microstructures and Enhanced Performance of Additively Manufactured Materials: *Olga Zinovieva*[1]; Aleksandr Zinoviev[1]; [1]University of New South Wales (UNSW)

Additive manufacturing (AM) enables the production of complex parts with tailored properties through microstructure control, offering benefits for aerospace, automotive, healthcare, and defence industries. However, the intricate physics of AM, influenced by numerous process parameters, poses challenges for predictability of part properties. To address this, process-structure-property (PSP) modelling has emerged as a powerful approach to understand and predict the relationships between manufacturing processes, microstructure evolution, and mechanical performance. This research employs melt pool scale thermal simulations coupled with cellular automata to analyse microstructure evolution. Microstructural data, including grain morphology and crystallographic orientations, informs crystal plasticity finite element models. The effects of beam profiles, nucleation parameters, and process variables on microstructures and mechanical behaviour, including microlattice performance, are analysed.

3:00 PM Break

3:30 PM

Validating a Simulation Toolchain to Predict Process-Structure-Property Maps for Additively Manufactured Aluminum Alloys: *Stephen DeWitt*[1]; John Coleman[1]; Alex Plotkowski[1]; [1]Oak Ridge National Laboratory

Given the vast processing space attainable through additive manufacturing, a trial-and-error approach to finding acceptable processing conditions is time-consuming and difficult for new alloys. Efficiently finding the optimal processing conditions that balance multiple considerations (e.g. minimize porosity and maximize yield strength) is even more difficult. In this presentation we discuss a simulation toolchain that combines thermal process simulations with analytic structure and property models to map standard laser powderbed fusion process parameters (e.g., power, velocity, hatch spacing, spot size) to common defects and mechanical properties. We demonstrate how this toolchain can be calibrated from simple single-track experiments and create process-structure-property maps for an example aluminum-copper-manganese-zirconium (ACMZ) alloy. Finally, we compare the predictions of the simulation toolchain to experimental characterization data for validation and discuss future research directions given these results.

3:50 PM

A Microstructure Modelling Framework for Multi-Laser Powder Bed Fusion of Ti-6Al-4V: *Hugh Banes*[1]; Prashant Jadhav[1]; Magnus Anderson[2]; Hector Basoalto[1]; [1]University of Sheffield; [2]Thermo-Calc Software AB.

Widespread adoption of additive manufacturing techniques for titanium alloys is currently limited by uncertainty in the microstructure variations introduced by the process. Novel heat sources, including Multiple-Laser Powder Bed Fusion (M-LPBF), have potential to improve part quality, however the relation between the processing parameters and final microstructure is not fully understood. To address this, an ICME framework has been developed, using a Representative Volume Element (RVE) approach to simulate the thermal fields induced by the laser-powder system, and two microstructure models. The Johnson-Mehl-Avrami-Kologorov (JMAK) description of the solid-state transformation in titanium, and a Cellular Automata (CA) description of the solidification and growth kinetics of the phase structure. This framework was applied to M-LPBF cases, with a series of scanning strategies computed and microstructures examined. The combination of single-track scans and multiple-layer hatches tested with focused and defocused additional lasers revealed that in certain cases beneficial microstructures could be achieved.

4:10 PM

Characterizing the Influence of Compositional and Thermocapillary Gradient Variations on the Temperature Profiles and Melt Pool Dimensions of LPBF-Processed Al 7xxx Alloys: *Chukwudalu Uba*[1]; [1]University of Louisiana Lafayette

Additive manufacturing (LPBF) is central to Industry 4.0, allowing the production of complex, high-precision parts across aerospace and manufacturing sectors. However, LPBF poses challenges in characterizing melt pool dynamics due to current experimental limitations. Concerning the LPBF of Al 7xxx alloys, the thermal–fluidic transport effects on the temperature distribution and melt pool characteristics have been ignored. This study proposes an integrated experimental–computational framework to address these challenges. Building on our previous study of CALPHAD-based Al 7xxx alloy design, the designed alloys' thermocapillary gradients were characterized using sessile drop experiments and CALPHAD. Finally, finite element-based heat transfer–fluid flow models were developed to simulate the LPBF process, utilizing the characterized thermocapillary gradient data. The results revealed that compositional and thermocapillary gradient variations affected the temperature distributions and melt pool dimensions. This model enhances the understanding of process–structure–property relationships in LPBF, aiding material design and process parameter optimization.

4:30 PM
Comparative Study of Melt Pool Dynamics and Keyhole Formation in Laser Powder Bed Fusion Process (LPBF) of SS316L and Ti-6Al-4V: *Amrita Dixit*[1]; Amarendra Singh[1]; [1]Indian Institute of Technology Kanpur

Understanding melt pool dynamics during laser-material interaction is critical to achieving high-quality mechanical properties in components produced through laser powder bed fusion (LPBF). This study examines the effects of constant versus variable absorptivity on keyhole formation predictions for Ti-6Al-4V alloy via numerical simulation. A mesoscale model is developed to incorporate key physical phenomena such as Marangoni convection, recoil pressure, convective losses, and vaporization losses, while a ray tracing method with Fresnel absorptivity simulates variable absorptivity. The constant absorptivity model is validated against existing data for SS316L alloy, whereas the variable absorptivity model is validated for Ti-6Al-4V alloy. Using the validated model, experimental data for SS316L alloy are further validated to identify processing parameters for keyhole formation. This will help in the optimization of the processing parameter for the control of melt pool dynamics. These insights enhance the understanding of melt pool dynamics in both conduction and keyhole melting modes.

4:50 PM
Multiphysics Modeling of Metal Matrix Composite (MMC) Additive Manufacturing Process including Melt Pool Characterizing and Grain Growth: *Mingyu Chung*[1]; Kang-Hyun Lee[1]; Jae Eun Park[1]; Gun Jin Yun[1]; [1]Seoul National University

Direct Energy Deposition (DED) is a widely utilized AM process to produce large components and repair damaged parts. Attempts have been made to obtain improved deposition-rates and mechanical properties by applying Metal Matrix Composite (MMC) powders to conventional DED process. However, the Multiphysics phenomena including melt pool evolution, nucleation, and phase transformation which are affected by the reinforcements are highly complex, and it hinders building PSP linkage for the MMC AM process. To fill this gap, computational analysis consisting of Thermo-Fluid and Cellular Automata model is constructed in this study; first one to estimate the melt pool formation and distribution of reinforcements in the melt pool, latter to predict the microstructure. Unlike previous studies, the results demonstrated that the analysis used in this study enables building linkage between Process and Structure for the MMC AM process and gives possibilities of optimizing the process to achieve the targeted quality and performance.

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): Artificial Intelligence and Machine Learning in ICME I

Tuesday PM
June 17, 2025

Room: Room E
Location: Anaheim Marriott

Session Chair: To Be Announced

1:30 PM Invited
Alloy Design for Additive Manufacturing: Expanding the Scope of Alloy 3D Printing for Resource-Constrained and Location-Specific Applications: *Wei Xiong*[1]; [1]University of Pittsburgh

Additive manufacturing becomes critical in advanced materials processing, allowing us to produce complex shape components. This study presents a novel approach to alloy design for additive manufacturing in resource-constrained environments. Utilizing a mixture of commercially available stainless steel 316L and Inconel 718 powders, the research demonstrates the creation of a functionally graded alloy through directed energy deposition. Post-heat treatment processes are optimized using Calphad-based ICME modeling, resulting in an alloy with properties comparable or superior to pure Inconel 718 at a reduced cost. A high-throughput heat treatment method is introduced, significantly accelerating design and optimization. This approach, combined with machine learning, offers a powerful pathway for rapid alloy development in additive manufacturing, particularly in resource-limited scenarios. The findings suggest this method can accelerate alloy design, enabling cost-effective, customized solutions for challenging environments while maintaining or enhancing material properties.

2:00 PM
Generative AI for Inverse Design of Inconel 718: Jarvis Loh[1]; Nigel Neo[2]; Zhidong Leong[1]; Wen Jun Wee[2]; Yang Hao Lau[1]; Xinyu Yang[1]; Mark Jhon[1]; Rajeev Ahluwalia[1]; Robert Laskowski[1]; *Wei-Lin Tan*[2]; [1]Institute of High Performance Computing (IHPC), Agency for Science, Technology and Research (A*STAR); [2]DSO National Laboratories

A challenge in employing machine learning for the inverse design of materials is explainability – many frameworks use property as input and processing parameters as output, resulting in a process-property 'black box' AI, bypassing microstructural information. In this work we attempt to plug the process-structure-property gap by using a Continuous Conditional Generative Adversarial Network (CcGAN) architecture to inversely generate microstructures corresponding to specified yield strengths. A convolutional neural network is then employed to predict the requisite processing parameters to attain these generated microstructures. To demonstrate this architecture, we generated an extensive training set of microstructures using phase field simulations to model the precipitation of γ' and γ" in Inconel 718, and a crystal plasticity model to calculate the corresponding yield strengths. Our methodology resulted in qualitatively well-aligned CcGAN-generated microstructures compared with those derived from physics-based calculations. Furthermore, the predictions for processing parameters achieve a root mean squared error within 7%.

2:20 PM
Inverse Alloy Design: An Alloy Composition Generation Framework With Flexibilities: Mohammad Abu-Mualla[1]; Ellis Crabtree[2]; Fredrick Michael[2]; Yayue Pan[1]; *Jida Huang*[1]; [1]University of Illinois Chicago; [2]NASA Marshall Space Flight Center

Inverse design, generating material compositions with targeted properties, offers a promising approach to material discovery. Machine learning has emerged as a key enabler for generative design. However, existing models face challenges such as non-uniqueness (multiple compositions yield the same property), the complexity of high-dimensional compositional spaces, and the generation of physically non-achievable alloys. This work proposes a latent diffusion generative model for the inverse problem and a Variational Autoencoder (VAE) to obtain the latent representation; we constrained the latent space to ensure the generation of physically valid alloys. Our framework successfully mapped both the composition-property and property-composition correlations, using the VAE for the forward and the latent diffusion model for the inverse design. The model is trained on the Granta Alloys dataset. Experimental results reveal the proposed framework could accurately predict both pathways and generate multiple feasible designs, providing flexibility for selecting compositions that meet target properties.

2:40 PM
Micromechanics Surrogate Model for Fatigue Life Prediction of Composites: *Brandon Hearley*[1]; Steven Arnold[1]; [1]NASA Glenn Research Center

Fatigue modeling of composites, particularly using a multiscale approach, can be very costly, due the number of iterations that must occur when evaluating the damage state of each constituent within each ply, thus making it difficult for engineering in early design stages to evaluate a large number of potential candidate material configurations. In this work, a machine learning surrogate model for ply level micromechanics fatigue damage of composites is presented, enabling S-N curve prediction of laminates for any arbitrary number of plies. Training data is created using they physics-based Micromechanics Analysis Code with Generalized Method of Cells (MAC/GMC) tool for a single ply under multiaxial loading, predicting the damage increment and corresponding cycles to damage for each ply. The developed machine learning model will allow engineers to quickly get a reasonably accurate estimate of the fatigue life a composite with any arbitrary number of plies subject to any multiaxial load.

3:00 PM Break

3:30 PM
Surrogate-Model-Assisted Multi-Objective Calibration of Crystal Plasticity Finite Element Method (CPFEM) Models: *Janzen Choi*[1]; Mark Messner[2]; Zhiyang Wang[3]; Tao Wei[3]; Tianchen Hu[2]; Jay Kruzic[1]; Ondrej Muransky[3]; [1]University of New South Wales; [2]Argonne National Laboratory; [3]Australian Nuclear Science and Technology Organisation

Crystal plasticity finite element method (CPFEM) models are powerful tools for simulating the deformation behaviour of polycrystalline materials, capturing the influence of a material's microstructure on its macroscopic properties. However, identifying a unique set of crystal plasticity parameters presents significant challenges due to the vast parameter space and the high computational cost associated with microstructure-informed finite element simulations. To address these challenges, a surrogate model is developed to approximate the CPFEM response, which is then integrated with a multi-objective genetic algorithm (MOGA) to determine the crystal plasticity parameters. This approach optimises the material parameters using multiple objective functions, such as for the stress-strain curve and grain rotation measurements obtained via in-situ electron backscatter diffraction (EBSD) during tensile loading. The calibration workflow is demonstrated using Alloy 617 at room temperature, showing that the calibrated CPFEM model can accurately capture the stress-strain behaviour, overall texture evolution, and reorientation trajectories of individual grains.

3:50 PM
Integrated Microstructure and Mechanism-Guided Multimodal Machine Learning for Advanced Steel Design: *Wei Xu*[1]; [1]Northeastern University

Machine learning is revolutionizing the material design community, especially for high-performing steels. However, emerging methods such as automated laboratories suffer from poor interpretability and requirements for huge amount of data. The current study combines physical metallurgy knowledge and microstructural data to accurately predict properties of steels and improve steel design. Guided by thermodynamic data, deep learning models achieve precise predictions for frictional work and the martensite transformation start temperature. For more complex scenarios such creep and fatigue, transfer learning is employed where source models are established to understand the relationship amongst composition, processing, and mechanical properties. These learned mechanisms are then used to predict fatigue and creep properties. Recognizing that most problems in steel design rely heavily on microstructural information, rapid quantification methods for microstructural images are developed, and multimodal information pertaining to the images is extracted to develop site-specific AI strategies, finally achieving a comprehensive integration of prediction capabilities.

4:10 PM
Linking Multiple Length Scales Using Material Data Driven Design (MAD3): *David Montes De Oca Zapiain*[1]; Hojun Lim[1]; [1]Sandia National Laboratories

Metal alloys used in stamping and forming processes exhibit polycrystalline structures at the lower length scale that cause the metal to display plastic anisotropy. Accurate predictions of the metal's plastic anisotropy are crucial in manufacturing given the effect it has on the macro scale. Material Data Driven Design (MAD3) is an innovative software that leverages the power of machine learning to link the micro and macro scales and thus modernize the forming and stamping processes of sheet metals by predicting the parameters that characterize the load-dependent behavior of a metal alloy 1000 times faster than existing solutions. This software is conveniently packaged in a simple and easy-to-use graphical user interface that is deployed using cloud computing. In this talk, we present the structure and functionality of MAD3 and how this technology can be obtained by external users. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. SAND2024-14838A

4:30 PM
High-Throughput Screening of Ti-V-Nb-Mo Carbide MXenes Using Machine Learned Potentials and Their Assessment as Catalysts for Hydrogen Evolution Reaction: *Mohammed Wasay Mudassir*[1]; Sriram Goverapet Srinivasan[1]; Mahesh Mynam[1]; Beena Rai[1]; [1]TCS Research and Innovation

MXenes, a versatile class of 2D materials, have shown great potential as catalysts for the hydrogen evolution reaction (HER). The recent discovery of high entropy (HE)-MXenes has significantly broadened the compositional landscape, suggesting potential diverse candidates with enhanced stability and functionality. Leveraging atomistic modeling, we systematically explored this vast design space by developing a Neural Network Potential (NNP) trained in an active learning fashion on Density Functional Theory (DFT) data for $(Ti_xV_yNb_zMo_p)_{n+1}C_n$ MXenes (where x+y+z+p=1; n=1,2,3). This NNP was utilized to identify thermodynamically stable compositions from a vast number of HE-MXenes and to examine how the arrangement of transition metals within and across layers influences stability. Additionally, we assessed the catalytic HER performance of these stable MXenes by calculating the hydrogen adsorption energy, $\Delta G(^*H)$ using DFT. In this presentation, I will discuss the NNP development workflow and study findings, highlighting new synthesizable HE-MXenes with catalytic potential for HER.

4:50 PM
Parameter-Efficient Quantized Mixture-of-Experts Meets Vision-Language Instruction Tuning for Semiconductor Electron Micrograph Analysis: *Sagar Srinivas Sakhinana*[1]; Venkataramana Runkana[1]; [1]Tata Research Development and Design Center

Semiconductors, crucial to modern electronics, are generally under-researched in foundational models. It highlights the need for research to enhance the semiconductor device technology portfolio and aid in high-end device fabrication. In this paper, we introduce sLAVA, a small-scale vision-language assistant tailored for semiconductor manufacturing, with a focus on electron microscopy image analysis. It addresses challenges of data scarcity and acquiring high-quality, expert-annotated data. We employ a teacher-student paradigm, using a foundational vision-language models like OpenAI GPT-4o, Google Gemini as a teacher to create instruction-following multimodal data for customizing the student model, sLAVA, for electron microscopic image analysis tasks on consumer hardware with limited budgets. Our approach allows enterprises to further fine-tune the proposed framework with their proprietary data securely within their own infrastructure, protecting intellectual property. Rigorous experiments validate that our framework surpasses traditional methods, handles data shifts, and enables high-throughputscreening.

The 7th International Congress on 3D Materials Science (3DMS 2025): 3DMS: Keynote Session

Tuesday PM
June 17, 2025

Room: Plenary Room
Location: Anaheim Marriott

Session Chair: To Be Announced

1:30 PM Introductory Comments

1:35 PM Keynote
3D X-Ray Observations Provide Striking Findings in Rubber Elasticity: *Vikram Deshpande*[1]; [1]Cambridge University

From Hooke's law in the 1660s to the 1930s work of Flory on polymer chains, the understanding of rubber elasticity was formalised via the Neo-Hookean model. This established the idea that, under isothermal conditions, stress is (non)linearly related to strain and no other state variable. Here, we suggest that this fundamental concept might need to be revisited. Using innovative X-ray measurements capturing the three-dimensional spatial volumetric strain fields, we demonstrate that rubbers and indeed many common engineering polymers, undergo significant local volume changes. But remarkably the overall specimen volume remains constant regardless of the imposed loading. This strange behaviour which also leads to apparent negative local bulk moduli is due to the presence of a mobile phase within these materials. The presentation will end with a broad overview of laboratory X-ray techniques including high-speed tomography and energy dispersive diffraction that might open new understandings for a range of materials.

2:05 PM Question and Answer Period

The 7th International Congress on 3D Materials Science (3DMS 2025): Emerging 3D Characterization Techniques and Instrumentation II

Tuesday PM
June 17, 2025

Room: Room C
Location: Anaheim Marriott

Session Chair: To Be Announced

2:20 PM Invited
High-Energy X-Ray Imaging and Diffraction With Intense Undulator Radiation: *Yujiro Hayashi*[1]; Jaemyung Kim[1]; Hirokatsu Yumoto[2]; Takahisa Koyama[2]; Haruhiko Ohashi[2]; Hiroshi Yamazaki[2]; Yasunori Senba[2]; Shunji Goto[2]; Ichiro Inoue[1]; Taito Osaka[1]; Kenji Tamasaku[1]; Makina Yabashi[1]; [1]RIKEN SPring-8 Center; [2]Japan Synchrotron Radiation Research Institute

Demands for synchrotron-based 3D characterization for materials in manufacturing industries are shifting from modeled specimens or small test pieces to mass-produced components without any cutting. The upgrade of SPring-8 named SPring-8-II will meet the demands of high-energy X-rays, because brilliant high-energy undulator radiation with an energy band width of 1% will be obtained without any monochromators. We have tested the concept of a so-called high-energy pink beam using a double multilayer monochromator designed for 100 keV. In this presentation, we show some results of 3D imaging and diffraction experiments using the 100-keV pink beam based on industrial demands. Computed laminography, for instance, enabled 3D imaging of voids in die-attach solder in a power semiconductor module for automotive applications. Laminographic 3DXRD enabled 3D orientation mapping for a 9-mm-thick steel plate as a milestone toward the characterization of plastic deformation, creep, and fatigue of polycrystalline materials embedded in manufactured components and products.

2:50 PM
Unconventional Applications of Scanning 3dxrd: Opportunities for Cementitious Materials: *Michela La Bella*[1]; [1]Danish Technical University (DTU)

Scanning 3dxrd is a newly developed technique that permits retrieving the crystallographic phase, orientation, shape, and size of individual grains in polycrystalline aggregates. Originally, it has been developed to deal with materials science challenges mostly related to metallurgy. However, scanning 3dxrd has proven to be a versatile and promising technique to be applied also in other materials science fields. In this talk, I will present two examples of the application of scanning 3dxrd in combination with other complementary techniques to study cementitious materials. The advantages of using this technique compared to more conventional ones will be addressed together with the perspectives on possible improvements toward broader fields of applications.

3:10 PM Break

3:40 PM Invited
Lab-Scale Diffraction Contrast Tomography (DCT): State-of-the-Art, Challenges, and Opportunities: *Nikhilesh Chawla*[1]; Eshan Ganju[1]; [1]Purdue University

The acquisition of high-fidelity 3D grain maps is essential for advancing our understanding of the micromechanical behavior of polycrystalline materials. Grain orientations, grain boundary misorientations, and grain shapes play a significant role in important phenomena such as slip transfer, corrosion, and grain growth. The past few years have seen considerable advances in the acquisition of high-reliability grain maps using laboratory-based Diffraction Contrast Tomography (LabDCT). Additionally, the microstructures of challenging sample geometries have become more accessible at the lab scale with recent developments in advanced Lab DCT acquisition strategies, such as helical phyllotaxis scanning and forward-based reconstruction. In this paper, we present the state-on-the-art of lab-scale DCT. The important strides over the years as well as challenges and opportunities will be presented. The use of machine-learning based techniques for rapid acquisition and high throughput will be discussed.

4:10 PM
Laboratory-Based 3D X-Ray Scattering Tensor Tomography: Azat Slyamov[1]; Adriaan van Roosmalen[1]; Kenneth Nielsen[1]; *Erik Lauridsen*[1]; [1]Xnovo Technology

Scattering (dark-field) X-ray microscopy methods advance fiber orientation analysis by mapping anisotropic structures without direct resolution, enabling an extended field of view (FOV). Two primary technologies—scanning small-angle scattering and full-field linear grating interferometry—have been used for fiber composites and biological materials. However, both methods have disadvantages with acquisition overhead: scanning methods require a focused beam to raster scan the sample, while linear gratings require linear and rotational shifts for 2D orientation sensitivity. A recent innovation using circular grating unit cells overcomes these limitations by enabling single-shot 2D orientation mapping. Each unit cell in the 2D grid provides localized scattering data, effectively simulating raster scanning, while the circular shape captures 2D orientation sensitivity in one frame. This approach, integrated into the Exciscope Polaris platform, allows for efficient in-lab X-ray tensor tomography (XTT). We successfully validate this technology against synchrotron results and demonstrate its applications in technological and biological composite materials.

4:30 PM
Investigating Martensitic Phase Transformations in CuAlNi and NiTi Shape Memory Alloys With In-Situ X-Ray Topotomography: *Janice Moya*[1]; Wolfgang Ludwig[2]; Timothy Thompson[1]; Jonathan Wright[2]; James Ball[2]; Adam Creuziger[3]; Ashley Bucsek[1]; [1]University of Michigan; [2]European Synchrotron Radiation Facility; [3]U.S. National Institute of Standards and Technology Science

To investigate reversible martensitic phase transformations in shape memory alloys (SMAs), this work leverages in-situ X-ray topotomography and diffraction contrast tomography measurements during mechanical cycling on copper-aluminum-nickel (CuAlNi) and nickel-titanium (NiTi) SMAs on beamline ID11 at the European Synchrotron Radiation Facility. These techniques are essential for uncovering microstructural mechanisms driving martensite transformations, specifically testing variant selection theories and observing interactions that guide transformation pathways. Topotomography allows for high spatial resolution imaging of the 3D morphology of austenite-martensite microstructures as they evolve during mechanical loading. This technique captures interactions between the formation of martensite and important microstructural features, including the nucleation of specific martensite variants at triple junctions, martensite interactions between neighboring grains across grain boundaries, and the formation of multiple, intersecting martensite variants. This work also aims to refine current reconstruction methods to improve martensite contrast in 2D projections and tomographic reconstructions, further advancing our understanding of complex SMA microstructures.

The 7th International Congress on 3D Materials Science (3DMS 2025): Methods of Materials Simulation and Modelling in 3D & 4D II

Tuesday PM
June 17, 2025

Room: Room D
Location: Anaheim Marriott

Session Chair: To Be Announced

2:20 PM
Conforming Mesh Generation from 3D Experimental Images: *Daniel Pino Munoz*[1]; Jean-Luc Bouvard[1]; Pierre-Oliver Bouchard[1]; Marc Bernacki[1]; [1]Mines Paristech, PSL University

Advancements in experimental techniques have led to an increased availability of three-dimensional (3D) microstructural data for various materials. However, voxelized representations of these data can limit the applicability of some numerical methods for microstructural analysis, including mechanics, damage, and phase transformation. In this study, we introduce a technique for generating conformal finite element meshes directly from microstructural images. Our method utilizes segmented images as input, where labeled phases are employed to generate signed distance functions that subsequently create the conformal mesh. This approach enables the application of advanced numerical techniques to study physical phenomena at the microstructural level without the constraints imposed by voxelized representations.

2:40 PM
A Versatile Tool for 3DMS, ICME and AI for MS Applications: Fast Fourier Transform (FFT)-Based Modelling of Microstructure/Property Relationships of Polycrystalline Materials: *Ricardo Lebensohn*[1]; Miroslav Zecevic[1]; [1]Los Alamos National Laboratory

Crystal plasticity (CP) models are extensively used to obtain microstructure/property relationships of polycrystalline materials. FFT-based methods, originally proposed by Moulinec and Suquet (1998) for composites, extended to polycrystals by Lebensohn (2001), and currently implemented for non-local large-strain elasto-viscoplasticity [1], are very competitive compared with CP-Finite Elements for some applications, due their higher efficiency and their direct use of voxelized microstructural images. In this talk, we will report recent progress on FFT-based polycrystal plasticity that expands its applicability, including strain-gradient plasticity, achieving geometric accuracy working with voxelized images, non-periodic extensions, and dynamic effects. We will show applications of these methods to micromechanics of nano-metallic laminates, multiscale coupling with Lagrangian hydrocodes, integration with 3DMS characterization methods, use for training and validation of AI models for material science applications, and an ICME application to optimize creep behavior of materials.[1] Zecevic M., Lebensohn R.A., Capolungo L. JMPS 173, 105187 (2023).

3:00 PM Break

3:30 PM
Investigating Effects of Particles and Voids in Plastic Deformation of Al2219 Using Crystal Plasticity and High Energy X-Ray Diffraction Techniques: *Hojun Lim*[1]; Javier Solano[2]; Philip Noell[2]; Michael Sangid[2]; [1]Sandia National Laboratories; [2]Purdue University

The effects of secondary particles and voids on the plastic deformation of aluminum alloy are investigated using crystal plasticity finite element (CPFE) simulations and high energy X-ray diffraction microscopy (HEDM) techniques. HEDM and X-ray computed tomography (XCT) are used to fully construct 3D microstructure of polycrystalline Al2219, identifying grain orientations and the spatial distributions of particles and voids. The CPFE model is utilized to simulate uniaxial tension of the characterized polycrystalline microstructure, both with and without defects. The predicted local fields are compared with experimentally measured grain-average elastic strains and therefore determine grain-level stresses. In addition, observed crack locations are analyzed in relation to CPFE simulations with and without voids and particles. This work demonstrates effects of incorporating realistic distributions of secondary particles and voids in finite element predictions of local response, as well as in understanding failure and fracture behavior.

3:50 PM
A High-Fidelity Fatigue-Life Modeling Framework Using Fast Fourier Transforms: *Nathan Searle*[1]; Krishna Logakannan[1]; Laura Vietz[1]; Benjamin Anglin[2]; Ashley Spear[1]; [1]University of Utah; [2]Naval Nuclear Laboratory

Early stages of fatigue crack evolution typically dominate total fatigue life and contribute to observed scatter in total life among components. Current fatigue modeling techniques at microstructure scale focus primarily on predicting either crack initiation or microstructurally small crack (MSC) propagation, relying on overly-conservative assumptions to then estimate total fatigue life. Development of a method that incorporates both initiation and MSC propagation stages of fatigue life has largely been prohibited by the computational costs of running more than a few cycles of loading, especially when using crystal plasticity-based finite element methods. Through use of Fast Fourier Transform (FFT) methods, this work aims to develop a framework that seamlessly integrates predictions of fatigue-crack initiation and subsequent MSC propagation in 3D polycrystals. By implementing back stress, fatigue indicator parameters, damage evolution, and crack propagation within a parallelized FFT code, the new framework enables computationally efficient, high-fidelity predictions of microstructure-sensitive fatigue crack evolution.

4:10 PM
Atomistic Simulations to Reveal HIP-Bonding Mechanisms of Al6061/Al6061: *Ankit Roy*[1]; Vineet Joshi[1]; Rajib Kalsar[1]; Miao Song[1]; Ayoub Soulami[1]; [1]Pacific Northwest National Lab

Molecular dynamics simulations were employed to understand the diffusion bonding process during hot isostatic pressing (HIP) of Al6061/Al6061 alloy. Simulations of the HIP process reveal atomistic phenomena that are difficult or unlikely to be observed experimentally and provide useful insights into the mechanism of diffusion and bonding. The results reveal that at the start of the HIP process, a massive incursion of oxygen atoms occurs from the pre-existing -Al2O3 to the 6061 region across the interphase interface. These oxygen atoms interact with the enriched Mg atom layer present at the existing -Al2O3 and 6061 matrix to form a secondary complex Mg2Al2O5 phase. Diffusion calculations also show that transport of atoms due to the applied pressure is 4–5 orders of magnitude higher than would occur in the absence of HIP conditions. The Mg2Al2O5 phase also provides efficient pathways for the rapid transport of Mg atoms.

4:30 PM
Modeling the Hardening and Damage Evolution of Additively Manufactured Metal Matrix Composites Using an Elasto-Viscoplastic FFT-Based Framework: *Claire Ticknor*[1]; Jamila Khanfri[2]; Alex Butler[2]; Josh Kacher[2]; Aaron Stebner[2]; Ashley Spear[1]; [1]University of Utah; [2]Georgia Institute of Technology

Additively manufactured (AM) particle-reinforced metal matrix composites (MMCs) combine two fundamental advantages: 1) the additive process can rapidly produce metal parts with complex geometries, and 2) metal matrix composites display enhanced mechanical strength relative to pure metal. A fundamental aspect of designing AM MMCs to meet mechanical performance targets includes high-fidelity models that effectively capture the hardening and damage response of the material, which is affected by the amount of reinforcement particles, process-induced microstructure, and presence of defects. We propose a modeling framework using a large-strain elasto-viscoplastic fast Fourier transform (EVPFFT) code that incorporates an AM MMC-specific work-hardening formulation coupled with triaxiality-based continuum damage mechanics. With this framework, the deformation and failure for multiple volume fractions of particle reinforcements and the resulting tradeoffs of strength and ductility in polycrystalline AM MMCs can be simulated. This work aids the understanding of the structure-to-property relationships of AM MMCs to enable performance-based designs.

Specialty Congress 2025: All-Congress Plenary Session: Wednesday Plenary Session

Wednesday AM
June 18, 2025

Room: Plenary Room
Location: Anaheim Marriott

Session Chair: To Be Announced

8:00 AM Introductory Comments

8:10 PM Plenary
Zentropy and Zentropy-Enhanced Neural Networks (ZENN) for Materials: *Zi-Kui Liu*[1]; Wenrui Hao[1]; [1]Pennsylvania State University

In thermodynamics, materials are considered systems. The properties of a system represent its responses to disturbances from its surroundings, observable as measurable quantities. Based on non-equilibrium thermodynamics, these responses reflect internal processes due to external disturbances and are related to derivatives of the system's energy or free energy. Consequently, accurate predictions of properties depend on the quantitative prediction of the system's free energy landscape, considering both internal and external variables. In this presentation, we will discuss the general framework of our quantitative predictive theories (DOI: 10.1088/1361-648X/ad4762), based on a multiscale entropy approach (recently termed zentropy theory) that integrates quantum mechanics and statistical mechanics. We will present their successful applications to magnetic and thermoelectric materials and melting, along with key challenges for complex systems. Additionally, we will explore potential paths forward, particularly the zentropy-enhanced neural networks (ZENNs) currently being developed by Liu's and Hao's groups.

8:50 AM Question and Answer Period

Joint Sessions of AIM, ICME, & 3DMS: Industrial Case Studies I: Joint Session of AIM & ICME

Wednesday AM
June 18, 2025

Room: Joint Sessions Room
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Introductory Comments

9:10 AM
Hydro Quebec Efforts Toward ICME: Characterizing the Microscale Tensile Behavior of Hydraulic Turbine Steels With Micro-Tensile and Nano-Indentation Tests: *Daniel Paquet*[1]; Pierre-Antony Deschênes[1]; Laurent Tôn-Thât[1]; Robert Wheeler[2]; Betty Huang[3]; Nabil Bassim[3]; [1]Hydro Quebec; [2]MicroTesting Solutions LLC; [3]McMaster University

Two different techniques are used to extract microscale elastoplastic properties of steels used for the fabrication and repair of hydraulic turbines. Martensitic stainless steels and carbon steels, composed of ferrite and pearlite, with significantly different macroscopic tensile behaviors, are characterized by micro-tensile and nano-indentation experiments. Those two intrinsically different techniques are complementary to each other. Micro-tensile tests are easier to analyze but more complex to perform. They require an expertise in FIB machining and an access to sophisticated in situ instruments. This experimental technique is well suited for constitutive relation calibration as it allows a better control over the applied strain field, which is homogeneous and uniaxial when neglecting microstructural effects. Inversely, nano-indentation tests are easier to execute but more complex to analyze because the introduced state of strain is inhomogeneous and triaxial. Nano-indentation is suitable for applications such as Microstructure Informatics for which high throughput experiments are desired.

9:30 AM
Efficient, Coupled Process-Structure-Property Simulations of Additive Manufacturing Using the "Materialize" Framework: *Brodan Richter*[1]; Joshua Pribe[2]; George Weber[1]; Edward Glaesssgen[1]; [1]NASA Langley Research Center; [2]Analytical Mechanics Associates

Process-structure-property (PSP) simulations have the potential to guide and supplement experiments through physics-based insight into the additive manufacturing (AM) process. However, implementing PSP simulations often requires difficult, bespoke coupling of various software packages that use a range of programming languages. This presentation introduces "Materialize", a Python-based framework recently developed by NASA Langley Research Center, to implement coupled physics-based PSP models and support integrated computational materials engineering workflows. Materialize was conceived to efficiently link computational materials models across length scales and PSP space, with a particular emphasis given towards supporting exploratory studies in AM applications. The use of Materialize to perform GPU-accelerated process-structure simulations of transient temperature fields and microstructure evolution during AM is presented. The linking of process-structure simulations to structure-property simulations is then discussed, and the full PSP pipeline will be highlighted. The results demonstrate capabilities of Materialize that are intended to streamline physics-based PSP simulations of AM.

9:50 AM

Uncertainty Quantification, Error Propagation, and Sensitivity Analysis for Synchrotron X-Ray Residual Stress Measurements: *Diwakar Naragani*[1]; Chris Budrow[2]; Kelly Nygren[1]; Paul Shade[3]; [1]Cornell University; [2]Budrow Consulting; [3]Air Force Research Lab

High-energy synchrotron X-rays can measure lattice strains in structural materials under an energy-dispersive or an angle-dispersive modality. During the experimental data collection and analysis workflows several choices are made about the instrumentation, scanning procedure, profile fitting, and material constants that can significantly affect the strain calculated from the diffraction signal. We can explore the impact of these choices within a structured Bayesian framework to deliver accurate and reliable measurements. First, Bayesian uncertainty quantification is used to augment the typical process of calibrating the experimental setup. Second, the determined uncertainty is propagated through the reconstruction software to ascertain error bars on the reported strains. Third, uncertainty due to the material, specifically due to the reference lattice and elastic constants, is also propagated to the predicted residual stress. Finally, a global sensitivity analysis is used to understand the relative importance of these choices for the reported uncertainty on residual stress.

10:10 AM

The HPC4EI Program Connects Industry Partners With National Lab HPC and AI/ML Resources: *Aaron Fisher*[1]; Nick Killingsworth[1]; Victor Castillo[1]; [1]Lawrence Livermore National Laboratory

The High Performance for Energy Innovation (HPC4EI) program fosters public-private partnerships by awarding funding to collaborative R&D projects between national laboratories and industry partners. Focused on addressing critical manufacturing challenges, HPC4EI leverages the Department of Energy's (DOE) supercomputing resources and expertise. A key strategy employed in numerous HPC4EI projects involves high-performance computing (HPC) simulations to develop digital twins of manufacturing processes. These simulations generate massive datasets used to train advanced machine learning tools and reduced-order models capable of real-time predictions. This capability enables analysis and optimization of complex processes, with the potential to save hundreds of millions of dollars and millions of metric tons of CO2 emissions. This presentation will showcase successful examples of past HPC4EI manufacturing projects and outline how prospective industry partners can engage with the program.

10:30 AM Break

10:50 AM

Faster Prediction With AI/ML for Manufacturing: Using Simulations and Production Data Develop Fast-Running Inference Models and Knowledge Tools for Manufacturing: *Victor Castillo*[1]; Yeping Hu[1]; Bo Lei[1]; [1]Lawrence Livermore National Laboratory

Manufacturing processes often involve numerous control parameters that influence final product quality. While computer simulations offer a significant advantage over physical experiments in navigating this high-dimensional control space, they can still be computationally expensive. This work leverages deep learning to develop fast-running surrogate models that accurately capture the dynamics of complex industrial processes. These surrogate models enable near-real-time predictions, facilitating efficient optimization of manufacturing parameters. Furthermore, a novel method is presented for integrating sparse manufacturing data with simulation outputs, enhancing the model's ability to predict actual production quality. The effectiveness of this approach is demonstrated through case studies involving both benchmark problems and real-world manufacturing systems.

11:10 AM

Materials Microstructure Design Integrated With Image-Based Simulation: Oliver Rimmel[1]; *Mike Marsh*[1]; [1]Math2Market

Imaging workflows that create digital twins of physical samples and then computationally measure the material properties of the samples through simulation are well-demonstrated and valuable characterization techniques. It is desirable to then digitally adjust the parameters of the sample (e.g. fiber volume content, fiber orientation, void content, etc) to derive new materials with improved properties. Here we show how to make digital twins of empirical samples, statistical twins with identical parameters, siblings with single-parameter changes, and cousins with multi-parameter changes. This approach informs the engineering design team of the material properties of a wide variety of samples. In this example, we systematically vary fiber volume content and void content in a fiber-reinforced composites application and solve the mechanical properties for each digital experimental variant, reaffirming the "Digital Transformation" pattern that provides clear economic and scalability advantages. The framework shown extends to conduction, flow, acoustic, and other properties characterization.

11:30 AM

Pinax: A Machine Learning Platform for Data-Driven Materials Development: *Satoshi Minamoto*[1]; Takuya Kadohira[1]; Masahiko Demura[1]; [1]National Institute for Materials Science

The National Institute for Materials Science (NIMS) is developing a robust platform to accelerate data-driven materials research. To date, NIMS has built an ecosystem that includes "RDE", an IoT-based data collection infrastructure; "MatNavi", a comprehensive materials database; and "MInt", a computational platform for solving complex scientific problems. Recently, we have developed "pinax", which functions as a centralized hub for data aggregation and machine learning playground. This platform provides advanced analysis provenance management, which improves the efficiency, reproducibility, and accuracy of model development. We aim to strengthen the interaction between these platforms and maximize the comprehensive capabilities of the research ecosystem.

11:50 AM

Architecture for Developing an Image Recognition Model Workflow for Workplace Safety Application: *Kyle Toth*[1]; Monika Singhal[1]; Chenn Zhou[1]; Chason Ault[2]; Matt Liddick[3]; [1]Purdue University Northwest; [2]Steel Dynamics, Inc.; [3]Charter Steel

This research presents a computer vision-based safety system using multiple models, utilizing the YOLOv8 architecture, to enhance safety by detecting workers and ensuring compliance with personal protective equipment (PPE) requirements. While the second model, trained on industry-specific and open-source data, detects PPE such as safety jackets and helmets with accuracy, the first model identifies workers. Additionally, the system monitors marked static hazard zones, issuing real-time alerts when workers enter these dangerous areas. This multi-model approach offers a practical solution for improving safety protocols and preventing accidents in steel manufacturing.

3rd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2025): Optimization of Manufacturing Processes I

Wednesday AM
June 18, 2025

Room: Room A
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Introductory Comments

9:10 AM
Application of Deep Learning Approaches to Model the Heat Treatment Process-Microstructure-Property Relationship: *Hoheok Kim*[1]; Junwoo Kang[1]; Sehyeok Oh[1]; Jaimyun Jung[1]; Sejong Kim[1]; Ho Won Lee[1]; Seong-Hoon Kang[1]; [1]Korea Institute of Materials Science (KIMS)

Designing materials to meet specific demands is essential in materials science, requiring a deep understanding of the process-structure-property (PSP) relationship. Traditional methods rely on feature engineering, while deep learning offers a framework that eliminates this need and enhances performance. This study introduces a deep learning framework to establish the PSP linkage for the heat treatment, microstructures, and mechanical properties of 42CrMo4 steel. We employed a conditional StyleGAN to generate microstructure images based on tempering temperatures and a ResNet algorithm to predict yield strength, tensile strength, and elongation from these images. Samples were heat-treated at various temperatures, revealing that lower temperatures resulted in tempered martensite, while higher temperatures increased ferrite content. Strength values decreased with rising tempering temperatures for both observed and generated images. The ResNet predictions aligned well with actual measurements, demonstrating the framework's ability to generate plausible microstructures and accurately predict properties under new conditions.

9:30 AM
ANN-Based Prediction of Steel Hardenability: *Hai-Lin Chen*[1]; Yunpeng Ma[1]; Qing Chen[1]; [1]Thermo-Calc Software

We present a general artificial neural network (ANN) model for predicting microstructure formation and hardness in continuously cooled steels based on composition and austenitization condition. The model includes specialized sub-models for start and finish transformation temperatures, fractions of individual phases (ferrite, pearlite, bainite, and martensite), and hardness, as well as additional critical quantities. Thermo-Calc calculations and principles of physical metallurgy were integrated to enhance model accuracy and generalization. Additionally, a robust algorithm was developed to enable rapid generation of Continuous Cooling Transformation (CCT) diagrams, detailing transformation temperatures and critical cooling rates, for any specific steel compositions and austenitization conditions. These predicted diagrams, along with phase fraction and hardness estimations, provide valuable guidance for optimizing steel heat treatments to achieve desired mechanical properties.

9:50 AM
A Study on Digital Tools for the Safe and Sustainable Design of Materials: *Andrea Gregores Coto*[1]; Christian Precker[1]; Santiago Muiños Landin[1]; Leticia Hernando Rodríguez[2]; [1]AIMEN; [2]UPV/EHU

The urgent need to replace toxic hard chromium coatings has led the MOZART project to propose nickel-matrix nanocomposite coatings, which provide high corrosion and wear resistance without harmful environmental impacts. However, these coatings typically rely on boric acid, which conflicts with EU REACH standards. Our approach leverages a Conditional Variational Autoencoder to map the latent space of potential molecular alternatives, with Genetic Algorithms guiding the search to regions likely to yield safe and sustainable substitutes. Additionally, we assess the importance of molecular representation to improve model training. This innovative use of machine learning to optimize latent space demonstrates a powerful pathway for sustainable materials discovery in manufacturing.

10:10 AM
Chemical and Materials Informatics for Rapid Toxin-Free Product Development: *James Saal*[1]; [1]Citrine Informatics

Discovering and/or designing replacements for toxic chemicals such phthalates and per- and polyfluoroalkyl substances (PFAS) from coatings and materials requires modeling capabilities to not only identify discrete small molecules that can mimic PFAS properties but also predict the highly-nonlinear interactions of these additives in coating and materials formulations that give rise to performance metrics of interest (e.g., resistance to wear, plasticization, and flammability). Citrine Informatics is a materials and chemicals informatics software company for accelerated design of novel products and manufacturing processes. Several relevant Citrine success stories will be shared, including the discovery of high-conductivity organic semiconductors with Panasonic and the development of non-phthalate plasticizers for polystyrene plastics with MIT. In each case, Citrine's tools were used to connect physics-based simulations and existing experimental data to predict real-world chemicals and materials performance and rapidly identify candidate materials for lab-scale validation, resulting in a significant acceleration of product development.

10:30 AM Break

10:50 AM
AI-Simulation Workflow to Accelerate Computational Discovery of Graphitization Product of Detonation Nanodiamonds: *Xiaoli Yan*[1]; Millicent Firestone[1]; Álvaro Vázquez-Mayagoitia[1]; Murat Keçeli[1]; Eliu Huerta[1]; [1]Argonne National Laboratory

Detonation nanodiamonds (DNDs) are known to exhibit diverse morphologies, including carbon dots and nano-onion structures, which depend on various post-detonation processing parameters. While experimental techniques used to study these structures are widely regarded as accurate, they are costly, labor-intensive, and often impractical for exploring the full design space of process parameters. In this work, we introduce an AI-assisted molecular dynamics simulation framework to accelerate the optimization and refinement of process parameters for DND synthesis. ReaxFF-based simulations are performed on nanodiamonds with different morphologies, enabling the exploration of their structural evolution under varying process conditions. To predict time-dependent morphological transitions, we develop a graph-diffusion model that integrates these simulation results, offering a predictive tool for understanding the impact of parameter combinations on nanodiamond properties. This AI-driven approach significantly enhances the efficiency of the design process, reducing reliance on expensive experimental trials and opening new avenues for tailored nanodiamond production.

11:10 AM

ML-Based Process Monitoring for Porosity Detection and Rectification in L-PBF of SS316: *Christian Gobert*[1]; Guru Madireddy[1]; Emir Beg[1]; Romeo Kwihangana[2]; Kyle Ryan[2]; [1]Sentient Science; [2]ARCTOS

Laser Powder Bed Fusion (L-PBF) process monitoring in the aim of porosity mitigation and consistent material performance is an outstanding issue in additive manufacturing. Sentient Science and ARCTOS have worked together to develop a ML-based process monitoring system and porosity rectification strategy for L-PBF. The ARCTOS' PANDATM L-PBF system is equipped with ARCTOS' AMSENSE sensor suite. Near-infrared optical tomography imaging, long wave infrared imaging, and visible wavelength imaging are all used to capture process signatures. Sentient Science has developed a machine learning (ML) based porosity detection model to identify pore based on collected in-situ monitoring data and process context features. Identified pores are rectified with Sentient Science's remelt rectification strategy, whereby a set of scan vectors and their parameters are selected according to apparent porosity size. The DC-IM and AMSENSE system is integrated into a layer wise closed loop system that monitors and repairs porosity in L-PBF automatically.

11:30 AM

Physics-Informed ML for Crystal Growth Manufacturing: *Katherine Colbaugh*[1]; Crystal Zhu[2]; Petia Koutev[1]; [1]Crystal Growth Solutions, LLC; [2]Case Western Reserve University

Single crystal materials are the functional components in a variety of applications including energy, semiconductor, medical imaging, nuclear detection, electrification, and telecommunication. The demands for crystal materials are rising, driving an increase in specifications that require higher levels of testing, design, data analysis, and operation. However, traditional data-driven AI methods are not effective due to the long cycle times - days to months, high cost of experimentation - high-temperature, precious metals, and rare-earth elements, and complexity of the crystal growth processes – multidisciplinary, many control parameters and measured variables. Here we have developed a deep-tech approach to combine physical domain knowledge and ML models. This benchmark study on industrial data validates the predictive capabilities of physics-informed ML for use in crystal growth manufacturing, including melt growth, solid-state synthesis, vapor deposition, and epitaxy. The methods developed in this work enable data-driven decision-making to increase yield, optimize parameters, and reduce crystal defects.

11:50 AM

Performance Analysis of Different Shaped Tool Electrodes During Electrical Discharge Machining of Inconel 718: *Shankar Singh*[1]; [1]Sant Longowal Institute of Engineering & Technology (SLIET), Longowal

Electrical discharge machining is used for machining electrically conducting material by thermal energy, which leads to local heating followed by melting and evaporation of the work surface, resulting in small craters. Complex geometries involve different shapes, and tool electrode plays a major role in reproducing the shape on component. The aim of the current study is to explore the effects of copper tool electrode shapes along with other main EDM process factors on the basic machining performance, during EDM of Inconel 718. The different cross sections of electrode used in the work include circular, square and hexagonal. The effect of different tool electrode geometry (TEG) (circular, square and hexagonal), pulse current (Ip), pulse-on time, gap voltage on material removal rate, tool wear rate, and surface roughness have been studied. L9 (34) orthogonal array was used to perform experimental runs, and the results were analysed using Regression Analysis.

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): ICME Application to Advanced Manufacturing III

Wednesday AM
June 18, 2025

Room: Room E
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM

Tailoring Microstructure in Functionally Graded NiTi Alloys Using In-Situ Alloying Directed Energy Deposition: *Chinnapat Panwisawas*[1]; [1]School of Engineering and Materials Science, Queen Mary University of London

Inhomogeneous non-equilibrium microstructures of NiTi alloys can be induced by additive manufacturing (AM), resulting in compromised performance and impeded functional applications. NiTi alloys with varying gradient compositions have been in-situ alloyed using directed energy deposition (DED): mixed powder NiTi, graded Ti/Ni, and graded Ti/NiTi, to achieve tailored microstructure gradients. The printability of these graded materials was evaluated to control intermetallic phase distribution. Systematic investigations of microstructural characterisation, phase transformation, and mechanical properties have been performed to obtain tailored microstructure. Computational modelling unveils the mechanisms governing dynamic temperature fluctuations, as well as thermal and mass transport within melt pools. Effective control over the formation and distribution of intermetallic compounds has been achieved by a broadening of the martensitic transformation interval through microstructure gradient design. This study provides valuable insights into the fabrication of AM graded NiTi alloys, thus enabling intricate structural designs tailored to meet specific functional requirements.

9:30 AM

ICME Modeling for Process-Structure-Property Toolchain Development for Laser Powder Bed Fusion: *Ranadip Acharya*[1]; Nitin Chandola[1]; Subham Mridha[1]; Boliang Zhang[1]; Vijay Jagdale[1]; [1]Collins Aerospace

This abstract presents an Integrated Computational Materials Engineering (ICME) approach for developing a comprehensive toolchain aimed at optimizing the laser powder bed fusion (LPBF) process. The toolchain integrates models that link processing parameters to resultant microstructure and material properties, enabling predictive capabilities for LPBF applications. By systematically analyzing the thermal, mechanical, and metallurgical behaviors during the LPBF process, this framework allows for the identification of optimal processing conditions tailored to specific material systems through fast-acting analytical models and a high-fidelity computational toolchain. The study employs computational fluid dynamics, cellular automata, phase field modeling and crystal-plasticity based finite element analysis to simulate the dynamic interactions between process variables and microstructural evolution resulting in property variation. Ultimately, this ICME framework provides a robust foundation for the future development of 'first-time-right' technologies in additive manufacturing.

9:50 AM

Enhancing the Printability of Laser Powder Bed Fusion-Processed Aluminum 7xxx Series Alloys Using Grain Refinement and Eutectic Solidification Strategies: *Chukwudalu Uba*[1]; [1]University of Louisiana Lafayette

Additive manufacturing, particularly LPBF, is vital to Industry 4.0, enabling high-precision part production across aerospace, biomedical, and manufacturing sectors. This layer-by-layer technology improves material properties over conventional methods, especially in high-performance alloys like titanium and steel. Al 7xxx alloys offer low density and high-specific strength yet face LPBF challenges such as hot cracking and porosity due to rapid solidification and thermal gradients. This study presents a computational and experimental framework to enhance Al 7xxx LPBF processibility via compositional modification. Using CALPHAD, printable Al 7xxx compositions were designed with V, Ti, and Mg additions to enable grain refinement and eutectic solidification. Subsequent LPBF/SLM experiments and characterization tests, such as metallography (SEM), SEM, EDS, XRD, and micro-CT scan, confirmed the production of refined microstructures with reduced porosity. This work supports the Materials Genome Initiative's goal to accelerate materials development, promoting crack-free, high-quality Al 7xxx components through an integrated computational materials engineering approach.

10:10 AM

Physics-Based Modeling for Fatigue Crack Initiation Predictions in Additively Manufactured AlSi10Mg Alloys: *Deepali Patil*[1]; Anthony Spangenberger[1]; Diana Lados[1]; [1]Worcester Polytechnic Institute

Additive manufacturing (AM) is rapidly becoming an essential manufacturing process across various industries due to its design flexibility and potential for substantial weight, cost, and energy savings. However, the use of AM for safety-critical components is limited by process-induced defects, which reduce fatigue lifetimes and increase variability. In this research, Stochastic Volume Elements (SVEs) of AM AlSi10Mg are developed for a given set of process parameters using a physics-based approach and fatigue loading is simulated via crystal plasticity simulations with FFT solvers. The stress-strain (S-S) response from these simulations is post-processed to obtain a Fatigue Indicator Parameter (FIP), aiding in predicting the Fatigue Crack Initiation (FCI) life of these alloys. This model is calibrated and validated with experimental fatigue data, allowing it to predict fatigue crack initiation life and S-N curves across the AM process parameter space. The feasibility of this approach and future modeling initiatives will be discussed.

10:30 AM

Effect of Random Porosities and Surface Roughness on Fatigue Life of Additively Manufactured Maraging Steel: Aditya Pandey[1]; *Vidit Gaur*[1]; [1]Indian Institute of Technology Roorkee

A combined approach of machine learning, computational fluid dynamics and analytical model was established to explore the interaction between porosity distribution and surface roughness on the fatigue life of additively manufactured components. A new fatigue life estimation model was proposed by introducing parameter gamma () by modifying the Murakami's model based on defect size and effective stress. A total of 100 fatigue test were conducted at different stress ratios followed by the post fracture defect analysis and surface roughness measurements. Different machine learning algorithms such as artificial neural network (ANN) and random forest (RF) etc. were employed to estimate the fatigue life. The results revealed that the randomly distributed subsurface porosities and surface defects increases the scatter in fatigue lives thereby leading to uncertainty in fatigue life prediction. Furthermore, the machine learning algorithms exhibit promising prediction performance, especially when considering the parameter gamma and combining surface roughness with porosity.

10:50 AM

Numerical Investigations on the 3D-Printed Porous Bone Tissue Engineering (BTE) Scaffolds Fabricated via Selective Laser Sintering (SLS) and Fused Filament Fabrication (FFF) Processes: *Ans Al Rashid*[1]; Muammer Koc[1]; [1]Hamad Bin Khalifa University

Additive manufacturing (AM), a.k.a 3D printing (3DP), processes allow for the rapid, on-site, and on-demand fabrication of complex, intricate, and customized patient-specific implants. Therefore, AM technology is now being widely explored and adopted for the fabrication of bone tissue engineering (BTE) scaffolds. However, the dimensional stability, control and accuracy of such structures are crucial to serve the desired functionalities, i.e., providing a template for cell adhesion, growth and proliferation. In this study, numerical modelling and simulation tools are employed to investigate the different unit cell designs for BTE scaffold fabricated via selective laser sintering and fused filament fabrication processes. In addition, the effect of using different materials (i.e., polyamide-12 and polyether ether ketone) on dimensional accuracy (warpages) and residual stresses is investigated. The results of this study will provide a basis for appropriate process and material selection for producing such structures beforehand fabrication for sustainable use of materials and resources.

11:10 AM

Modeling the Effect of Powder Reuse on Meltpool Dynamics and Defect Formation in Additively Manufactured Components: *Pranjal Chauhan*[1]; Amarendra Singh[1]; [1]Indian Institute of Technology Kanpur

The reuse of metal powder in additive manufacturing provides economic and environmental advantages through reduced raw material consumption and minimized waste. However, repeated powder reuse introduces variability in material properties, impacting melt pool stability and potentially compromising the structural integrity of manufactured parts. A 2D numerical model is developed to address these challenges by simulating the Electron Beam Melting (EBM) process with powder bed composed of a mixture of virgin and reused alloy powders. Overall, an ICME-based approach is implemented to optimize the blend ratios of virgin and reused powders, aiming to reduce defect formation and improve cost efficiency. This framework provides insights into powder management strategies to limit defect formation by optimizing the mixing ratio of virgin and reused powders for consistent part performance in additively manufactured EBM components.

11:30 AM

Computational Investigation on the Combined Effect of Surface Roughness and Pore Attributes on Strain Concentrators in Metal Additively Manufactured Materials: *Erick Ramirez*[1]; George Weber[2]; Saikumar Yeratapally[3]; Kenji Shimada[1]; [1]Carnegie Mellon University; [2]NASA Langley Research Center; [3]Science and Technology Corporation

Metal additive manufacturing (AM) provides a pathway for creating highly optimized components. However, porosity and surface roughness (SR) continue to be prevalent issues for fatigue performance despite best efforts in optimizing process parameters and postprocessing techniques. This work uses finite element analysis to conduct a parametric study to link various pore attributes (i.e., size, aspect ratio, orientation, and location) to strain concentration factors (SCFs) in the presence of SR under elastic/plastic deformation during uniaxial loading. Keyhole and lack-of-fusion pores are idealized by prolate and oblate ellipsoids, respectively, while SR is reconstructed from high-resolution X-ray computed tomography images of an AM tensile specimen. Each simulation of the parametric study assumes a single pore in a Ti-6Al-4V material, modeled with J2-plasticity. This investigation reveals how isolated porosity increases SCF at the rough surface and how variability in SR geometry results in variability in SCF at the pore.

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): ICME for Materials and Process Design I

Wednesday AM
June 18, 2025

Room: Room F
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Invited
An Approach to Implementing Sustainability Into Structural Materials Design: *Carelyn Campbell*[1]; [1]National Institute of Standards and Technology

The demand for more sustainable alloys and processes requires a new element in the well-defined processing-structure-property-performance systems approach. As the design process is always a balancing of various conflicting objectives, several key challenges in incorporating sustainability and recyclability into the design process are considered. What are the available tools to evaluate different processes methods and end-life recyclability of the designed material? What tools are needed to evaluate available scrap materials that may reduce cost, energy consumption, and emissions? How can the amount of scrap material be increased in the primary alloy content without impacting the desired performance? How does one identify critical materials and design for replacement alloying elements? Much of the infrastructure required to meet these new challenges have been developed through the Materials Genome Initiative. Some examples of the tools available to meet these challenges are applied to different Al, steel, and superalloy designs.

9:30 AM
Rapid and Flexible Design of Alloys Using The Alloy Optimization Software (TAOS): *Nicholas Ury*[1]; Brandon Bocklund[1]; Vincenzo Lordi[1]; Aurelien Perron[1]; [1]Lawerence Livermore National Laboratory

The Alloy Optimization Software (TAOS) is a user-friendly tool that allows for rapid design of alloys through black-box optimization. By coupling with Calphad-based software packages such as PyCalphad and Thermo-Calc, users can leverage their own private or unencrypted databases, commercial databases, or a combination thereof to meet their specific alloy optimization needs. With a "bring-your-own-model" feature, TAOS also allows users to go beyond Calphad-based calculations and incorporate custom properties into their alloy design. In addition, TAOS provides bi-objective optimization and sensitivity analysis that enables visualizing the relationships between the composition and desired properties. Case studies will be presented to showcase TAOS's user-friendly interface and how users are able to create their own models and utilize these new features to aid in their alloy design efforts. TAOS can be directly licensed by end users: https://softwarelicensing.llnl.gov/product/taos.Prepared by LLNL under Contract DE-AC52-07NA27344.

9:50 AM
Predicting the Color of Gold-Based Alloys Using a CALPHAD-Based Model: Incorporating Composition, Heat Treatment, and Viewing Conditions: *Xin Wang*[1]; Bartek Kaplan[2]; Clay Houser[1]; Paul Mason[1]; Andreas Markstrom[2]; [1]Thermo-Calc Software Inc; [2]Thermo Calc Software Ab

We present a CALPHAD-based computational model for predicting the color of gold alloys, considering critical factors such as alloy composition, heat treatment temperature, illuminant wavelength distribution, observer viewing angle, and material thickness. This model leverages thermodynamic databases to account for the presence of intermetallic compounds, enabling comprehensive simulations of gold-based alloy colors. Core methodology involves the calculation of the dielectric function for each phase present in the alloy, which is then used to predict the material's optical properties. For single-layer systems, the Fresnel equations are applied to model light reflection and transmission. For more complex structures, such as multi-layered configurations, a transfer matrix method is utilized. This multi-faceted approach allows for precise color predictions under varying conditions, providing a robust tool for designing gold alloys with tailored aesthetic properties. Our model offers significant advancements in the prediction and design of gold alloys where precise control over material appearance is essential.

10:10 AM
Intelligent Materials Design for Rhenium Refractory Complex Concentrated Alloys: *Abdelrahman Garbie*[1]; [1]University of Louisiana Lafayette

This study focuses on the computational design of Refractory Complex Concentrated Alloys (Re-RCCAs), leveraging ICME frameworks to integrate empirical data, machine learning models, and alloy design methodologies. Our approach optimizes Re-RCCA compositions for extreme environments requiring mechanical strength, thermophysical stability, and radiation tolerance. We employ CALPHAD simulations, high-throughput semi-empirical calculations, and machine learning-based modeling to minimize waste and enhance efficiency. Machine learning predicts optimal compositions while reducing experimental iterations and material waste, following a Lean Six Sigma approach.The ICME workflow involves literature review, element selection, HEAPS screening, and CALPHAD modeling to predict phase stability. Machine learning then co-optimizes alloy compositions, significantly reducing trials. This efficient, cost-effective process maximizes resource use and minimizes loss of expensive powders, highlighting ICME's potential in advanced alloy design.

10:30 AM Break

10:50 AM
Design Principles for Controlling the Miscibility in Refractory Multi-Principal Component Alloys: *John Cavin*[1]; Pravan Omprakash[1]; Rohan Mishra[1]; [1]Washington University in St. Louis

The high-dimensional compositional space of multi-principal component alloys (MPCAs) challenges traditional methods for efficiently predicting phase stability to design alloys. For applications like catalysis, single-phase miscible solid solutions are desirable, whereas hard precipitates in a solid solution matrix suit high-temperature structural uses. Design principles to deliberately control the miscibility of MPCAs and rapidly identify regions in the multidimensional space where single phase or mixed phase microstructures are expected to be thermodynamically stable are of interest. We address this need through a thermodynamic model that generates high-dimensional convex hulls of alloy free energies using polynomial enthalpy models fit to the free-energy of equimolar and non-equimolar solid solutions and precipitates derived from density-functional theory calculations. We present results on refractory high entropy alloys with up to six elements that exhibit promising miscibility predictions, along with design principles for selecting additive elements to stabilize otherwise immiscible equimolar alloys and vice-versa.

11:10 AM
Exploring Alloying Strategies for Enhanced Strength and Ductility in High-Temperature Additively Manufactured Lightweight Alloys: *Avik Mahata*[1]; [1]Merrimack College

Additive manufacturing (AM) of high-strength aluminum alloys faces significant challenges due to rapid melting and solidification, leading to brittleness from excessive intermetallics and reduced ductility under tensile stress at elevated temperatures. To overcome these limitations, we explore novel alloying strategies by introducing elements such as Ti, Zr, Ni, Sc, Mn, and Ce into the aluminum matrix. Utilizing density functional theory (DFT) and molecular dynamics (MD) modeling, we investigate how targeted alloying can stabilize intermetallic phases, prevent coarsening, and refine microstructures to enhance tensile ductility. By forming thermally stable, nanoscale precipitates and optimizing the balance between soft and hard phases, we aim to reduce brittleness and improve deformability without compromising strength. This research provides a computational framework for designing aluminum alloys capable of withstanding the thermal and mechanical demands of high temperature AM applications.

11:30 AM
Computationally Guided Alloy Design for Refractory Complex Concentrated Alloys With Tensile Ductility Made by Laser Powder Bed Fusion: Dillon Jobes[1]; Daniel Rubio-Ejchel[1]; Jacob Hochhalter[2]; Amit Misra[2]; *Liang Qi*[1]; Yong-Jie Hu[3]; Jerard Gordon[1]; [1]University of Michigan; [2]University of Utah; [3]Drexel University

Single-phase body-centered cubic refractory complex concentrated alloys (RCCAs) retain strength at high temperatures but typically lack room-temperature ductility, causing cracking and premature failure when processed by laser-based additive manufacturing (AM). We developed an alloy design framework for enhancing tensile ductility in non-equimolar RCCAs within the Ti–V–Cr–Nb–Zr–Ta system. Density functional theory (DFT) and machine learning screened ~10 alloy compositions for ductility, followed by Scheil solidification modeling to exclude compositions prone to micro-segregation and cracking. Two alloys, Ti0.4Zr0.4Nb0.1Ta0.1 and Ti0.486V0.375Ta0.028Cr0.111, were selected, fabricated via laser powder bed fusion (L-PBF) AM, and evaluated for solidification defects, microstructure, and mechanical properties. Both alloys achieved tensile yield strengths >800 MPa and failure strains >5%. Premature failure due to un-melted high melting point elements was observed, highlighting areas for further optimization. These results demonstrate the framework's effectiveness in designing ductile RCCAs for AM applications.

11:50 AM
Study on Hydrogen Embrittlement in Steels Using First Principles Calculations: Sanyam Totade[1]; *Abhishek Thakur*[1]; Appa Chintha[1]; [1]Tata Steel

Hydrogen embrittlement leads to serious degradation in toughness and strength of steels. This poses an important aspect for industries to mitigate hydrogen embrittlement in steels to increase their usability and prevent failure especially under hydrogen environment. In this context, using first-principles calculations, we have studied the energetics of hydrogen in different structural traps, such as voids, dislocations, and grain boundaries, present in BCC Fe. Hydrogen stability under the presence of common solute atoms present in steel has also been studied. Finally, hydrogen behavior at Fe/precipitate interface has been investigated with a focus on different carbides potentially present in steel. Our findings show that tetrahedral voids present in Fe stabilizes hydrogen more as compared to the octahedral voids. Also, the presence of Si, Co, Cr, Mn, and S among other common solutes traps hydrogen efficiently within Fe.Keywords: Hydrogen Embrittlement; First-principles calculations; Structural traps; Precipitates.

The 7th International Congress on 3D Materials Science (3DMS 2025): Multimodal, Multiscale, and/or Correlative 3D Characterization

Wednesday AM
June 18, 2025

Room: Room D
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Invited
In-Situ Characterization of Martensitic Phase Transformations During Mechanical Cycling Using In-Situ Topotomography and Dark-Field X-Ray Microscopy: *Ashley Bucsek*[1]; Celeste Perez[1]; Janice Moya[1]; Adam Creuziger[2]; Can Yildirim[3]; Carsten Detlefs[3]; Jon Wright[3]; Wolfgang Ludwig[3]; [1]University of Michigan; [2]National Institute of Standards and Technology; [3]European Synchrotron Radiation Facility

Reversible martensitic phase transformations enable the functional properties of many "switchable" multiferroic materials. Due to the complex, transient, and 3D nature of martensitic phase transforming microstructures, understanding these behaviors is a significant scientific challenge. In particular, hysteresis and functional fatigue associated with interfacial stress fields at the phase interfaces remain major technological barriers. Our goal is to investigate the cyclic activation and propagation of martensitic microstructures in situ and in 3D using electron backscatter diffraction, diffraction contrast tomography, topotomography, and dark-field x-ray microscopy during mechanical cycling. The results show the 3D emergence and evolution of the 3D microstructures, individual phase interfaces, and interfacial stress fields. The results will lead to a new framework for understanding martensitic phase transforming materials that emerges from a multiscale understanding of stress-activated habit plane variant selection, incorporates the important role of defects, interfacial stress fields, and has broad implications for imperative crosscutting micromechanics challenges.

9:30 AM
Multimodal Assessment of Mechanically Induced Transformation and Damage in TRIP Steels Using X-Ray Nanotomography and Pencil-Beam Diffraction Tomography: *Hiroyuki Toda*[1]; Kyosuke Hirayama[2]; Hiro Fujihara[1]; [1]Kyushu University; [2]Kagawa University

A comprehensive multimodal measurement environment integrating X-ray nano- and micro-tomography techniques and a special X-ray diffraction technique has been developed and was applied for the first time to practical metallic materials. The X-ray diffraction method used is a special one in which a collimated X-ray beam of 1 micron in diameter is scanned as the sample is rotated, hitting all microscopic regions of the sample from all directions. The three techniques were installed on a single synchrotron beamline (BL20XU at SPring-8) and the deformation, phase transformation, damage and fracture processes of a single TRIP steel specimen were visualised and analysed. The transformation behaviour of a large number of austenite grains was analysed individually to identify the factors controlling the behaviour. It was found that the phase transformation rate is influenced by the crystallographic orientation and dislocation density of individual austenite grains, and that this also affects subsequent damage behavior.

9:50 AM

3D Investigation into the Effects of Microstructure on Humid-Air Environmentally Assisted Cracking in 7xxx Aluminium Alloys: *Matthew Curd*[1]; Jack Donoghue[1]; Cameron Grant[1]; Ryan Euesden[1]; Philip Prangnell[1]; Timothy Burnett[1]; [1]University of Manchester

7xxx series aluminium alloys are commonly utilised as structural materials in aerospace applications due to their high specific strength and fracture/fatigue resistance. However the latest generation of these alloys suffers from poor humid-air (hydrogen) environmentally assisted cracking (EAC) performance. To better understand the influence of microstructure on EAC, two short (~400um) cracks produced in warm humid air within old and new generation 7xxx alloys have been serially sectioned using a femtosecond (fs-) laser system coupled to an SEM. The resulting large volume, high resolution, multimodal datasets allow the crack paths through the grain structures to be visualised and key parameters of the crack-interacting grains to be assessed, and compared. The morphology of the cracks (including branching and deflections) is explored and these are compared to crack tip regions. Finally, we briefly show how the microstructural information collected can inform modelling efforts, linking crack tip hydrogen production to EAC rates.

10:10 AM

3D Reconstruction of a HighEnergy Diffraction Microscopy Sample Using MultiModal Serial Sectioning With HighPrecision EBSD and Surface Profilometry: *Gregory Sparks*[1]; Simon Mason[2]; Michael Chapman[3]; Jun-Sang Park[4]; Hemant Sharma[4]; Peter Kenesei[4]; Stephen Niezgoda[2]; Michael Mills[2]; Michael Uchic[3]; Paul Shade[3]; Mark Obstalecki[3]; [1]University of Dayton Research Institute; [2]The Ohio State University; [3]Air Force Research Laboratory; [4]Argonne National Laboratory

High-energy diffraction microscopy (HEDM) combined with in-situ mechanical testing is a powerful nondestructive technique for tracking the evolving microstructure within polycrystalline materials during deformation. However, it is known that HEDM can fail to identify certain microstructural features, particularly smaller grains or twinned regions. Characterization of the identical sample volume using high-resolution surface-specific techniques, particularly electron backscatter diffraction (EBSD), can not only provide additional microstructure information about the interrogated volume but also highlight opportunities for improvement of the HEDM reconstruction algorithms. In this study, a sample fabricated from undeformed "low solvus, high refractory" nickel-based superalloy was scanned using HEDM. The volume interrogated by HEDM was then carefully characterized using a combination of surface-specific techniques, including epi-illumination optical microscopy, zero-tilt secondary and backscattered electron imaging, scanning white light interferometry, and high-precision EBSD. Custom data fusion protocols were developed to integrate and align the microstructure maps captured by these surface-specific techniques and HEDM.

10:30 AM Break

10:50 AM

Scaling Ductility From Microscale to Bulk by Coupling Crystal Plasticity Simulations With Deep Learning: *Laura Vietz*[1]; Rebecca Divine[1]; Carter Cocke[2]; Ashley Spear[1]; [1]University of Utah; [2]California Institute of Technology

Characterizing ductile fracture in bulk materials can be challenging and cost-prohibitive, namely for materials used in harsh environments like nuclear reactors. In these cases, experimental characterization is limited to sample sizes below the representative volume element (RVE), called statistical volume elements (SVEs), which exhibit scatter in mechanical properties due to size effects. The RVE is the smallest volume of material above which a property of interest converges to bulk behavior. This research aims to link microstructure-dependent SVE-derived mechanical properties to bulk-scale properties by combining crystal plasticity simulations with deep learning. As a proof-of-concept, a generated 3D dataset trained a convolutional neural network to predict RVE ductility from SVE responses. The dataset is populated with different-sized SVEs and their corresponding stress-strain responses for four materials simulated using a damage-enabled large-strain elasto-viscoplastic FFT model for ductile fracture. This work could enable a cost-effective method for characterizing bulk properties using small-scale test specimens.

11:10 AM

Multiscale Microstructure and Strain Characterisation in Aluminium Using Dark-Field X-Ray Microscopy: *Adam Cretton*[1]; Albert Zelenika[2]; Johann Haack[1]; Felix Frankus[1]; Sina Borgi[1]; Flemming Grumsen[1]; Can Yildirim[3]; Carsten Detlefs[3]; Grethe Winther[1]; Henning Friis Poulsen[1]; [1]Technical University of Denmark; [2]Institute for Applied Materials, Karlsruhe Institute of Technology; [3]European Synchrotron Radiation Facility

Using Dark-Field X-ray Microscopy (DFXM), this study captures the multimodal evolution of strain and dislocation dynamics in bulk aluminium samples, revealing insights into deformation mechanisms. DFXM enables simultaneous in-situ 3D mapping of dislocation density, local orientation, and elastic strain fields, capturing the complex scale-bridging interactions that govern plasticity. Observations show that dislocation cells form stochastically at low strains but exhibit a transition near 5.20% strain, where strain accommodation progresses through the emergence of geometrically necessary boundaries (GNBs) that accommodate larger strain gradients. By tracking boundary evolution and strain accommodation across deformation steps, this multimodal approach demonstrates scaling behavior and highlights universal stochastic processes in dislocation structuring under strain. We extend these findings with ongoing work in 4D tracking, analysing evolving dislocation patterns and providing data applicable to dislocation dynamics and crystal plasticity models.

11:30 AM

Multimodal Characterisation of Calcite Crystals Precipitated From Bio-Cementation: *Marilyn Sarkis*[1]; Carsten Detlefs[1]; James Ball[1]; Can Yildirim[1]; [1]European Synchrotron Radiation Facility

Bio-cementation is a process during which calcite crystals are precipitated in the sand medium thanks to bacterial activity. These crystals will then bond the sand particles together and make the material cohesive, making this process suitable as a soil-reinforcement technique. However, the growth and the microstructure of these crystals remain unstudied to this day. This study proposed a multimodal approach in order to characterize the precipitated calcite crystals, and uses X-ray computed tomography (CT), 3D X-ray diffraction (3DXRD) as well as Dark-Field X-ray Microscopy (DFXM) on ID03 at the ESRF. Preliminary results show that the precipitated crystals are polycrystalline and grow by stacks on top of each other as the process of bio-cementation goes on. The grains also present elastic strain, that is mainly due to growth. Further investigation will include 3D strain mapping in the calcite crystals, to see the effect of the mechanical loading on the microstructure.

11:50 AM

3D In-Situ Characterization of Twinning Inside Individual Mg4Al Grains Using DarkField X-Ray Microscopy: *Sangwon Lee*[1]; Michael Pilipchuk[1]; Can Yildirim[2]; Duncan Greeley[3]; Qianying Shi[1]; Tracy Berman[1]; Adam Creuziger[4]; Evan Rust[4]; Carsten Detlefs[2]; Veera Sundararaghavan[1]; John Allison[1]; Ashley Bucsek[1]; [1]University of Michigan; [2]European Synchrotron Radiation Facility; [3]Los Alamos National Laboratory; [4]National Institute of Standards and Technology

Magnesium (Mg) alloys, being lighter than aluminum, offer potential for reducing fuel consumption in vehicles. Enhancing their mechanical properties depends on understanding deformation twinning mechanisms influenced by local stress fields. However, characterizing these local stresses before, during, and after twinning remains challenging. We present the first three-dimensional (3D) in-situ characterization of deformation twinning inside individual Mg-4wt.%Al grains under mechanical loading, using dark-field X-ray microscopy (DFXM) coupled with crystal plasticity finite element analysis. This method provides 3D spatially resolved maps of misorientation, dislocation density, and twin morphology with 100 nm resolution. Our results reveal that triple junction geometry may influence twin variant selection, twin growth is irregular and multidirectional, and twin-related junctions are sites of localized dislocation accumulation—a precursor to crack initiation. These insights into the micro-mechanisms of plastic deformation in Mg alloys can inform strategies to enhance their mechanical performance.

The 7th International Congress on 3D Materials Science (3DMS 2025): Time Resolved 3D Characterization II

Wednesday AM
June 18, 2025

Room: Room C
Location: Anaheim Marriott

Session Chair: To Be Announced

9:00 AM Invited

Capturing the Emergence of Hierarchical Microstructures in Metallic Materials: *Ashwin Shahani*[1]; [1]University of Michigan

Microstructure is the 'fingerprint' that identifies the unique characteristics of a material. Oftentimes that microstructure shows a hierarchy of length-scales, from point and line defects at the atomic scale to secondary phases at the mesoscale. This raises an important question about how various classes of defects emerge and interact with each other during processing. In this talk, I will focus on the microstructural complexity of metal matrix nanocomposites and shape memory alloys, highlighting efforts by my group in understanding and controlling that complexity to meet technological demands. Our work is made possible by real-time, three-dimensional imaging with synchrotron x rays, which enables us to obtain key insights on the evolution of microstructure, and ultimately, to test the predictions of simulations and theory. I will also explore future directions at the intersection of multimodal characterization and artificial intelligence to analyze next generation engineering materials and their hierarchical microstructures.

9:30 AM

Watching Real-Time Eutectic Solidification to Understand the Crystal Morphology Formation and Habit Plane Selection: *Paul Chao*[1]; Shanmukha Aramanda[2]; Xianghui Xiao[3]; Ashwin Shahani[2]; [1]Sandia National Laboratories; [2]University of Michigan; [3]Brookhaven National Laboratory

Our study utilizes synchrotron transmission x-ray imaging at the nanoscale to observe the eutectic solidification dynamics of the Al-Al3Ni alloy in real-time. This process reveals the simultaneous emergence of two solid crystals from the liquid, forming a periodic pattern influenced by solute diffusion and capillary effects. The investigation focuses on the formation of facets under various freezing conditions, a critical aspect for understanding and technological applications. High-resolution imaging of dynamic interfaces presents challenges, prompting the development of alternative imaging strategies. We discuss how the growth front shapes of the Al-Al3Ni eutectic relate to the 3D shape of Al3Ni crystals in the solid state. Additionally, we explore the orientation relationship and habit planes between solid Al and Al3Ni crystals, using Electron Backscatter Diffraction (EBSD) for quantification. This research provides insights into the microstructural evolution during solidification, emphasizing the interplay between phase transformation dynamics and microstructure development.

9:50 AM

Study of Grain-Scale Plastic Events in Ti-7Al Alloys With Far-Field High-Energy Diffraction Microscopy and Graph Theory: *Yuefeng Jin*[1]; Xiongye Xiao[2]; Peiyu Zhang[2]; Wenxi Li[1]; Amlan Das[3]; Katherine Shanks[3]; Paul Bogdan[2]; Ashley Bucsek[1]; [1]University of Michigan; [2]University of Southern California; [3]Cornell High Energy Synchrotron Source

Although plasticity is traditionally modeled as a smooth process in space and time, in some hexagonal close-packed materials like \945-phase titanium-aluminum alloys, plasticity can occur in localized, grain-scale bursts, even before macroscopic yield. These grain-scale plastic events are important for understanding room-temperature creep and dwell fatigue. In this work, we use far-field high-energy diffraction microscopy (ff-HEDM) to characterize such events in a Ti-7Al sample during creep loading. To study the mechanisms, we apply graph analysis, where each node represents a grain, and the edge represent the grain connectivity. We analyze both local features of event-prone regions and global characteristics across the grain network. By examining the feature distributions and changes during loading, we gain insights into the initiation, propagation, and evolution of grain-scale plastic events, enhancing our understanding of how localized deformation contributes to material failure. This work is funded by the NSF STC Center of Complex Particle Systems (COMPASS).

10:10 AM

3D Characterization of Hydrogen-Induced Damage in X70 Steel Using Synchrotron X-Ray Tomography: *Victor OKUMKO*[1]; Thilo Morgeneyer[2]; Yazid Madi[2]; Henry Proudhon[2]; Andrew King[1]; [1]Synchrotron Soleil; [2]Mines Paris PSL -Centre des Matériaux.

Hydrogen embrittlement significantly degrades the mechanical properties of metals, affecting ductility, fracture toughness, and fatigue resistance. This study examines the initiation and propagation of hydrogen-induced damage in X70 stainless steel, utilizing smooth and round-notched tensile samples to evaluate stress triaxiality effects. High-resolution synchrotron X-ray tomography and Scanning Electron Microscopy were employed to analyse surface and internal damage under varying hydrogen pressures and strain rates. In-situ tensile tests at the PSICHE beamline facilitated simultaneous mechanical testing and imaging. Results from smooth tensile samples indicate that cracks primarily initiate at the surface under moderate strain rates, while low strain rates promote deeper hydrogen diffusion, leading to internal damage. The ongoing investigation of round-notched samples aims to elucidate geometry's role in stress concentrations and hydrogen impact on crack nucleation and growth. These findings will enhance the development of a multiscale numerical model for safer hydrogen infrastructure design under the European project HyWay.

10:30 AM Break

10:50 AM
Dynamics of Individual Dislocations During Plastic Deformation: *Felix Frankus*[1]; Adam Cretton[1]; Sina Borgi[1]; Albert Zelenika[1]; Anter El-Azab[2]; Henning Poulsen[1]; Grethe Winther[1]; [1]Technical University of Denmark; [2]Purdue University

The plasticity of metals is fundamental to manufacturing, yet our understanding of the micromechanics of work-hardening remains incomplete due to complex, multiscale interactions between dislocations. Validating theoretical dislocation interaction models requires time-resolved, 3D experimental datasets that represent bulk behaviour. Recently, Dark-Field X-Ray Microscopy (DFXM) has enabled the imaging of such datasets across hundreds of micrometres within in-situ strained, millimetre-sized specimens. We present DFXM movies of aluminium tensile specimens, capturing dislocation interactions combined with meso-scale structural evolution at low strain levels, including pileups and dislocation boundaries over volumes exceeding several hundred cubic micrometres. Analysis of strain fields around dislocation lines allowed extraction of line directions and Burgers vectors, providing a detailed description of dislocation structure.We tracked a dislocation pileup configuration from formation through rearrangement to dissolution. These identified configurations serve as input for discrete dislocation dynamics simulations, allowing comparisons between experimental observations and predictions for stress fields and dislocation velocities.

11:10 AM
Grain Boundary Migration in Mesoscale Polycrystals: *Zipeng Xu*[1]; Robert Suter[1]; Gregory Rohrer[1]; [1]Carnegie Mellon University

During thermally activated grain growth, the grain boundary migrates to reduce the system's total excess free energy. Although the classical theory describes the migration behavior in bicrystals, recent studies show that this is not the case in polycrystals. In this talk, we will discuss grain boundaries' migration behavior in polycrystals from impurities and energy anisotropy effects, using two high-energy diffraction microscopy (HEDM) measured polycrystals with multiple time steps. We found that, both on average and locally around the triple junction, grain boundary energy anisotropy affects the grain growth process such that low energy grain boundaries tend to replace and grow at the expense of neighboring high energy grain boundaries. With those observations, we proposed a new mechanism of grain boundary migration, which potentially can explain the inconsistency from the classical theory. The findings suggest the importance of energy anisotropy during grain growth.

11:30 AM
High Speed High-Energy Diffraction Microscopy During Ti64 Dwell Fatigue: *Kenneth Peterson*[1]; Kelly Nygren[2]; Sven E. Gustafson[2]; Arthur Woll[2]; Paul Shade[3]; Mark Obstalecki[3]; Darren C. Pagan[1]; [1]Pennsylvania State University; [2]Cornell High Energy Synchrotron Source; [3]Air Force Research Laboratory

Dwell fatigue failure has been proposed to initiate from stress concentrations resulting from accumulated slip during dwell. However, to date, a challenge to determining precise conditions at failure nucleation stem from the difficulty of resolving the transient interplay of deformation mechanisms at appropriate time scales. Fortunately, the next generation of synchrotron-compatible load frames and wide dynamic-range X-ray area detectors have enabled diffraction data collection in situ with unprecedented speed and fidelity. This new capability allows for investigation into 3D deformation processes that had previously been inaccessible, like the subtle evolution of stress that occurs within individual grains during dwell. Here, we utilize these technological advancements to perform far-field high energy X-ray diffraction microscopy (ff-HEDM) continuously within individual dwell periods during dwell fatigue testing of Ti-6Al-4V at room temperature. FF-HEDM measurement times are reduced from approximately 10 minutes to 10 seconds, enabling unprecedented views of microscale deformation behavior during dwell.

11:50 AM
Investigating the Influence of Strain Rate on Hydrogen Embrittlement in Steel Sub-Size Tensile Specimens Using X-Ray 3D Tomography: *Luciano Santana*[1]; Victor Okumko[2]; Andrew King[2]; Thilo Morgeneyer[1]; Jacques Besson[1]; Yazid Madi[1]; [1]Mines Paris PSL - Centre des Matériaux; [2]Synchrotron SOLEIL

This study examines the effect of strain rate on hydrogen embrittlement in steel sub-size tensile specimens using X-ray 3D tomography. Tensile specimens were subjected to various strain rates in both air and a 100 bar hydrogen environment, with tests interrupted before fracture. High-resolution tomography revealed strain-rate-dependent differences in damage distribution and orientation. At moderate strain rates, damage initiates from the surface as flat ellipses perpendicular to the specimen's longitudinal axis, indicative of brittle hydrogen-induced cracking, and in the bulk as elongated ellipsoids aligned with longitudinal axis, typical of microvoid coalescence. At low strain rates, hydrogen diffuses more deeply, causing embrittlement throughout the specimen, with brittle damage parallel to the longitudinal axis observed both in bulk and at the surface. This research advances understanding of the mechanical response and damage progression in steel exposed to gaseous hydrogen.

3rd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2025): Optimization of Manufacturing Processes II

Wednesday PM
June 18, 2025

Room: Room A
Location: Anaheim Marriott

Session Chair: To Be Announced

1:40 PM
AI Guided Discovery of Lunar Derived Materials for a Sustainable Ecosystem: *Eddie Gienger*[1]; Michael Pekala[1]; Nam Le[1]; Alex New[1]; Greg Canal[1]; Karun Kumar Rao[1]; Milena Graziano[1]; Morgan Trexler[1]; Christian Sanjurjo-Rodriguez[1]; Steven Storck[1]; Elizabeth Pogue[1]; Mary Daffron[1]; Greg Bassen[2]; Aaron Baumgarten[1]; Brandon Wilfong[2]; Denise Yin[1]; Wyatt Bunstine[2]; Elizabeth Reilly[1]; Leslie Hamilton[1]; Tyrel McQueen[2]; Christopher Stiles[1]; Christopher Stiles[1]; [1]Johns Hopkins University - Applied Physics Laboratory; [2]Johns Hopkins University

One key challenge for lunar missions is manufacturing materials directly on the Moon using in situ resources. By integrating AI, high-throughput synthesis, and large language models (LLMs), we advance materials discovery, design, and fabrication in the Moon's harsh environment, reducing dependence on Earth-based resources. The core "predict-make-measure" framework utilizes AI-driven predictions, experimental synthesis, and rapid characterization, creating a closed-loop system that iterates efficiently from material concept to production. An AI-powered knowledgebase enables efficient search and optimization of lunar resources. This database aids in discovering high-hardness, high-silicon materials composed of lunar-abundant elements, while generative models and a physics-based AI screening pipeline refine composition candidates. Utilizing directed energy deposition (DED) over 250 unique materials have been synthesized. The samples are characterized with quick assessments of mechanical properties like hardness and qualitative ductility scoring. This approach sets a foundation for autonomous, sustainable material synthesis in resource constrained environments.

2:00 PM

A Data-Driven Approach to Print Performance Prediction: *Jennifer Ruddock*[1]; James Hardin[1]; [1]Air Force Research Laboratory

DIW 3D printing is a useful additive manufacturing technique for high-mix, low-volume manufacturing because the process parameters can be adapted to new materials and geometries. However, the link between printer parameters, ink properties and printed part performance is often not straightforward, resulting in a costly trial-and-error approach to print process adaptation. To avoid this onerous process, we aim to determine what minimal test print pattern can be used to predict useful print performance metrics such as the geometric fidelity (avoiding slumping, voids, etc.) and minimize overall print time. This work will first build a core dataset of potential test prints and representative print challenges then seek to link test prints to print behavior using combinations of data-driven tools.

2:20 PM

Simulation-Based Optimization of Additive Manufacturing Toolpaths to Reduce Distortion: *Ashley Gannon*[1]; Stephen DeWitt[1]; James Haley[1]; Bruno Turcksin[1]; Lauren Heinrich[1]; Thomas Feldhausen[1]; Alex Beatty[1]; Alex Roschli[1]; Andres Marquez Rossy[1]; Leah Jacobs[1]; Cameron Adkins[1]; Callan Herberger[1]; Michael Borish[1]; Liam White[1]; [1]Oak Ridge National Lab

Minimizing residual stresses and the resulting geometric distortion is important for enabling a wider adoption of additively manufactured parts. The toolpath during printing, including the dwell time between layers, is known to have a significant impact on the residual stress. We present a workflow that combines toolpath planning, simulation, in-situ monitoring, and optimization techniques to refine dwell control for improved geometric accuracy. This workflow integrates finite element analysis with real-time monitoring data to iteratively calibrate and validate simulation predictions, forming a feedback system that minimizes distortion. To quantify deviations, we use a structured blue light scanner to capture the geometry of printed part and compare the scanned geometry to the original CAD. This comparison allows us to assess distortion quantitatively and verify the effectiveness of optimized dwell parameters in reducing distortion. Additionally, this workflow can be adapted for convergent manufacturing processes, enhancing the accuracy and efficiency of hybrid production methods.

2:40 PM Break

3:10 PM

Effects of Raster Angle on the Properties of Fused Filament Fabricated Conductive Particles Reinforced Thermoplastic Polyurethane Composite and Prediction of Properties Using Artificial Neural Network: *Imran Khan*[1]; Ans AlRashid[1]; Muammer Koç[1]; [1]Hamad Bin Khalifa University, Qatar

Polymer composites find widespread industrial applications due to their high strength-to-weight ratio, low cost, easy processing, functional properties, etc. The mechanical properties of polymer composites are critical in real-world applications. 3D printing can be utilized for the fabrication of polymer composites. This study investigates the effect of raster angle (a critical process parameter) on the mechanical properties of conductive particles reinforced thermoplastic polyurethane polymer composite fabricated via fused filament fabrication (FFF). The properties of the composite were predicted using generic machine-learning algorithms based on an artificial neural network. Microscopic analysis was also performed on the test samples. It was observed that the raster angle significantly affected the composites' mechanical properties. The optimum raster angle for the composite fabrication via FFF is also suggested and verified. It was observed that machine learning can be applied to 3D printing, especially for predicting the properties of the fabricated polymer composite.

3:30 PM

Utilizing Time-Series Data for Improved Prediction of End-Point Temperature and Carbon in Basic Oxygen Furnace With a Large Industrial Dataset: *Jianbo Zhang*[1]; Maryam Ghalati[1]; Hongbiao Dong[1]; [1]University of Leicester

The Basic Oxygen Furnace (BOF) is crucial in the steelmaking process, converting molten iron into stee by elevating temperature, reducing carbon content, and controlling composition. This stage generates extensive production data, including tabular data and time-series data such as off-gas data and oxygen blowing data. Using domain knowledge, the data was carefully filtered and preprocessed, and 6517 samples were used to train, validate and test. A neural network model was designed to integrate both tabular data and time-series data as input, creating predictive models for end-point temperature and end-point carbon content separately. Several advanced time-series algorithms, including LSTM, GRU, RNNs and CNNs, were tried and compared, with LSTM yielding the best results. After model optimization, the models achieved 93.94% (±0.02%) accuracy for carbon prediction and 89.03% (±15°C) accuracy for temperature prediction on testing data, underscoring the significant improvement achieved by incorporating time-series data.

3:50 PM

Fatigue Life and Fatigue Crack Growth Rate Prediction of Additively Manufactured Al 2024 Alloy Using Generative AI and Machine Learning Models: Sneha Jayaganthan[1]; *R Jayaganthan*[2]; Saurabh Gairola[2]; [1]Stanford University; [2]Indian Institute of Technology Madras

This study investigates the prediction of fatigue life and fatigue crack growth rate behaviour in additively manufactured Al 2024 alloy using machine learning (ML). The fatigue behaviour of the additively manufactured alloy is influenced by a variety of factors such as defect size and location, columnar microstructure, surface finish, residual stress, etc. Hence, it is difficult to predict the fatigue behaviour using conventional methods. Key test variables, including stress amplitude, build orientation, stress ratio, and post-processing condition, were used as input variables. Experimental data were employed to train various ML models, including Support Vector Machines, Random Forests, Decision Trees, and Convolutional Neural Networks (CNN). Given the limited availability of experimental data, the training dataset was augmented with generative AI models. The pre-processed dataset, comprising both experimental and generative AI data, was utilized to train the above ML models, with hyperparameter tuning performed using kernel functions.

4:10 PM

On the Use of Decoder-Only Transformers to Model Time-Series based Silicon Data: *Ricardo Calix*[1]; Tyamo Okosun[1]; Hong Wang[2]; [1]Purdue University Northwest; [2]Oak Ridge National Laboratory

Silicon prediction in a steel blast furnace is crucial for maintaining high-quality metal production and optimizing furnace operations. In this study, we explore the use of decoder-only transformer neural networks (GPT-like models) for modeling time-series silicon data collected from a Midwestern steel blast furnace. While transformers are traditionally associated with text processing, we adapt the decoder architecture to directly ingest numerical tabular time-series data. Our experiments involve training a GPT model from scratch on silicon data, implementing various data preprocessing techniques, and evaluating different architectural modifications. We find that the model exhibits learning capability and, in some cases, produces promising predictions. However, further refinements are needed to enhance consistency and accuracy. We discuss the advantages of decoder-only transformers for time-series forecasting, the challenges encountered, GPU operational conditions, and potential future improvements. Our findings suggest that transformer-based architectures could play a significant role in time-series modeling for industrial applications.

4:30 PM
Estimation of SOC in Electric Vehicle Batteries Using Machine Learning Models: *Bhanu Sree Vijayanand*[1]; Shrishail C Prabhakar[1]; Jayaganthan R[1]; [1]Indian Institute of Technology Madras

The estimation of the State of Charge (SOC) of lithium-ion(LFP) batteries is critical for enhancing the performance of electric vehicles (EVs). Conventional SoC estimation methods utilise coloumb counting and SoC vs OCV measurements. In EV applications, the OCV determination is challenging as the battery pack will be in closed circuit condition during drive cycle. It is important to utilise SOC datasets of LFP batteries obtained under various drive cycles and environmental factors, which could enhance the robustness of predicting its ageing behaviour. In the present work, the SOC data of Li-ion battery (LFP) estimated with the simulated actual drive cycles, were used to train Machine learning models such as Support vector Machine (SVM), XG-Boost, CNN, LSTM for predicting the aging behaviour. The comparative study is made on predictive accuracy of these ML models used in the present work. The mechanisms on aging behaviour of Li ion battery is discussed.

4:50 PM
Development of a Massively Parallel Reduced-Order Model Based Design/Optimization Tool for Power Generation Using Natural Gas-H2 Blended Fuels: *Shashikant Aithal*[1]; Nick Killingsworth[2]; Bob Schrecengost[1]; Aaron Fisher[2]; Victor Castillo[2]; [1]Argonne National Laboratory; [2]Lawrence Livermore National Laboratory; [2]Department of Energy

Hydrogen use in power generating equipment such as gas turbines or internal combustion engines, traditionally fueled by natural gas, promises to reduce the generation of CO2. The fraction of hydrogen in the fuel mixture has a significant impact on the overall combustion characteristics and can pose unique operational challenges such as flashback in gas turbines and knocking in IC engines. Design and optimization of such power generation equipment fueled by NG-H2 blends present unique challenges on account of the large design space and conflicting constraints. We present the development of a massively parallel framework for generating data needed for AI-based models. Open-source code Cantera was used to generate over 1600 data points predicting ignition delay, flame-speed, burned gas temperatures and/or emissions over a range of conditions relevant to the operation of engines/gas turbines to generate a fast-running ROM. We will discuss current applications and possible future work.

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): Artificial Intelligence and Machine Learning in ICME II

Wednesday PM
June 18, 2025

Room: Room E
Location: Anaheim Marriott

Session Chair: To Be Announced

2:10 PM Invited
Recent Advances in Structure-Property Correlations and Their Impact on ICME-Driven Accelerated Design of Materials and Products: *Amarendra Kumar Singh*[1]; Satyam Shukla[1]; [1]Indian Institute of Technology Kanpur

The Integrated Computational Materials Engineering (ICME) approach has transformed the design, development, and deployment of materials and products by enabling the prediction and optimization of composition, microstructure, and processing paths to meet specific property and performance targets, which may include strength, ductility, and corrosion resistance, depending on the application. Structure-property relationships used in ICME workflows are primarily based on experimental data, which significantly limits the capability for inverse design. Recent advances in modeling and simulations, high-throughput experimentation, and machine learning-based tools provide a promising alternative approach. Data from ab initio calculations, crystal plasticity, and representative volume element (RVE)-based simulations supplement the experimental data, now enhanced through high-throughput experiments. Advanced machine learning models are employed to develop predictive tools that capture complex relationships among composition, microstructure, and properties. This enables a more robust platform for inverse design of materials and products. A few illustrative examples will be presented.

2:40 PM
Exploring Novel Alloys With Superior Specific Hardness Using Data-Driven Approaches: Taeyeop Kim[1]; Wook Ha Ryu[2]; Geun Hee Yoo[2]; Donghyun Park[1]; Ji Young Kim[2]; Eun Soo Park[2]; *Dongwoo Lee*[1]; [1]Sungkyunkwan University; [2]Seoul National University

The discovery of advanced alloys using experimental data-driven approaches is hindered by the challenges of managing large compositional design spaces and the risk of overfitting machine learning (ML) models. This study combines ML predictions with thin-film base high-throughput experimental verification to accelerate the discovery of novel ternary alloy systems with exceptional specific hardness. By applying ensemble learning to a dataset from combinatorial experiments, we efficiently explored a composition space involving 28 metallic elements and discovered tens of new compositions exhibiting superior specific hardness compared with previously reported alloys. The property was consistently observed in 2 mm thick ribbon samples, demonstrating scalability. Explainable AI revealed that elemental dissimilarities significantly enhance solid-solution strengthening and phase formation, offering key insights into the underlying mechanisms. This iterative ML-driven process provides a reliable approach for discovering high-performance alloys and could serve as a useful framework for future materials development.

3:00 PM Break

3:30 PM
Machine Learning Models for Predicting 3D Microstructure--Property Relationships From 2D Images: Guangyu Hu[1]; Sheila Whitman[1]; *Marat Latypov*[1]; [1]University of Arizona

Engineering properties of structural alloys depend on both alloy composition and 3D microstructure. Modeling the engineering properties requires access to 3D microstructure information, which can be obtained either from direct (yet expensive) 3D experiments or reconstruction from 2D section(s). In this contribution, we present machine learning (ML) approaches to modeling effective properties of heterogeneous materials directly from 2D sections. To this end, we consider statistical learning models based on spatial correlations and microstructure representations obtained with vision transformers as well as deep learning with convolutional neural networks. We train all models on data obtained from micromechanical 3D simulations. Upon training, the presented models only need 2D sections as input, whose experimental acquisition is much more accessible compared to 3D characterization.

3:50 PM
Deep Learning-Based Platinum Particle Analysis for Corrosion Insights in BWR Systems: *Txai Sibley*[1]; Ryan Jacobs[2]; Dane Morgan[2]; Kevin Field[1]; Elizabeth Holm[1]; [1]University of Michigan; [2]University of Wisconsin-Madison

This research investigates the use of deep learning-based image analysis models to detect platinum particles on Boiling Water Reactor (BWR) system components. These platinum particles, added through noble metal chemical addition (NMCA), are essential for preventing stress corrosion cracking by controlling water chemistry, thereby extending the lifespan of reactor parts. The study utilizes a segmentation model trained on a limited set of images to analyze platinum particles on reactor surfaces. By linking microstructural attributes with electrochemical potential (ECP), we aim to better understand corrosion behaviors and refine NMCA effectiveness evaluation. This work lays the groundwork for improving segmentation accuracy, reducing data collection and annotation costs, and deepening our comprehension of how platinum particles influence BWR reactor performance.

4:10 PM
Machine Learning for the Computational Design of Single-Crystal Superalloys: *Matthieu Degeiter*[1]; Edern Menou[2]; Armand Barbot[1]; Patricia Klotz[1]; Sami Ben Elhaj Salah[2]; Didier Locq[1]; Yohan Cosquer[3]; Mikael Perrut[1]; [1]ONERA; [2]SAFRAN TECH; [3]DGA TA

High Pressure Turbine (HPT) blades in gas turbines are designed with single crystal nickel-base superalloys, as their microstructure provides the blades with exceptional mechanical properties at high temperature. In service, the thermomechanical loadings imposed on the blade induce microstructure evolutions which eventually degrade the blade macroscopic properties. Improving the blade service life requires to develop new superalloy grades with improved creep resistance at high temperature. The fundamental mechanisms underlying the macroscopic behavior of materials are often complex, take place over extended ranges of length and time scales, and are strongly nonlinear. When the equations driving these mechanisms are not known, data-driven methods are particularly effective in guiding metallurgists and engineers. In this context, our work focuses on the construction of gaussian process models based on experimental data to estimate the creep life of superalloys as a function of their chemical composition and testing conditions.

4:30 PM
Machine Learning Models for Predicting Thermoelectric Properties in Cu-Based Alloys and Composites: *Novana Hutasoit*[1]; [1]Swinburne University of Technology

The composition of elements in alloys and metal-matrix composites plays a crucial role in defining their functional properties. Thermoelectricity, the conversion of heat into electricity, is a key characteristic for materials used in energy conversion applications. While thermoelectric properties are traditionally predicted using computationally expensive methods such as density functional theory (DFT), machine learning (ML) offers a more cost-effective alternative when paired with appropriate predictors. This study explores the use of physical properties of elements to develop ML models for predicting the thermoelectric performance of Cu-based alloys and composites. By employing data-driven techniques, this study aims to expedite the discovery and design of novel, low-cost, and environmentally sustainable thermoelectric materials.

4:50 PM
Multi-Modal Machine Learning Framework for Property Prediction in Ni-Based Superalloys and Aluminum Alloys Using Integrated Characterization Data: *Jiwon Park*[1]; Chang-Seok Oh[1]; [1]Korea Institute of Materials Science

Multi-modal machine learning approaches have emerged as powerful tools for integrating diverse materials characterization data to advance materials discovery and optimization. In this study, we present a novel framework that combines microstructural images, X-ray diffraction patterns, compositional data, and processing parameters to predict properties of Ni-based superalloy and aluminum alloys. Our model architecture employs parallel neural network branches to process each data modality independently before fusion: convolutional neural networks for microstructure image analysis, XRD data without peak and phase assessments, and fully connected layers for composition and process variables. The fused representation enables both property prediction and interpretable feature importance analysis across modalities. This work demonstrates the potential of multi-modal learning to leverage complementary materials characterization techniques for enhanced materials informatics and accelerated alloy development.

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): ICME Award Session

Wednesday PM
June 18, 2025

Room: Plenary Room
Location: Anaheim Marriott

Session Chair: To Be Announced

1:30 PM Introductory Comments

1:35 PM Keynote
ICME Industry Implementation Award: Randy Beals: **ICME-Driven Development of Magna Aural 5M and Sustainable Aural 5R Aluminum Alloys for Structural Automotive Applications:** *Randy Beals*[1]; [1]Magna International

Magna International utilized Integrated Computational Materials Engineering (ICME) to develop Aural 5M, a modified primary aluminum alloy designed for structural automotive components. Through a combination of theoretical modeling and experimental validation, Thermo-Calc and JMatPro software's were used to predict phase stability, enhance castability, and improve manufacturability while eliminating heat treatment to reduce environmental impact. Experimental results demonstrated that Aural 5M exhibited superior castability and lower porosity compared to the baseline Aural 5S. This research accelerated the development of next-generation secondary Aural R alloys, which incorporate 100% recycled content with increased levels of iron, copper, and zinc for enhanced sustainability. The evolution of Aural 5R highlights its potential for broad automotive applications and facilitates technology transfer across the industry. ICME's integration of materials data with performance and manufacturing simulations significantly reduced development time, underscoring its role in advancing innovation, optimizing material properties, and promoting sustainable practices in automotive alloy design.

2:05 PM Question and Answer Period

The 7th International Congress on 3D Materials Science (3DMS 2025): 3D Imaging at the Nano-Scale

Wednesday PM
June 18, 2025

Room: Room D
Location: Anaheim Marriott

Session Chair: To Be Announced

1:30 PM Invited
Characterizing Nanoscale Ordering Using Bragg Coherent Diffraction Imaging: Nathan Warren[1]; Chloe Skidmore[1]; Wonsuk Cha[2]; Katherine Harmon[2]; Jon-Paul Maria[1]; Stephan Hruszkewycz[2]; *Darren Pagan*[1]; [1]Pennsylvania State University; [2]Argonne National Laboratory

The amount of local ordering in many metallic alloys is sensitive to the thermal processing route that they have undergone. Of current importance for alloy design is controlling this ordering to optimize an alloy's mechanical properties for a desired application. However, before ordering can be controlled, new means to quantitatively characterize its presence are needed as this remains an on-going challenge. In this study, we use Bragg coherent diffraction imaging to reconstruct morphology and lattice displacement in model Cu3Au nanocrystals (~10 nm spatial resolution) that have been heat-treated at temperatures below, within, and above the order-disorder transition temperature range. The magnitudes and distributions of the scattering amplitudes (proportional to electron density) and lattice strains within these crystals are then analyzed to correlate them to the expected amount of short-range ordering present.

2:00 PM
Experimental and Modelling Study of Mechanical Failure in 400 nm Porous Glass Using In Situ Nanoscale 3D X-Ray Microscopy: *Stephen Kelly*[1]; Sebastian Schafer[2]; François Willot[3]; Hrishikesh Bale[1]; Mansoureh Norouzi Rad[1]; Dirk Enke[4]; Juliana Martins de Souza e Silva[5]; [1]Carl Zeiss RMS; [2]Martin-Luther-Universität Halle-Wittenberg; [3]Mines ParisTech; [4]Universität Leipzig; [5]Fraunhofer Institute for Microstructure of Materials and Systems IMWS

Porous glasses find uses in optics, heterogeneous catalysis, sensors, chromatography, and as hosts for nanoparticles and biocompounds mainly due to their high specific surface area and high thermal and chemical resistances. For these uses, the mechanical stability of porous silica is a requirement to guarantee resilience, load-bearing capacity, and fatigue resistance. With pore and strut sizes in the nanometer to micrometer range and a bicontinuous 3D structure, understanding the relationship between structure, processing, and mechanical properties is challenging. In this study, we used nanometer resolution X-ray computed tomography (nano-CT) to image a controlled pore glass (CPG) with 400 nm-sized pores under in-situ uniaxial compression. Critically, by combining 3D imaging data with computational tools, we quantitatively analyze the microstructural changes within the CPG sample, mapping displacements and strain fields, and show agreement with FFT/Phase Field simulations in explaining the appearance of cracks and brittle failure.

2:20 PM
Application of a Multilayer Laue Lens for Full-Field Tomography and DFXM: Nis Gellert[1]; *Steffen Staeck*[1]; Henning Friis Poulsen[1]; Carsten Detlefs[2]; Can Yildirim[2]; Innokenty Kantor[3]; Rajmund Mokso[1]; [1]DTU; [2]ESRF; [3]MAX IV

Multilayer Laue lenses (MLL) are diffraction-based X-ray optics that are especially suitable for the hard X-ray range. They exhibit a larger numerical aperture, NA, than compound refractive lenses and conventional Fresnel zone plates. In this work, we first present the implementation and characterization of an MLL at the DanMAX tomography beamline at MAX IV. Here the MLL is used for tomography via phase-contrast projection holography for materials science and bio-imaging. Coupled with a 150 Mpixel camera in the so-called Xtreme-CT setup, a large field-of-view (2 mm) is coupled with high spatial resolution (100 nm).Next, we present the plans and status for implementing an MLL as an objective at the dedicated DFXM beamline ID03 at ESRF. Here the aim is to improve the spatial resolution to 30 nm. In addition, the larger NA will also improve data acquisition speed.

2:40 PM
Quantitative Analysis of Vacancy Distribution In Metals: Experiments and Simulations: *Michal Dagan*[1]; Bpatiste Gault[2]; Julien Guénolé[3]; George Smith[1]; Paul Bagot[1]; Michael Moody[1]; [1]Oxford University; [2] Max-Planck-Institut für Eisenforschung GmbH; [3]Université de Lorraine

Vacancies are critical to understanding materials evolution in service, however, imaging of vacancy distribution in metallic materials remains a challenge. We construct an automated reconstruction procedure to retrieve precise information on vacancies distributions from field ion microscopy data. FIM uses an intense electrostatic field to ionise inert gas atoms in the vicinity of the surface of a cryogenically-cooled needle-shaped specimen, biased to a few kV. A FIM micrograph is a direct-projection image, revealing the atomic arrangement at the surface of the sample. As the field is increased the removal of surface atoms is enabled and FIM becomes a 3D technique.By developing image processing to extract 3D locations of vacancies within ion-irradiated tungsten (a leading candidate for plasma facing components in fusion reactors), we demonstrate the distribution of individual vacancies inside the sample. We compare results with SRIM and MD simulations, showing qualitative agreement in vacancy depth and distribution profiles.

3:00 PM Break

3:30 PM
Synchrotron X-Ray Nanotomography Uncovers Microstructure of a Three-Phase Eutectic Solidified in Microgravity: *Soumyadeep Dasgupta*[1]; Xianghui Xiao[2]; Melis Serefoglu[3]; Ulrike Hecht[4]; Ashwin Shahani[1]; [1]University of Michigan; [2]Brookhaven National Laboratory; [3]Marmara University; [4]Access e.V.

Microstructure selection of two-phase eutectics is reasonably well understood, but the same cannot be said about three-phase eutectics. Our study aims to advance fundamental understanding of pattern formation in the Al-Ag-Cu system during invariant eutectic solidification. Using synchroton x-ray nanotomography with high spatial resolution (~50 nm), we investigate in 3D the microstructural arrangement of (Al), AgAl, and AlCu eutectic phases following directional solidification (DS) under diffusive conditions in a microgravity environment aboard the International Space Station. With the wealth of 3D data, we quantify various attributes of the three-phase pattern during a velocity jump in DS: the phase fractions, eutectic length scales, phase connectivities, and interfacial shapes. Our research offers new insights into the selection of eutectic morphology and topology under DS, with implications to a wide array of multi-phase systems.

3:50 PM
Microstructural Influences on Crystal Plasticity Model Predictions Using High Energy X-Ray Diffraction Microscopy and TriBeam Tomography: *Justine Schulte*[1]; Dalton Shadle[2]; James Lamb[1]; McLean Echlin[1]; Kelly Nygren[2]; Matthew Miller[2]; Tresa Pollock[1]; Irene Beyerlein[1]; [1]University of California, Santa Barbara; [2]Cornell University

High energy x-ray diffraction microscopy (HEDM) is a valuable technique to study deformation in polycrystals as it provides 3D microstructure reconstructions and time-resolved micromechanical data. In the literature, this technique has been paired with full field models by providing initial microstructures and fine-scale validation. However, it is known that HEDM cannot consistently resolve small grains and twins, which arises as a consideration when interpreting results and a possible source of discrepancy in validation efforts when paired with microstructure-sensitive models in FCC materials. To quantify how missing features affect predicted values, a SEM-based TriBeam tomography dataset was collected on an IN718 sample that was monitored during a loading experiment using near-field and far-field HEDM. These overlapping reconstructions will be used to quantify differences in the captured grains. Additionally, crystal plasticity finite element (CPFE) simulations will be run with both reconstructions to observe any deviations in predicted values due to microstructural differences.

4:10 PM Cancelled

4:30 PM
3D-EBSD Characterization of the Microstructure Around a Crack Initiation on an Inconel 718DA Fatigue Sample: *Frédéric Adamski*[1]; Florent Coudon[1]; Ditoma Satera[2]; Henry Proudhon[2]; [1]Safran; [2]Centre des Matériaux - Mines de Paris - PSL

Inconel 718DA is an alloy widely used in the aerospace industry for manufacturing high-pressure turbine discs, for which damage results from fatigue stresses. Fatigue crack initiation remains a mechanism that needs to be studied to improve our understanding. To this end, an interrupted fatigue test was carried out on a specimen with a flat surface in order to initiate a large number of short cracks with a length of a few tens of micrometers. One of these cracks was then selected for full EBSD-3D FIB-SEM characterization of the microstructural volume in its vicinity. This talk will first focus on the protocol for generating, identifying and preparing the crack to be characterized. Next, the steps involved in reconstructing the volume from the 2D slices will be explained. Finally, the analysis of the microstructure and the crack path will provide further insight into the fatigue damage mechanisms of this alloy.

The 7th International Congress on 3D Materials Science (3DMS 2025): Time Resolved 3D Characterization III

Wednesday PM
June 18, 2025

Room: Room C
Location: Anaheim Marriott

Session Chair: To Be Announced

1:30 PM Invited
Texture Tomography for Non-Destructive Microtexture Imaging of Highly Deformed Metals: *Mads Carlsen*[1]; William Hearn[1]; Ulrich Lienert[2]; Marianne Liebi[1]; [1]Paul Scherer Institut; [2]DESY

Texture tomography is a recently developed framework for reconstructing three dimensional maps of the crystallographic texture of polycrystalline samples from scanning-beam experiments using synchrotron x-rays equivalent to X-ray diffraction computed tomography (XRD-CT) and scanning-beam x-ray diffraction (s3S-XRD). Texture tomography is a compliment to these other techniques that works well for small-grained and textured samples, where the individual grains are not resolved by the experiment and for highly deformed microstructures where the grains are resolved but the process of peak-finding is difficult due to significant overlap of diffraction peaks from different grains.We present the results of the first in-situ experiment using texture tomography to characterize a 3D-printed steel sample displaying twinning induced plasticity (TWIP). We obtain grain-maps from the bulk of the same sample at before and after deformation as well as measure the development of twinning.

2:00 PM
In-Situ Laser Powder Bed Fusion of a Novel Aluminum Alloy: *Katrin Bugelnig*[1]; Bechir Chehab[2]; Ravi Shahani[2]; Pierre Lhuissier[3]; Elodie Boller[4]; Guillermo Requena[1]; [1]German Aerospace Center (DLR); [2]Constellium Technology Center; [3]Laboratoire SIMaP, Université Grenoble Alpes ; [4]ESRF

The Laser Powder Bed Fusion (LPBF) process for the novel structural AL-Fe-Zr alloy, Aheadd® CP1, by Constellium was investigated in-situ during synchrotron x-ray microtomography at the ESRF/BM18 beamline using a miniature LPBF machine. The data obtained provides information on defect morphology and size distribution, as well as build quality as a function of printing strategy and geometry. Moreover, information about the porosity history from layer to layer that cannot be easily obtained by other methods was acquired. It was observed that the LPBF process is a partially self-healing process, i.e., pores formed in one location can heal after a few more layers are built up, while other pores form. This experiment allows for the understanding of the underlying mechanisms and provides suitable data, such as morphology and distribution of defects depending on material, printing parameters and sample geometry, for the validation of AM simulation models.

2:20 PM
Investigation of Phase-Field 4D Reconstruction for X-Ray In Situ Observation of Dendrite Solidification: Ayano Yamamura[1]; Shinji Sakane[1]; Hideyuki Yasuda[2]; *Tomohiro Takaki*[1]; [1]Kyoto Institute of Technology; [2]Kyoto University

Time-resolved X-ray computed tomography (4D-CT) is a powerful tool for observing three-dimensional dendrite growth during alloy solidification. However, reconstruction becomes difficult when the growth rate is high. In this study, we investigate the possibility of 3D reconstruction using phase-field simulation. Here, we use data assimilation to introduce the X-ray transmission images into the phase-field simulation. As the simulations in data assimilation becomes large-scale, we performed parallel computation using multiple GPUs on a GPU supercomputer.

2:40 PM
Industry-Ready Residual Stress Measurements at CHESS's Structural Materials Beamline: *Kelly Nygren*[1]; Paul Shade[2]; Chris Budrow[3]; Matt Miller[1]; Edwin Schwalbach[2]; [1]Cornell University; [2]Air Force Research Laboratory; [3]Budrow Consulting LLC

Synchrotron X-rays provide a powerful probe to non-destructively measure elastic lattice strains inside crystalline materials. Critically, an attractive combination of spatial resolution and measurement efficiency enables researchers to evaluate the 3D residual stress within parts through mapping of these elastic lattice strains. Optimized for X-ray diffraction of metals, the Structural Materials Beamline (SMB) routinely measures residual stress in parts with complex geometries using both angle-dispersive and energy-dispersive X-ray diffraction. SMB is part of the Materials Solutions Network at CHESS (MSN-C): a sub-facility of CHESS created to provide critical measurements and research products to the U.S. Department of Defense (DoD) ecosystem. SMB has focused on the development of standards, automation, hardware, and maturing measurement and analysis workflows to transform X-ray techniques from specialized tools into accessible engineering solutions for industry. Current capabilities will be presented with results for an additively manufactured part with complex geometry.

3rd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2025): Large Language Models - Information Extraction and Materials Design

Thursday AM
June 19, 2025

Room: Room A
Location: Anaheim Marriott

Session Chair: To Be Announced

8:30 AM
Advancing Materials Discovery and Manufacturing Optimization Through Large Language Models: *Avik Mahata*[1]; [1]Merrimack College

The integration of large language models (LLMs) into materials science and manufacturing offers unprecedented opportunities for accelerating innovation and enhancing efficiency. We demonstrate how LLMs can automatically extract and synthesize valuable information from vast unstructured texts, including experimental procedures, material properties, and synthesis conditions, thereby building comprehensive datasets for machine learning applications. In materials discovery, we leverage LLMs to generate hypotheses for novel compounds by predicting plausible chemical structures and estimating their properties using natural language descriptions. For manufacturing processes, LLMs analyze technical manuals, operational logs, and maintenance records to optimize process parameters, improve predictive maintenance, and reduce downtime. Case studies highlight the successful identification of new high-temperature superconductors and the optimization of additive manufacturing settings for aerospace-grade alloys. Our results underscore the potential of LLMs to revolutionize materials research and industrial manufacturing by providing sophisticated tools for data-driven decision-making and innovation acceleration.

8:50 AM
Enhancing Data Acquisition in Manufacturing: Leveraging LLMs for Effective Material Property Databases: *Inés Pérez Couñago*[1]; Lara Suárez Casabiell[1]; Gabriel Novas Domínguez[1]; Santiago Muíños Landín[1]; Pilar Rey Rodriguez[1]; Félix Vidal Vilariño[1]; [1]AIMEN Technology Center

Large Language Models (LLMs) enable the creation of up-to-date material property databases, offering significant potential for identifying materials with desired properties, proposing alternatives to costly options, resolving discrepancies in reported values, and automating inputs for tools like Finite Element Analysis (FEA). This work explores Multimodal Retrieval-Augmented Generation (RAG) for extracting information from Wire Arc Additive Manufacturing (WAAM) and Sheet Moulding Compound (SMC) documents. Given that material property data is often tabular, a benchmark was developed for parsing tools capable of handling diverse PDF layouts. Tables, images, and text were extracted using multimodal embeddings and table2text techniques, enabling the retrieval of relevant material information. The extracted data was processed into structured formats, including automatic detection and conversion into SI units, and LLM outputs were evaluated using standard metrics, as well as a custom metric. These advancements enhance workflow efficiency and decision-making by providing rapid, traceable access to manufacturing information.

9:10 AM
LLM-Assisted Data Curation in Starrydata: An Open Database of Material Properties Extracted From Published Plots: *Yukari Katsura*[1]; Tomoya Mato[1]; Yu Takada[1]; Dewi Yana[1]; Eiji Koyama[1]; Erina Fujita[2]; Yoshihiro Sakamoto[3]; Naoto Saito[1]; Fumikazu Hosono[1]; Atsumi Tanaka[1]; Masaya Kumagai[4]; [1]National Institute for Materials Science; [2]Institute of Statistical Mathematics; [3]RIKEN; [4]SAKURA Internet Inc.

We developed the Starrydata web system (https://www.starrydata2.org) as an open database of experimental materials data collected by tracing plot images from scientific literature. This platform enables users, including our data curators, to share experimental data extracted from published papers. The data hosted on Starrydata are publicly available and can be freely downloaded and used for both commercial and non-commercial purposes, provided our paper is cited. Starrydata includes datasets for functional materials such as thermoelectric, magnetic, and battery materials. The thermoelectric materials project comprises data for approximately 50,000 physical samples reported in around 10,000 papers, including more than 130,000 curve data on the temperature dependence of thermoelectric properties. We will present our efforts to accelerate data curation in Starrydata by developing an automated retrieval system using commercial Large Language Models (LLMs). Tasks such as figure labeling and the extraction of experimental processes from text have proven effective in assisting data curators.

9:30 AM
Harnessing Large Language Models for Information Extraction and Material Design: Shuozhi Xu[1]; Xin Wang[1]; *Kun Lu*[1]; Haiming Wen[2]; [1]University of Oklahoma; [2]Missouri University of Science and Technology

Since the advent of ChatGPT in November 2022, the field of large language models (LLMs) has seen an explosive development. In the scientific community, LLMs have been employed to automate literature reviews, assist data analysis, and generate hypotheses. In the materials science community, there is a rapid surge in the interest in LLMs because the majority of information concerning materials exists as text, aligning closely with the text-centric nature of LLMs. In this work, we explore the abilities of LLMs for two tasks: information extraction and material design. In the first task, we employed an LLM to extract information including chemical compositions, processing conditions, microstructures, and properties. The LLM was shown to significantly outperform a conventional rule-based method. In the second task, we utilized an LLM to establish the relationship between structures and properties in a couple cases. The LLM-based relationship was compared favorably with machine-learning based ones.

9:50 AM Break

10:10 AM
Utilizing Large Language Models for Interpreting & Interfacing With Instance Segmentation Results of Metallic Powder Micrographs: *Stephen Price*[1]; Kiran Judd[1]; Kyle Tsaknopoulos[1]; Danielle Cote[1]; [1]Worcester Polytechnic Institute

Powder characterization is key to the efficient optimization of additive manufacturing techniques such as cold spray. To accomplish this, computer vision has proven to be effective at predicting and segmenting cold spray powder from SEM micrographs. However, while good at identifying and analyzing powders, outputs are large, complex, and difficult to analyze. This work presents a novel post-processing step utilizing a large language model (LLM) to interface with these outputs, making them more interpretable for real-world applications. This framework can process and analyze these results, answering practical questions about various morphological characteristics, such as area, eccentricity, sphericity, etc. Additionally, this approach can be used to compare multiple powders, enabling the user to query which characteristics are most similar or most different between samples. By embedding computer vision results in a readable format, an LLM improves the accessibility and interpretability of computer vision results for powder characterization.

10:30 AM
Application of LLMs in Understanding Advanced Materials Properties and Manufacturing Processes: *Jamiu Odusote*[1]; Salihu Tanimowo[1]; Kamardeen Abdulrahman[1]; [1]University of Ilorin

Traditional large language models (LLMs) have limited capabilities in comprehending specialized datasets related to materials or manufacturing fundamentals, such as microstructures, phase changes, and thermomechanical properties. This study aims to integrate multimodal data; images, sensor readings, and numerical data, with textual descriptions for better understanding of Advanced Materials Properties and Manufacturing Processes (AMPMP). A complete picture of the domain was constructed when multiple modalities is combined, enabling the development of rich representations that capture the complexities inherent in AMPMP. The results showed that multimodal approaches have potential to significantly improve the modeling and analysis of these specialized domains compared with LLMs. Integration of diverse data sources could lead to models with lower variance and improved generalization than those that rely solely on a single modality. This means that a multimodal approach can provide a more comprehensive understanding of AMPMP, with practical implications for various applications in materials science and engineering.

1050 AM
Salvaging of Materials Fatigue Data from Literature Using Language Model Systems: *Ali Riza Durmaz*[1]; Jyoti Mohanty[2]; Akhil Thomas[2]; [1]University of California - Santa Barbara, Fraunhofer IWM; [2]Fraunhofer IWM

Materials fatigue has been researched since the 18th century which has led to a wealth of data and information contained in scientific literature. Associated cyclic testing of a single material often requires months to years. Thus, design of safety-critical components is often constrained to few thoroughly characterized materials or relies on rather crude estimates. Comprehensive extraction of fatigue information from publications into a structured and harmonized format could support building predictive models in the future.

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): ICME for Materials and Process Design II

Thursday AM
June 19, 2025

Room: Room E
Location: Anaheim Marriott

Session Chair: To Be Announced

8:00 AM Invited
ICME-Based Materials and Manufacturing Development: *Qiaofu Zhang*[1]; [1]University of Alabama

The Integrated Computational Materials Engineering (ICME) approach has been developed and demonstrated as a cost-effective and time-efficient strategy for the development of novel materials and advanced manufacturing processes over the past decade. This talk will present examples of new materials design and advanced manufacturing process development through the integration of ICME modeling with experiments, replacing the conventional trial-and-error strategy. It includes two main aspects: 1) the development of ICME models to link the materials' process-structure-property relationships through CALPHAD-based (CALculation of PHAse Diagram) microstructure modeling, physics-based models, and machine learning approaches; 2) iterative designs that combine ICME-based computer design with lab-scale prototyping. Specific examples will include the development of high-performance conductive alloys for energy applications, ceramic-metal composite for extreme environment applications, and innovations in advanced manufacturing.

8:30 AM
AI-Enhanced Integrated Computational Materials Engineering Framework for Efficient Alloy Design in Continuous Design Spaces: Osman Mamun[1]; *Bhuiyan Shameem Mahmood Ebna Hai*[1]; [1]Fehrmann MaterialsX GmbH, Fehrmann Tech Group

The rapid discovery of multi-component alloys with optimized properties is challenging, requiring both computational efficiency and precision. Recent Bayesian optimization (BO) advancements in continuous design spaces enhance alloy composition optimization, identifying novel alloys with targeted properties. Multi-objective BO acquisition functions like TSEMO, parEGO, and qNEHVI are benchmarked for efficiency and robustness. To accelerate development, an ICME framework integrates CALPHAD-based simulations for phase stability and thermodynamic predictions, autonomously selecting acquisition functions based on material properties and objectives. Design of Experiments (DOE) strategies minimize validation iterations, reducing timelines, while pool-based active learning enables concurrent computational and experimental work in high-throughput environments. Multi-scale modeling correlates microstructure with performance, with uncertainty quantification ensuring robustness. Data-driven machine learning enables real-time predictions and feedback loops, refining optimization iteratively. This framework, combining advanced optimization, simulations, and experimental validation, provides a scalable solution for rapid discovery and qualification of novel alloys.

8:50 AM
An Integrated Computational Material Engineering Approach to Characterize Mechanical Properties of Cu-Ni-Cr Alloys for Advanced Manufacturing: Pouria Nourian[1]; Ahsanul Alam Kabhi[1]; Md Ashfaq Siddiquee[1]; *M Shafiqur Rahman*[1]; [1]Louisiana Tech University

Cu-Ni-Cr alloys are prized for their strength, corrosion resistance, and adaptability in demanding sectors like aerospace and energy. This study applies an Integrated Computational Material Engineering (ICME) approach, combining molecular dynamics (MD) simulations, finite element analysis (FEA), and machine learning (ML), to discover alloy compositions with optimized mechanical properties. First, MD simulations calculate key properties—elastic modulus, ultimate tensile strength, bulk modulus, shear modulus, and Poisson's ratio—across various compositions, validated against experimental trends. These data feed into the macroscale FEA for tensile and bending tests, simulating performance under realistic loads. Using these results as optimization objectives, ML identifies compositions predicted to offer superior mechanical balance. This ICME approach significantly accelerates alloy discovery by reducing dependence on physical testing, enabling rapid optimization across a broad compositional space. The findings advance materials design for high-performance applications, providing a scalable framework adaptable to diverse alloy systems.

9:10 AM
Inverse Design by the MInt System Implementing Materials Integration: *Masahiko Demura*[1]; Satoshi Minamoto[1]; Takuya Kadohira[1]; Kaita Ito[1]; [1]National Institute for Materials Science

The MInt system embodies the concept of Materials Integration, linking processing, structure, property, and performance in a unified computational framework. By integrating this system with optimization algorithms, such as artificial intelligence, materials and processes can be designed based on targeted performance requirements. This study demonstrates the effectiveness of this approach through two case studies: the design of aging heat treatment processes for nickel-based dual-phase alloys and the optimization of welding processes to mitigate creep life degradation in heat-resistant steel welded joints. These examples highlight how the MInt system enables inverse design, offering a powerful tool for material development and process optimization.

9:30 AM Break

9:50 AM
Multi-Disciplinary Robust Co-Design Exploration Framework for Materials, Products, and Manufacturing Processes: *H M Dilshad Alam Digonta*[1]; Mathew Baby[1]; Anand Balu Nellippallil[1]; [1]Florida Institute of Technology

Conventional manufacturing processes involve the complex interactions between stakeholders from manufacturing, materials, and product disciplines to realize the final product. Effectively designing this complex system requires a multi-disciplinary design approach that emphasizes coordinating the interactions between the different disciplines. This necessitates the capability to co-design, which involves simultaneously exploring a wide range of "satisficing" robust design solutions across multiple disciplines by managing uncertainties.In this paper, we present a multi-disciplinary, robust co-design exploration framework for design space exploration involving multiple disciplines and management of uncertainty. The framework uses multi-disciplinary robust design constructs and a machine learning-based visualization tool to explore the robust multi-disciplinary design space simultaneously. The efficacy of the framework is demonstrated using the hot rod rolling problem, which considers the interactions between material microstructure and manufacturing processes. The framework is generic and supports the co-design exploration of systems characterized by multi-disciplinary interactions and the presence of uncertainties.

10:10 AM
Enhancing Robust Design Using Improved Variance Estimation in Design Capability Index: *Pooja Mukundan*[1]; H M Dilshad Alam Digonta[1]; Mathew Baby[1]; Anand Balu Nellippallil[1]; [1]Florida Institute of Technology

The simulation-based design of material systems involves uncertainties in design variables that must be managed. One approach for managing design variable uncertainties involves using the Design Capability Index (DCI) metric for Robust Design, which allows designers to identify robust solutions that are relatively insensitive to uncertainties. In DCI, the variance of responses due to uncertainties is computed using the first-order Taylor Series expansion, which fails to eliminate 'uncertainty sensitive' maxima/minima points from the robust solution space. First-order Taylor Series Expansion will also potentially result in errors for non-linear/multimodal response functions. To address these drawbacks, we explore alternative variance estimation methods – the second derivative, multiple derivative, and multiple-point methods, in the DCI metric. We employ the hot rod rolling problem to explore the effect of these alternate methods on DCI. This exploration is facilitated using the machine learning-based visualization technique - interpretable Self-Organizing Map (iSOM).

10:30 AM
Co-Designing Products, Materials, and Manufacturing Processes for ICME Together With Their Supply Networks: *Mathew Baby*[1]; Anand Balu Nellippallil[1]; [1]Florida Institute of Technology

Satisfying customers' requirements for products involves various stakeholders making decisions regarding materials and their processing to realize products with targeted properties and the supply of these products to customers. These decisions are interrelated and made across multiple levels of a decision hierarchy. Therefore, delivering products to meet customer requirements requires 'co-designing' a multilevel system comprising the products, materials, manufacturing processes, and product supply network to simultaneously consider conflicting multilevel stakeholder requirements.In this paper, we present a framework to support the systematic co-design of products, materials, manufacturing processes, and the product supply network. The framework supports designers in systematically modeling the multilevel stakeholder decisions and their relations. We illustrate the efficacy of the proposed framework using a steel rod manufacturing and supply example problem. This problem involves the manufacture of steel rods using hot-rod rolling processing and its supply to customers through a supply network comprising the manufacturer and distributors.

10:50 AM
ICME Framework for Design of Micro-Alloyed Electrical Steels: Akash Gupta[1]; Shalini Koneru[1]; *Akash Bhattacharjee*[1]; Surya Ardham[1]; Sandeep Pusuluri[1]; Ish Jha[1]; [1]Tata Consultancy Serives (TCS), Research

Electrical steels are widely used in electric drives and vehicles to meet sustainability regulations, among this non- grain oriented electrical steels (NOES) are used in various soft magnetic core applications. B-H (magnetic hysteresis) curve is a crucial characteristic of magnetic materials along with desired mechanical properties. An ICME based alloy design framework is developed to account for the influence of microalloying elements on engineering the microstructure and crystallographic texture of NOES for improving magnetic and mechanical properties. Here, we employed cellular automata (CA) based model coupled with equilibrium precipitation model to predict the microstructure and texture of NOES during annealing process. This is further used for prediction of magnetic and mechanical properties, using object-oriented micromagnetic model framework (OOMMF) integrated with Ubermag and mesoscale models like crystal plasticity, respectively. A closed feedback loop is then used to integrate these models to optimize chemistry and processing parameters for achieving target properties.

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): PSP Linkages: Multiscale/Multiphysics Modeling IV

Thursday AM
June 19, 2025

Room: Room F
Location: Anaheim Marriott

Session Chair: To Be Announced

8:00 AM Invited
Observing and Predicting Grain Growth in Polycrystals: *Gregory Rohrer*[1]; [1]Carnegie Mellon University

Predictive models for grain growth during annealing would be useful in the ICME context because they have the potential to speed the development of new materials. Recent three-dimensional studies of grain growth have shown no correlation between curvature and migration velocity, contradicting the observed migration behavior of individual grain boundaries in bicrystals. Two types of simulations, atomistic molecular dynamics and continuum threshold dynamics have been instantiated with experimental observations and used to simulate growth under different conditions. Both of these simulations reproduce the independence of curvature and velocity observed in the experiment, as well as a reduction in energy by the replacement high energy grain boundaries with lower energy grain boundaries. A more realistic driving force for grain growth will be proposed and the prospect for predictive grain growth simulations will be discussed.

8:30 AM

Optimizing Non-Oriented Electrical Steel for Energy-Efficient Drives: The Role of Final Annealing in Microstructure Design: *Masoud Sistaninia*[1]; [1]Materials Center Leoben Forschung Gmbh

Non-oriented (NO) electrical steel is vital for applications in rotating electrical drives due to its uniform magnetic properties. The efficiency of these drives depends on optimizing processing routes like hot-rolling, cold-rolling, final annealing, and shear cutting. Our research focuses on designing high-performance NO electrical steels by controlling their microstructure and crystallographic texture through precise thermomechanical processing. This study highlights the critical role of final annealing in defining the steel's magnetic properties. We show how specific annealing conditions influence microstructure and magnetic performance. By conducting extensive annealing experiments, we identified optimal parameters that balance grain size and texture, improving both magnetic and mechanical properties. This presentation will discuss the methodologies used, including advanced simulation tools, to support the development of NO electrical steels aimed at enhancing energy-efficient applications and promoting a sustainable energy future through optimized materials for electric drives.

8:50 AM

Recapturing and Reusing Published Mg Alloy Texture Data: Benjamin Begley[1]; *Victoria Miller*[1]; [1]University of Florida

Crystallographic texture is a rich data source, but when published in typical forms, e.g. as pole figures, it does not adhere to FAIR data principles. By publishing the data as an image, its reusability is severely limited. The texture encodes the effects of alloying and processing on relative deformation mode activities, making quantitative comparisons crucial. For example, during rolling the extent of basal pole splitting can be related the activity of pyramidal <c+a> slip. In this talk, we present a method for quantitatively reconstructing an ODF based on pole figure images. A variety of Mg alloy textures from the literature are recaptured and quantitatively compared. Using polycrystal plasticity simulations, their predicted mechanical behavior is evaluated. The relationships between alloying, processing, and texture features are discussed.

9:10 AM

Microstructure Evolution, the Influence on Material Properties, and the Optimized Processing Parameters Search in Additive Manufacturing: *Wei Huang*[1]; [1]Gatech

The primary aim of this investigation is to study the microstructural changes that affect material properties, such as elastic modulus and Poisson's ratio, and then how to search for the optimized processing parameters. To achieve this, the characterization of the microstructure of materials, mainly the surface/textures, grain size, and defects, if necessary, is of great importance. The texture and grain size simulation for multi-phase materials systems is conducted based on the modeling of processing by physical stimuli. The influence of defects on the material properties, texture, and grain size is also considered. Specifically, thermal dynamics, Bunge calculation, and the CET model initially simulate the texture. The visco-plastic self-consistency model gains the properties of the impacted materials after determining the texture distribution. Afterward, artificial intelligence is utilized to search for the optimized processing parameters or predict material properties so that this work could offer better instruction to natural industries.

9:30 AM Break

9:50 AM

Connecting the In-Plane Strength Anisotropy of Hot Rolled Line Pipe Steel to Its Microstructural Equivalent: *Chetan Kadgaye*[1]; [1]Iit Roorkee

This study looks at how precipitates affect hot-rolled X-65 Line pipe steel's in-plane tensile behavior, including strain hardening. On the RD-TD plane, tensile samples were made in four different orientations: 0°, 30°, 60°, and 90° to the RD. Superior mechanical characteristics, including improved yield continuity and an ideal strength-ductility balance, were demonstrated by the 90° sample. Grain boundary properties, dislocation-precipitation interactions, and elastic-plastic incompatibility at grain boundaries all contribute to the yielding behavior and tensile response. The improved characteristics of the 90° sample are mostly due to the interaction of dislocations with tiny precipitates as well as variations in Elastic Modulus (EM) and Schmid Factor (SF) across high-angle grain boundaries (HAGBs).

10:10 AM

ICME-Driven Synthesis of Nanosheets and Applications in Solar Energy Harvesting and CO<SUB2-CH$_4$ Separation in Biogas: *Ping Wu*[1]; Shunnian Wu[1]; P.V.T. Weerasinghe[1]; H.L. Senevirathna[1]; H.N. Thenuwara[1]; W.P.C. Lee[1]; [1]Singapore University of Technology and Design

This presentation showcases two studies leveraging Integrated Computational Materials Engineering (ICME) to tackle challenges in material synthesis and renewable energy. The first study utilizes ICME for the entropy-driven synthesis of 2D mica nanosheets from 3D non-Van-Der-Waals crystals. Through first-principles calculations, biaxial straining models, and experiments, we address barriers in exfoliating strongly bonded materials, focusing on their application in solar energy harvesting. The second study presents bio-inspired nanocomposites of magnesium oxide and hydroxide, modeled after the water-harvesting strategies of Namib Desert beetles, to enhance CO-CH separation in biogas. Using density functional theory (DFT) and gas-composite interface modeling, the nanocomposites exhibit superior CO adsorption and selective gas capture, with minimal CH adsorption. These studies demonstrate ICME's potential in optimizing material properties for energy applications by linking processing, microstructure, and performance, offering innovative solutions in solar energy and biogas processing.

10:30 AM

Multiscale Modeling of Mechanical Deformation in Metal-Matrix Nanocomposites Enabled by Machine Learning: *Wenwu Xu*[1]; Colin Delaney[1]; Ethan Morrison[1]; Sky Soltero[1]; Marivel Alfaro[1]; Md. Shahrier Hasan[1]; [1]San Diego State University

We present an innovative multiscale modeling framework for Metal-Matrix Nanocomposites (MMNCs), integrating Machine Learning (ML) with Molecular Dynamics (MD) simulations and the Finite Element Method (FEM). This approach effectively captures the mechanical influence of nano-scale inclusions on the macroscopic behavior of MMNCs. Initially, MD simulations are conducted under various conditions to generate a comprehensive dataset reflecting the mechanical responses of MMNCs. This data is subsequently used to train ML models, which enhance the accuracy and computational efficiency of FEM-based analyses. Our method accurately predicts the deformation behavior of MMNCs across scales, showing strong agreement with experimental results and theoretical predictions. By seamlessly bridging atomistic and continuum modeling, this work provides a scalable and robust solution for the analysis of advanced composite materials, advancing the capabilities of predictive modeling in materials science.

10:50 AM

An Integrated Material Model for ICME-Based Process Simulations: Capturing Plasticity and Damage Evolution in Laser-Assisted Hole Flanging Process: *Karthik Ramalingam*[1]; Christian Haase[2]; Ulrich Krupp[1]; [1]IEHK Institute - RWTH Aachen; [2]TU Berlin

This study presents a material model tailored for Integrated Computational Materials Engineering (ICME)-based process simulations. The model integrates plasticity and damage evolution mechanisms, offering a refined approach to simulate material behavior under complex deformation conditions. Central to this work is the use of evolution equations for dislocation densities, enabling precise tracking of the microstructural state throughout processing and capturing critical interrelationships among process parameters, microstructure, and properties. By simulating the growth of dislocation densities and development of void fractions in each step, the model ensures accurate transfer of deformation history across sequential stages. Implemented for laser-assisted hole flanging—a multistep process where shear cutting and laser heating influence component quality and performance—this model enhances the fidelity of process simulations. Ultimately, it advances ICME by providing a reliable framework for microstructure-sensitive material modeling in thermomechanical processing.

11:10 AM

An Integrated Experimental and Computational Study on the Role of Material Interfaces in Mediating Plastic Flow in Amorphous/Crystalline Composites: *Ashraf Bastawros*[1]; Amir Abdelmawla[1]; Liming Xiong[2]; [1]Iowa State University; [2]North Carolina State University

In this work, we study the deformation behavior in amorphous/crystalline metallic composites (A/C-MCs) through nanoindentation experiments and molecular dynamic (MD) simulations. The atomic deformation processes in both crystalline (C-) and amorphous (A-) phases near the amorphous-crystalline interface (ACI) are investigated and correlated with the material's overall constitutive behavior at the microscale. Our major findings are (i) the ACIs enable a co-deformation of the A- and C-phases through "stiffening" the soft phases but "softening" the stiff phases in A/C-MCs through different micro-mechanisms; (ii) there exists an ACI-induced transition zone with a thickness of~10 nm; (iii) the strong coupling between shear transformation zones (STZs) and dislocations can be quantified through carefully designed indentation experiments and simulations; and (iv) the nanoscale MD-simulation-predicted mechanisms can be mapped to the "pop-in" or "excursion" events on the force–indentation depth curves extracted from microscale experiments, although there is a length-scale gap in between.

The 7th International Congress on 3D Materials Science (3DMS 2025): 3D Characterization and Modeling in Advanced Manufacturing

Thursday AM
June 19, 2025

Room: Room D
Location: Anaheim Marriott

Session Chair: To Be Announced

8:00 AM

Measuring Intragranular Orientation-Strain Fields and Residual Stresses in As-Built Additively Manufactured Stainless Steel Using Scanning 3DXRD: *Jerard Gordon*[1]; [1]University of Michigan

Although laser-based metal additive manufacturing (LAM) is a disruptive technology enabling near-net shaped part production of metallic materials, its widespread adoption has been largely stymied due the occurrence of process-induced thermal residual stresses. To better understand the incidence of microscale residual stresses within bulk metal LAM materials, we employed novel 3d scanning x-ray diffraction (s3DXRD) to directly measure the full elastic strain tensor and orientation for ~500 grains within a bulk LAM sample. This measured strain data was used to estimate the residual elastic stress tensor components and von Mises stresses within the sample volume using the single crystal elastic constants. Interestingly, von Mises stress distributions appear to follow grain boundary networks and show significant localizations in regions of the microstructure containing fine grains. Overall, these results suggest that residual stress distributions within LAM materials are intimately connected to local solidification behaviors.

8:30 AM

Strain Field Mapping of a New Generation of Polycrystalline Chromium Coated Zirconium Claddings for Nuclear Application by Synchrotron Based Laue Microdiffraction: *Clement Ribart*[1]; Jean-Sebastien Micha[2]; Raphaelle Guillou[3]; Samuel Tardif[1]; Joel Eymery[1]; Jean-Luc Bechade[4]; [1]CEA Grenoble DEPHY/MEM/NRX; [2]UMR SYMMES CRNS CEA; [3]CEA Saclay SRMA; [4]CEA Saclay SRMP

We present a study probing the local in bulk micro-mechanical fields at the chromium-zirconium interface of a new generation of coated nuclear fuel claddings designed for improved resistance to hypothetic accidental high temperature transients Light Water Reactors. The chromium is deposited by DC-MS and/or HiPIMS-PVD processes, which results in a complex polycrystalline microstructure, textured and with heterogeneous internal stress state. The scanning diffraction µLaue technique, available at the ESRF on beamline BM32, is able to discriminate contributions of each crystallographic phase and to reconstruct raster maps of the locally integrated orientation and strain fields for each grain along the depth. Furthermore, the DAXM variant allows to resolve the signal along this latter direction, leading to 3D maps down to sub-micron voxel resolution. These techniques give valuable insight on the mechanical state of complex interfaces, which is an important parameter to further rely on the coated materials mechanical behavior.

8:50 AM

The Interest of Lab-Based DCT for the 3D Characterization of Monocrystalline Nickel-Based Alloys: *Alexiane Arnaud*[1]; Jun Sun[2]; Florian Bachmann[2]; Vladimir Esin[3]; Henry Proudhon[4]; [1]Safran Group; [2]Xnovo Technology; [3]Université de Lorraine; [4]Mines Paris - Centre des Matériaux

In the aerospace industry, single crystal nickel-based is used to manufacture high-pressure turbine blades, which are the most critical part of the engine. These alloys have a dendritic microstructure, usually produced by Bridgman furnace, where each dendrite can be associated with a crystalline orientation. Thus, this dendritic network is actually represented by subgrains separated by low-angle grain boundaries. The 3D characterization of a monocrystalline René N5 superalloy has been performed by lab-based diffraction contrast tomography (DCT). This experiment has demonstrated the precise capabilities of lab-based DCT in resolving subgrain boundaries with a misorientation angle of less than 1°, achieving an angular accuracy as fine as 0.1°. A slice from the 3D reconstruction has been compared with standard electron backscatter diffraction (EBSD) mapping. Obtaining the 3D microstructure non-destructively enabled the segmentation of the network of single-crystal dendrites, opening up new opportunities for studying crystal mosaicity.

9:10 AM
Analysis of 3D Grain Orientations in Additively Manufactured 316L: *David Rowenhorst*[1]; [1]Naval Research Laboratory

The additive manufacturing process promises to provide new and highly customized processing methods for metal alloy components. Due to the large thermal gradients and resultant residual stresses built up in the printing process, the grain morphologies and structures are far from the typical alloy microstructures. In this presentation, we will examine the orientation gradients present in additively manufactured 316L, as measured by automated mechanical serial-sectioning with electron backscattered diffraction (EBSD) maps, with a data set that encompasses over 30,000 grains. We will show that while the grain sizes can have a very wide distribution, with the largest grains reaching over millimeters in length, the local orientation gradients within those grains lead to grain-spread distributions of over 20°. We will also discuss proper metrics for analyzing these gradients by normalizing for the local grain size within the structure.

9:30 AM Break

9:50 AM
The Distribution of Carbides in the Heat Affected Zones of an Austenitic Steel: *Patrick Callahan*[1]; Keith Knipling[1]; [1]US Naval Research Laboratory

A novel FCC austenitic steel with high strength is under development for potential structural applications. The high strength is primarily achieved through precipitation of nanoscale vanadium carbides. The heat affected zones in welded material has recently been assessed using both Gleeble simulated thermal cycles and gas tungsten arc welds. The morphology and distribution of the carbides was determined in 3D using atom probe tomography. The relationship between the carbide distribution and the peak temperatures reached and the processing history in the heat affected zones will be discussed, as well as compared with the local mechanical properties and computational predictions from ThermoCalc.

10:10 AM
Three-Dimensional Characterization of Dislocation Networks and Orientation Gradients in LPBF CoNi-Based Superalloys: *James Lamb*[1]; Evan Raeker[1]; Nicolò Maria della Ventura[1]; McLean Echlin[1]; Tresa Pollock[1]; [1]University of California Santa Barbara

Laser powder bed fusion (LPBF) creates complex thermomechanical conditions that introduce significant residual stresses in printed parts. As a result, dense cellular dislocation networks and severe orientation gradients develop in the as-printed material, often leading to increased strength and work hardening when compared to traditionally manufactured components. Grain-scale and cell-scale misorientations are characterized in 3D using TriBeam tomography on LPBF prints of a CoNi-based superalloy. The resulting EBSD data enables calculation of geometrically necessary dislocation (GND) densities and grain-based misorientation metrics. Dislocation cells are observed to transition between orthogonal growth directions across melt pool boundaries. Concurrently, significant intracellular orientation gradients develop along the growth axis of solidification cells and between neighboring cells. Cell-scale misorientations accumulate along the build direction, creating larger orientation gradients, upwards of 50° over 500 µm, at the grain scale. These findings reveal fundamental relationships between processing conditions, microstructural evolution, and residual stress development during LPBF.

10:30 AM
A Crystal Plasticity Finite Element Study on the Strengthening Mechanisms in Additively Manufactured Precipitate Strengthened Alloys: *Ezra Mengiste*[1]; Jacob Strain[1]; Luke Brewer[1]; Matthew Kasemer[1]; [1]University of Alabama

The design of modern engineering components requires the development of innovative manufacturing techniques. In parallel, design engineers increasingly design components closer to their failure limits due to sustainability and performance demands, necessitating better predictions of mechanical behavior. Additive friction stir deposition (AFSD) has emerged as a solid-state additive manufacturing method which allows for the construction of near-net-shape components. When employed with precipitate-strengthened alloys, AFSD tends to lead to a loss of material strength due to changes in the morphology of the precipitates. In our work we utilize a crystal plasticity finite element model informed by experimental material characterization and mechanical testing performed on samples before and after AFSD processing. We discuss the contribution of the crystallographic texture on the yield strength of the material and the implementation of a precipitate strengthening model used to account for the effects due to the presence of precipitates.

The 7th International Congress on 3D Materials Science (3DMS 2025): Emerging 3D Characterization Techniques and Instrumentation III

Thursday AM
June 19, 2025

Room: Room C
Location: Anaheim Marriott

Session Chair: To Be Announced

8:00 AM Invited
Diffraction Microstructure Imaging at the Materials Science Beamline, ID11, at the ESRF: *Jon Wright*[1]; Haixing Fang[1]; Wolfgang Ludwig[1]; James Ball[1]; [1]European Synchrotron Radiation Facility

Synchrotron instrumentation has not stopped improving. New sources are coming online so that the X-ray flux and beam properties are better than ever before. Fast photon counting detectors are widely available and these offer a range of novel diffraction-tomographic methods for imaging microstructures in 3D. At beamline ID11 at the ESRF, there is now a suite of complementary methods that combines imaging detectors for tomographic imaging and DCT grain mapping together with far-field detectors for 3DXRD and scanning tomography. We have optimized the instrument at ID11 for beam sizes down to about 150 nm and high-energy X-rays (40-70 keV). The largest samples are typically a few millimeters in diameter. This contribution will discuss the latest developments at the beamline and the different ways that these are being exploited to address a range of different scientific questions, in a wide range of disciplines, from metallurgy to earth sciences.

8:30 AM
Colour X-Ray Imaging: 5D Non-Destructive Elemental Mapping of Materials: *Tim Burnett*[1]; Nicola Wadeson[1]; Amin Garbout[1]; Matthieu Boone[2]; Jan Aelterman[2]; [1]University of Manchester; [2]Ghent University

The next dimension of X-ray imaging is here! Five dimensional Colour X-ray Imaging enables non-destructive 3D and 4D images to be complemented by a fifth chemistry dimension. Whilst the fundamental technology has been demonstrated it is, at present, inaccessible to most researchers due to the difficulty of acquisition and the processing of the vast multidimensional datasets it generates. We have recently built a new lab-based Colour X-ray CT scanner utilising a large detector array and a commercial cabinet-based system and are embarking on refining many of the data processing workflows. A 640 x 160 pixel hyperspectral HEXITEC detector with CdTe crystal has been integrated into a Nikon XTH 225 scanner. We have already demonstrated the capability of the detector for large-field-of-view bright-field imaging using absorption edge detection and are now moving to superresolution imaging using detector shifting. Initial applications include minerals, stained biomaterial, electronic waste and rare earth magnets.

8:50 AM
3D Large Volume Non-Destructive Grain Structure Characterization in Metallic Alloys Using Lab-Based Diffraction Contrast Tomography (LabDCT): *Kaushik Yanamandra*[1]; Nathan Johnson[1]; Hrishikesh Bale[1]; Jette Oddershede[2]; Jun Sun[2]; [1]Carl Zeiss Microscopy; [2]Xnovo Technology

The grain boundary(GB) are essential information to analyze grain boundary related behaviors such as preferential precipitation or intergranular cracking in polycrystalline materials. Accessing the necessary parameters to describe a GB on the mesoscopic scale is beyond the reach of 2D characterization techniques and is only achievable through a 3D approach. With the capability to map the grain morphology and crystallographic orientation non-destructively in 3D, lab-based diffraction contrast tomography (DCT) using X-rays provides the necessary information to analyze the crystallographic parameters describing grain boundaries on the mesoscopic scale, including grain boundary misorientation angle/axis and plane inclination. In this work, we will present the results of using lab-based DCT to investigate the grain boundary characters in polycrystalline materials including ceramic examples, with further discussion of how the grain boundary properties are related to grain boundary behaviors such as grain boundary wetting and cracking.

9:10 AM
Interrogating 3D Grain Morphology and Crystallographic Texture via Automated Polarized Light Microscopy: *Paul Chao*[1]; Rhianna Oakley[1]; Andrew Polonsky[1]; [1]Sandia National Laboratories

Polycrystalline materials exhibit properties that are directly influenced by the morphology and crystallographic orientation of their constituent grains. In this work, we interrogate the 3D grain morphology and texture of polycrystalline materials (such as alpha titanium) via polarized light microscopy (PLM) within a commercially available automated serial-sectioning system platform. PLM leverages optical birefringence in anisotropic/uniaxial crystalline materials to assess crystal inclination relative to the incident polarized light beam, resulting in image contrast that reveals grain orientation. The serial-sectioning process automates conventional metallographic preparation, and we implement automated control routines to collect large image montages at various polarization states by rotating the sample to discrete angular intervals. We introduce data reconstruction techniques to rapidly determine the grain morphology and crystallographic texture in centimeter-scale volumes. Details of novel approaches to analysis will be presented. Applications to macroscale texture quantification and understanding mechanical properties in lower-symmetry and multi-phase systems will also be discussed.

9:30 AM Break

9:50 AM
Accelerating 3D Data Collection in TriBeam Microscopes: *McLean Echlin*[1]; James Lamb[1]; Andrew Polonsky[2]; Nicolò Maria della Ventura[1]; Kalani Moore[3]; Jorge Filevich[4]; Will Lenthe[5]; Steven Randolph[6]; Remco Geurts[4]; Chris Torbet[1]; Daniel Gianola[1]; Marc De Graef[7]; Tresa Pollock[1]; [1]University of California Santa Barbara; [2]Sandia National Laboratory; [3]Direct Electron; [4]Thermo Fisher Scientific; [5]EDAX-Gatan; [6]Oak Ridge National Laboratory; [7]Carnegie Mellon University

The latest generation of TriBeam microscope's high current PFIBs and multi-wavelength femtosecond laser sources enable faster material sectioning than previous generation systems. By combining these material removal modalities, procedures for limiting subsurface damage across ever widening classes of materials is possible. For instance, 3D datasets from polymer composites, biological samples, and battery materials have been collected at various institutions with this new instrument. However, improvements to the process of building TriBeam experiment workflows would vastly increase data collection and make these instruments accessible more broadly to researchers. Furthermore, the collection of information from a wider range of modalities, such as newly developed EBSD detectors that directly detect electrons, will require control software that can flexibly incorporate new hardware APIs. These new developments in instrumentation, data modalities, and opportunities for future iterations will be discussed.

10:10 AM
Enhancement of Multi-Modal Mechanical Polishing Serial Sectioning Technology: *Michael Uchic*[1]; Michael Scott[2]; Gregory Sparks[3]; Michael Chapman[2]; [1]Air Force Research Laboratory; [2]BlueHalo LLC; [3]University of Dayton Research Institute

Automated mechanical polishing serial sectioning (MPSS) experiments have been matured over the past two decades to provide accurate volumetric reconstructions of microscale feature ensembles within centimeter-scale and larger samples. However, the availability of MPSS data–especially multimodal data–is still somewhat limited. The vast majority of automated MPSS systems operate on only one sample at a time, and often with limited feedback or analysis during the experiment. This presentation will discuss the development of a novel multimodal MPSS system as an alternative to the current state-of-the-art. The system is comprised of multiple preparation systems, microscopes, and a mobile sample transfer robot, which can be used for MPSS workflows that accommodate numerous samples concurrently, including use of minimal surface damage methods such as vibratory polishing. Additionally, we discuss the implementation of "on-the-fly" analysis to further improve MPSS data uniformity and quality, and present experimental data to demonstrate these improvements.

10:30 AM
Automated Mechanical Serial Sectioning: A Robust Data-Driven Approach as Applied to a RoboMet.3D: *Rhianna Oakley*[1]; Paul Chao[1]; Andrew Polonsky[1]; [1]Sandia National Laboratories

The RoboMet.3D, a semi-automated mechanical serial sectioning (MSS) tool, enables the acquisition of microstructural data across macroscopic length scales by layer-wise material removal and imaging, generating a 3D structure representation of complex multi-material components. This process unveils features and failure mechanisms hidden from traditional 2D and non-destructive methods. However, achieving uniform material removal is hindered by system inconsistencies, often demanding manual adjustments by skilled operators, thus extending data collection and necessitating extensive post-processing. We introduce a novel one-step model predictive control (MPC) framework integrated with a run-to-run (R2R) controller, designed to automate parameter adjustments, enhancing material removal precision through iterative feedback and disturbance management. This data-driven R2R-MPC controller ensures consistent removal rates, adapting seamlessly to varying material properties. Its superiority is validated against traditional methods through both simulations and empirical results, showcasing significant advancements in efficiency and reliability for 3D microstructural analysis.

10:50 AM

3D Intragranular Orientation Mapping in Cold-Rolled Ferrite at Industrially Relevant Deformation Levels: *Aditya Shukla*[1]; Mads Carlsen[2]; N. Mavrikakis[3]; Virginia Sanna[1]; Marilyn Sarkis[1]; Carsten Detlefs[1]; Yaozhu Li[1]; Can Yildirim[1]; [1]European Synchrotron Radiation Facility - ESRF; [2]Paul Scherer Institut; [3]OCAS

Thermomechanical processing of metals introduces high dislocation densities, altering material properties through mechanisms such as work hardening. Non-destructive 3D mapping of deformation microstructures remains a challenge due to limitations in characterization tools. This study combines Dark-Field X-ray Microscopy (DFXM) and texture tomography (TT) to investigate deformation structures in 50% and 65% cold-rolled ferrite. DFXM enables non-destructive 3D mapping of intragranular deformation structures, resolving dislocation cells with elevated densities and misorientation values up to 5˚, at a resolution of 100 nm. TT complements this by providing 3D grain orientation data, aligning grains relative to the rolling direction and bridging the effects of neighboring grains on deformation. These data are also validated with complementary Electron backscatter diffraction (EBSD) measurements. The combined approach reveals the evolution of intragranular deformation structures, cell size distributions, and strain hotspots as a function of deformation, advancing our understanding of plasticity and the interplay between local and global deformation behaviors. This framework offers critical insights into deformation mechanisms and recrystallization in metals.

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): PSP Linkages: Multiscale/Multiphysics Modeling V

Thursday PM
June 19, 2025

Room: Room F
Location: Anaheim Marriott

Session Chair: To Be Announced

12:30 PM Cancelled

12:50 PM

Combination of Equilibration Preserving Machine Learning approaches With DOFKILL/DOFALIVE Multiphysics Approaches With Damage Partitioning: *Deepankar Pal*[1]; Anupam Neogi[1]; Junyan He[1]; Grama Bhashyam[1]; [1]ANSYS

Integrating equilibration-preserving deep learning (DL) techniques that satisfy equilibrium in the strong form with DOFKILL/DOFALIVE-based multiphysics frameworks offers a promising approach for modeling complex material behaviors related to structural, thermal, and diffusion physics under damage. Equilibration-preserving DL, such as Machine Learning enabled Stiffness (MLeS), ensures that learned approximations maintain physical constraints, making it suitable for multiphysics analogs of structural damage analysis. A combination (MLeS/traditional approach) with DOFKILL/DOFALIVE methods—where degrees of freedom (DOF) are selectively activated or deactivated based on combined metrics of damage and multiphysics—enables efficient partitioning of damage into brittle and ductile forms. This synergy allows the model to dynamically adapt its complexity, activating DOFs only where needed, reducing computational load without sacrificing accuracy. An example in Hydrogen Embrittlement (HE) will demonstrate damage partitioning and how coupled physics influences partitioning, order, and extent of damage. In addition, the accuracy, speedup, and DOF dropout/pickup aspects will be further discussed.

1:10 PM

Crystal Plasticity Analysis of Microstructure Effect on Formability of AA5052 Aluminum Alloys: *Minh Tien Tran*[1]; Han-Jun Lee[1]; Hoang Cuong Phan[1]; Hoang-Hai-Nam Nguyen[1]; Dong-Kyu Kim[2]; Ho Won Lee[1]; [1]Korea Institute of Materials Science; [2]Konkuk University

This study presents virtual material testing via crystal plasticity finite element method (CPFEM) coupling with the Marciniak-Kuczynski (MK) model to predict macroscopic mechanical behavior of aluminum alloy sheets, particularly investigating effect of microstructure on forming limit diagrams (FLD) of AA5052 aluminum alloys. Firstly, the CPFEM simulation is conducted to identify the hardening parameters for CPFEM-MK analysis of FLD. The predicted FLDs are consistent with experimental data, revealing a significant degradation of FLD as material thickness decreases. Secondly, the microstructures varied in crystallographic texture, grain shape together with grain size are fully considered in the CPFEM-MK analysis of forming limits. Results reveal a noticeably apparent influence on formability, primarily due to distinct stress-strain heterogeneities associated with the formation of local hotspots. The present study provides significant insight into the role of microstructure in localized deformation behavior and potential failure points, emphasizing the importance of microstructural control to enhance formability.

1:30 PM Break

1:45 PM

Incorporating Process-Induced Heterogeneity for Predicting Anisotropy in Aluminum Alloys: *Jinheung Park*[1]; Jinmo Koo[2]; Reza Rezaei[1]; Steven Long[3]; Amir Asgharzadeh[3]; Robert Dick[3]; Myoung-Gyu Lee[2]; Taejoon Park[1]; Farhang Pourboghrat[1]; [1]The Ohio State University; [2]Seoul National University; [3]Kaiser Aluminum

Plastic anisotropy in materials primarily depends on the texture evolution resulting from manufacturing processes. Numerous efforts have been made to predict plastic anisotropy using crystal plasticity finite element (CPFE) analysis based on these textures. However, accurately predicting plastic anisotropy remains challenging due to material heterogeneity. In this study, we introduce a computational framework capable of accurately predicting the plastic anisotropy of cold-rolled aluminum alloy sheets. We first simulated the rolling process using CPFE analysis to predict heterogeneity in dislocation density and crystal orientations after cold rolling and developed a representative volume element (RVE) incorporating this heterogeneity. By conducting CPFE virtual tensile tests on the generated RVEs, we then predicted r-values and normalized yield stresses in various loading directions. The proposed framework demonstrated improved prediction accuracy compared with conventional approaches, emphasizing that accurate prediction of plastic anisotropy requires considering the effect of manufacturing processes.

2:05 PM

Investigation of Sources of Discrepancies in Crystal Plasticity Simulations by Leveraging High-Fidelity Characterization Datasets: *Saikumar Reddy Yeratapally*[1]; George Weber[2]; Diwakar Naragani[3]; Paul Shade[4]; Edward Glaessgen[2]; [1]Science and Technology Corporation; [2]NASA Langley Research Center; [3]Cornell High Energy Synchrotron Source; [4]Air Force Research Laboratory

The advent of high-fidelity characterization techniques has provided valuable insights into the influence of microstructure on deformation and damage accumulation in polycrystalline alloys. Concurrently, the development of crystal plasticity (CP) models has provided complementary insights into various attributes (e.g. accumulation and evolution of subsurface plastic strain) that cannot be readily measured using advanced characterization techniques. However, missing physics, ignoring residual stresses, applying incorrect boundary conditions, and ignoring subsurface microstructure can lead to discrepancies between measurements and predictions from CP simulations. This presentation focuses on demonstrating how each of the aforementioned factors can result in discrepancies while predicting elastic modulus, grain-average elastic strains, stress relaxation and active slip systems. Validation data obtained from various high-fidelity measurements like high-energy X-Ray diffraction microscopy and high-resolution digital image correlation were used.

2:25 PM

A Modeling Framework to Inform the Fabrication of U-10Mo Monolithic and U3Si2 Fuel: *Ayoub Soulami*[1]; Kyoo Sil Choi[1]; Lei Li[1]; William Frazier[1]; Yucheng Fu[1]; Taylor Mason[1]; Vineet Joshi[1]; Curt Lavender[1]; [1]Pacific Northwest National Laboratory

Low-enriched uranium alloyed with 10 wt% molybdenum (U-10Mo) has been identified as a promising alternative to highly enriched uranium as fuel for the United States high-performance research reactors. U3Si2 dispersion fuels to be used in the High Flux Isotope Reactor (HFIR) have complex fuel geometries which creates challenges in Manufacturing. Fabricating these fuel plates consists of multiple complex thermomechanical processes, which lead to changes in the microstructure and can lead to defects. The integrated computational materials engineering (ICME) concept supports building a microstructure-based framework to investigate the effect of manufacturing processes on the material microstructure. In this presentation we will discuss how series of models have been informing the fabrication process. The models have directly impacted the fabrication and have been used to optimize the rolling schedule, reduce time and cost of fabrication, eliminate fabrication defects, and meeting the specifications.

The 7th International Congress on 3D Materials Science (3DMS 2025): 3D Data Processing, Software, and Reconstruction Algorithms III

Thursday PM
June 19, 2025

Room: Room C
Location: Anaheim Marriott

Session Chair: To Be Announced

12:30 PM

Uncertainty in High-Angular-Precision 3D-EBSD Orientation Measurements Using Spherical Harmonic Indexing and Global Pattern Center Optimization on Deformed and Undeformed Samples: *Gregory Sparks*[1]; Michael Uchic[2]; Paul Shade[2]; Mark Obstalecki[2]; [1]University of Dayton Research Institute; [2]Air Force Research Laboratory

In previous work, we demonstrated the use of high-precision EBSD orientation measurements from spherical harmonic indexing (SHI) combined with global pattern center (PC) optimization in 3D-EBSD reconstruction of an undeformed Ni superalloy sample. In this talk, we discuss the layer-to-layer consistency of the orientations measured using this technique both from the previous undeformed sample and a separate, deformed Ni superalloy sample, and compare this with the consistency of repeated measurements on a single layer for both samples. We also investigate the difference between orientation measurements from a Si wafer at 70° tilt (using the same technique of high-precision SHI with PC optimization) and orientation measurements from the same Si wafer at 0° tilt (obtained from matching experimental electron channeling patterns (ECP) with simulated ECP) as a potential explanation for residual rigid-body orientation errors in 3D-EBSD relative to other orientation measurement modalities.

12:50 PM

On the Inverse Problem of Recovering Admissible Intragranular Strain Fields From High-Energy X-Ray Diffraction Data: *Carter Cocke*[1]; Andrew Akerson[1]; Sara Gorske[1]; Katherine Faber[1]; Kaushik Bhattacharya[1]; [1]California Institute of Technology

Recovering strain fields from high-energy X-ray diffraction data is a challenging inverse problem that is commonly simplified to only obtain grain-averaged strains. Advanced techniques that obtain sub-granular strain fields often relax the requirement of either strain compatibility or stress equilibrium. Here, we present two methods that strongly enforce these requirements. The first approach is a post-processing step using grain-averaged strains and microstructural information from preexisting reconstruction algorithms. Using a finite-element formulation, the problem is posed as a linearly constrained least-squares problem that may be efficiently solved. We demonstrate the method through synthetic and experimental examples and recover intragranular strains with low error. Eschewing the need for a pre-reconstruction step, the second method directly inverts raw diffraction measurements. We discuss preliminary results and the associated challenges. The methods presented highlight that mechanical admissibility significantly constrains the solution space, which may be exploited to recover intragranular strains with high accuracy.

1:10 PM

Enhancing Polycrystalline-Microstructure Reconstruction From Diffraction Microscopy With Phase-Field Post-Processing: *Marcel Chlupsa*[1]; Zach Croft[1]; Katsuyo Thornton[1]; Ashwin Shahani[1]; [1]University of Michigan

A new protocol using a phase-field model processes 3D reconstructions of polycrystalline microstructures from synchrotron-based high-energy X-ray diffraction microscopy (HEDM) data. These reconstructions face challenges such as heterogeneous grain sizes, detector limitations, and overlapping Bragg peaks, among other errors. The noise often results in non-physical roughness at grain boundaries (GBs), complicating property measurements like tortuosity, curvature, and GB character. Such uncertainties hinder estimates of diffusivity, corrosion resistance, electrical resistance, and fracture strength. To address these issues, we employ phase-field equations to create a space-filling grain map that adheres to the physics of the microstructure. It penalizes high-energy grain shapes and configurations while promoting GB smoothing. High-confidence regions are preserved using a completeness-based mobility parameter in the phase-field model. This protocol offers an alternative to conventional image processing-based approaches. It can be applied to any diffraction-based, 2D or 3D reconstruction with grain and confidence data, including polyphase materials.

1:30 PM Break

1:45 PM
Identifying SOFC Triple Phase Boundaries From 3D FIBSEM: *Alexander Hall*[1]; Chengge Jiao[1]; Bartomiej Winiarski[1]; Patrick Barthelemy[1]; [1]Thermo Fisher Scientific

Electrochemical reactions at Triple Phase Boudaries (TPB) largely determine the efficiency of Solid Oxide Fuel Cells (SOFC). SOFC microstructure can be viewed in 3D using FIB-SEM. Specifically, the combination of Backscattered Electron (BSE) and Through-the-Lens Detector (TLD) Secondary Electron (SE) images allows easy identification of the three phases in a SOFC electrode sample. By using a plasma ion source, we reconstructed a sample volume roughly ten times larger than prior efforts. Additionally, we used deep learning segmentation of the Pore, YSZ, and Ni phases of the SOFC electrode. With this information, we characterized the volume fraction, two-phase interface densities, and TPBs from a volume large enough to be representative of the sample. Our work represents many technical improvements to SOFC characterization, but also a standardized workflow on which future SOFC characterization efforts can be based.

2:05 PM
Multimodal Microstructural Image Segmentation of Low-Temperature Sn3Ag0.5Cu7Bi Solder Using Multi-Channel Deep Learning: *Eshan Ganju*[1]; John Wu[1]; Nikhilesh Chawla[1]; [1]Purdue University

High-throughput and accurate semantic segmentation of electron microscopy data is crucial for efficient microstructural analysis, particularly in complex low-temperature solders. To obtain a complete picture of a materials system, various complementary streams of data are often required. By combining backscattered electron images, secondary electron images, and energy dispersive spectroscopy data as input for a deep learning-based approach, we can effectively exploit the complementary information provided by each imaging modality. When applied to a 3D dataset, this approach capitalizes on the unique material contrast from backscatter, surface topography from secondary electrons, and precise elemental distribution from compositional maps, leveraging the power of a multi-channel Unet++ inspired architecture to improve segmentation accuracy. Evaluation on an Sn3Ag0.5Cu7Bi dataset demonstrated that the multi-channel approach performs well and enables accurate identification and quantification of microstructural features. This study highlights the potential of multi-channel deep learning for advanced characterization of complex microstructures.

2:25 PM
Unlocking 3D Nanoparticle Shapes From 2D HRTEM images: Deep Learning for Classification and Denoising at Atomic Resolution: *Romain Moreau*[1]; Hakim Amara[1]; Maxime Moreaud[2]; Jaysen Nelayah[3]; Adrien Moncomble[3]; Christian Ricolleau[3]; Damien Alloyeau[3]; Riccardo Gatti[1]; [1]Université Paris-Saclay, ONERA, CNRS, Laboratoire d'Étude des Microstructures, 92320; [2]IFP Énergies Nouvelles, 69360; [3]Université Paris Cité, CNRS, Laboratoire Matériaux et Phénomènes Quantiques (MPQ), 75013

The study focuses on leveraging Deep Learning (DL) to enhance the analysis of nanoparticles (NPs) using High Resolution Transmission Electron Microscopy (HRTEM), down to atomic resolution. A Convolutional Neural Network (CNN) model was developed to automate the identification of 3D NP shapes from 2D images, overcoming challenges related to manual post-processing and noise. The model was trained on a carefully curated dataset of simulated HRTEM images, capturing various orientations, defocuses and NP sizes. Additionally, a UNet-type model was created for denoising and enhancing contrast between NPs and substrates, addressing limitations in image clarity due to microscope aberrations and environment. Even though this denoising model gives accurate predictions while processing simulated images, we have noticed that the inference on experimental images could sometimes fail. Therefore, we have added a segmentation model to improve the robustness of predictions on experimental micrographs.

2:45 PM
Classification of Abnormal Grain Growth Using 3D Convolutional Neural Networks: *Woohyun Eum*[1]; Yi Wang[2]; Amanda Krause[2]; Michael Tonks[1]; Joel Harley[1]; [1]University of Florida; [2]Carnegie Mellon University

Understanding what triggers abnormal grain growth (AGG) remains a challenge, as conventional descriptors do not fully explain it. This paper hypothesizes that more complex descriptors play a role in driving AGG. To test this, we train a 3D convolutional neural networks (CNN) to identify abnormal grains (identified manually after heat treatment) from the microstructure boundaries as-sintered Nickel samples before heat treatment, where human experts cannot visually distinguish abnormal grains. Our results demonstrate that the model achieves a 81.6% accuracy, as compared with a 66% accuracy for classifier based only on grain size. Note our input data does not contain orientation information, implying that abnormal grain growth may be observed from the grain boundary network alone. This work marks the first use of 3D CNNs with 3D measurements to capture multi-dimensional information about microstructures, highlighting their critical role in predicting AGG at early stages, without relying on traditional metrics.

3rd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2025): Posters

Tuesday PM
June 17, 2025

Room: Poster Room
Location: Anaheim Marriott

Session Chair: To Be Announced

Analysis of an Intelligent Characteristics of the Blast Furnace Peripheral Zone: *Sumaila Omeiza Jimoh*[1]; [1]Federal University of Technology, Babura

It is known that the minimum flow of coke rate is reached when CO use is at a maximum in the blast Furnace. This is achieved when the Peripheral Zones carries the Furnace maximum permissible load and is operating with an open center. The Aim of this research was to study an intelligent characteristics of heat emissions and recovery work in the Peripheral zone of the blast furnace. The developed model to calculate the gas temperature and its recovery in the peripheral zone of the BF can be used to optimize the thermal state of the shaft furnace in the peripheral zone.Keywords: Blast Furnace, coke rate, Carbon monoxide, Artificial intelligence (AI), Heat loss, peripheral zone.

Deep Learning for Industrial-Scale Modeling of the Basic Oxygen Furnace Process: *Maryam Khaksar Ghalati*[1]; Zhou Daniel Hao[1]; Jianbo Zhang[1]; Hongbiao Dong[1]; [1]University of Leicester

The basic oxygen furnace (BOF) steelmaking process is a cornerstone of modern steel production, where accurate modeling is critical for optimizing operations, improving process control, and enhancing energy efficiency. This study investigates the application of advanced deep learning models, including deep transformers, to model the BOF process. Representing the first extensive deployment of such architectures on BOF operational data, we evaluated multiple state-of-the-art models using a comprehensive dataset comprising over 10,000 samples from a large-scale industrial setting. Our research introduces novel approaches tailored to the complexities of BOF data, leveraging insights from exploratory data analysis to enhance predictive performance. The proposed models demonstrated improvements in accuracy compared to traditional methods, highlighting the transformative potential of deep learning in optimizing industrial processes.

Development of Milling State Assessment System Using Machined Surface Images and Engineer's Sensory Evaluations as Supervised Data: *Ryo Tanaka*[1]; Tatsuya Furuki[1]; [1]Chubu University

Milling manufacturing for products such as mold or medical products requires high-quality machined surfaces, engineers have achieved stable and efficient production by visually evaluating the appearance of machined surfaces and tools. However, such tacit intellectual skills are difficult to pass on. In this study, we attempted to develop a digital triplet-typed machining condition evaluation system based on a machine learning algorithm with excellent human interpretability, such as decision trees, using images of machined surfaces and the engineer's sensory evaluation as training data. Furthermore, milling produces scaly cutting mark patterns, although if variations of cutting mark shapes occur, the product's appearance like the glossiness deteriorates. Therefore, the developed system recognizes the shape of cutting marks and matches the pattern to evaluate the stability of the machined surface. This system enables unskilled engineers to know the results of evaluating superior engineers simply by taking pictures of the cutting surface.

Ontology-Based Digital Representations of Materials Testing in the MaterialDigital Initiative: *Hossein Beygi Nasrabadi*[1]; Birgit Skrotzki[2]; Harald Sack[1]; [1]FIZ Karlsruhe — Leibniz Institute for Information Infrastructure; [2]Bundesanstalt für Materialforschung und -prüfung (BAM)

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). In recent years, PMD achieved lots of progresses for developing the data ecosystem for digital materials research. The fundament of the data ecosystem is ontology-based digital representations of materials characteristics. 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 several mechanical testing use cases.

Optimization of Machining Conditions for Improved Machining Quality Based on a Digital Twin of Machine Tools: *Beomsik Sim*[1]; Jae-Eun Kim[1]; Wonkyun Lee[1]; [1]Chungnam National University

Optimizing machining conditions is essential for enhancing machining quality. This study proposes an approach to optimize machining conditions using a digital twin of a machine tool. The digital twin integrates key components, including the controller, feed drive system, and physical models based on cutting theory to estimate machining quality. It enables virtual experiments that incorporate the machine's dynamic behavior and control characteristics, offering a more accurate representation of the machining process. Based on these virtual experiment results, optimization techniques adjust the feed rate and spindle speed. This approach provides precise optimization by calculating machining quality as influenced by control characteristics and dynamic behavior, which traditional methods, such as design of experiments or basic models, cannot account for. The method is validated by comparing machining quality and machining time between non-optimized and optimized conditions, along with assessing the accuracy of the digital twin's predictions.Acknowledgment: This work was supported in part by the Technology Development Program for Smart Controller in Manufacturing Equipment (No. 20012834, Development of Smart CNC Control System Technology for Manufacturing Equipment) funded by the Ministry of Trade, Industry & Energy (MOTIE, Korea) and in part by a Korea Institute for Advancement of Technology (KIAT) grant funded by the Korean Government (MOTIE) (No. P00020616, The Competency Development Program for Industry Specialist).

Process Control System and Cloud Simulation Platform for Continuous Casting Based on Digital Twin Technology: *Cheng Ji*[1]; Bochun Liang[1]; [1]Northeastern University

In this work, a digital twin system is architected which predicts in real time the 3D temperature field, full-section reduction deformation and micro-structure evolution of the continuous casting. In temperature prediction, thermophysical parameters can be loaded in real time based on the specific location of the billet in 3D space, which ensured the prediction accuracy of solidification process. For deformation prediction, based on three-dimensional thermal/mechanical coupled FEM data-driven and mechanism-driven, a model for online prediction of deformation characteristics during the continuous casting process is established, with the calculation process employing nodal stress accumulation to determine pressure force. In micro-structure evolution, the precipitation of Mns, Ti(C, N) and ect were predicted by coupling microegregation with saturated solid solution product . In the practice, the digital twin system can control of process parameters rapidly, and it was appied in slab and bloom continuous casting process control more than 15 casters.

Quantum Machine Learning: Revolutionizing Fatigue Fracture Mode Prediction of Laser Powder Processed Inconel 625: *Ravindranadh Bobbili*[1]; Chitti Babu N[1]; [1]DRDO

The present study employs a quantum machine learning approach to predict the fatigue test failure of laser powder processed Inconel 625 alloy. In this research, four machine learning models were applied for fatigue fracture modeling. The machine learning algorithms (logistic regression, random forest, gradient boosting and QLattice) are trained and tested for fracture prediction. The input features are porosity (%), alternated stress, cycles, defect size (Area 1/2), respectively. The QLattice, gradient boosting and random forest models have the best performance as far as ROC-AUC curves are concerned. In addition, the shapley additive explanations (SHAP) is introduced to improve the interpretability of model. This cutting-edge approach offers unparalleled efficiency, accuracy, and cost-effectiveness compared to traditional experimental testing methods. Its ability to harness the power of quantum computing to predict fatigue fracture of laser powder processed Inconel offers immense potential for improvingmaterials design and manufacturing processes.

Unsupervised Learning for Low Dimensional Corrosion Quantification of Aluminum Films: *Sarah Firestone*[1]; Nathan Brown[1]; David Montes de Oca Zapiain[1]; Aditya Venkatraman[1]; [1]Sandia National Laboratories

Environmental corrosion at small length-scales can be assessed by the manual evaluation of topographical images of component surfaces using an Oxford-AFM. However, this process is time-consuming and subject to bias introduced by the researcher. In this work we address these challenges by developing an efficient and data-driven analysis of the images. Our proposed solution involves using unsupervised learning to identify trends of dynamic surface corrosion activity based on 2D topographical images of the samples subjected to harsh environments. Specifically, we leveraged computational techniques such as Generalized Extreme Value Distribution, binarization, spatial correlations, Principal Component Analysis, and K-Means clustering. Our protocols demonstrate excellent efficacy in identifying the evolution of corrosive features, even for previously unseen images. As a result, we have successfully established a continuum of corrosive states within the latent space, which allows for rapid, preemptive identification and facilitates localized mitigation. SNL is managed and operated by NTESS under DOE-NNSA-contract-DE-NA0003525.SANDNo.SAND2024-14510A

8th World Congress on Integrated Computational Materials Engineering (ICME 2025): Posters

Tuesday PM
June 17, 2025

Room: Poster Room
Location: Anaheim Marriott

Session Chair: To Be Announced

Advancing Materials Discovery: A Novel Generative Model for Inverse Design of Vanadium Oxide Crystal Structures: Danial Ebrahimzadeh[1]; Sarah Sharif[1]; *Yaser 'Mike' Banad*[1]; [1]University of Oklahoma

The discovery of high-performance materials is vital for addressing technical challenges in modern industries. Inverse design methodologies have revolutionized the search for tailored materials. We present a novel generative model combining an enhanced Generative Adversarial Network (GAN) and improved Variational Autoencoder (VAE) for invertible crystal structure encoding. Unlike traditional methods, our model excels in generating and optimizing crystal structures, validated in V-O compositions. Comparative analysis shows superior efficiency, achieving lower loss and better convergence than previously used GAN model. Our model discovered 151 stable and 107 metastable structures of 1394 DFT-evaluated structures within the stability and metastability range, derived from the Materials Project (MP) dataset. Additionally, our findings suggest updates to the stability range in the convex hull of MP. This work marks a significant advancement in inverse design, paving the way for transformative developments in materials science

Cerium's Effect on the Mechanical Characteristics and Transformation Kinetics of Low Carbon Steels: *Chetan Kadgaye*[1]; [1]Iit Roorkee

This study examines the detailed dilatometric and electron microscopic analysis of austenite formation and its subsequent decomposition in two cerium (Ce)-modified steels containing 0.6 and 0.03 wt% Ce. In the high-Ce steel (0.6 wt% Ce), austenite forms rapidly during heating, despite a prolonged incubation period. In contrast, the low-Ce steel (0.03 wt% Ce) promotes early austenite nucleation but exhibits a significant delay in completing the transformation. A similar pattern is observed during austenite decomposition upon cooling, where the low-Ce steel initiates the transformation early but with slower kinetics. The influence of Ce on the overall austenite transformation kinetics during the heating–cooling cycle is discussed from both a thermodynamic perspective and nucleation probability. Engineering stress–strain curves indicate that the low-Ce steel offers a better balance of strength and ductilitycompared to the high-Ce steel.

Development of Cu-S Interatomic Potentials for Time- and Length-Scale Bridging: *Thomas Hardin*[1]; [1]Sandia National Laboratories

Sulfidation of copper in the presence of sulfuric gases causes embrittlement and degradation of electrical properties. We report the development and validation of a "ladder" of copper-sulfur interatomic potentials representing a variety of speed/accuracy tradeoffs; we find that by additively decomposing the potential energy surface into effects captured by the Embedded Atom Method (EAM) and a machine learned correction term, risk of overfitting is reduced and overall accuracy is improved. Finally, we report on progress towards bridging time- and length-scales by extracting kinetic process rates from atomistic simulations based on these potentials. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525 (SAND2024-14710A).

Dissipative Triatomic Metamaterial for Broadband Asymmetric Elastic-Wave Transmission: *Sagr Alamri*[1]; Li Bing[2]; [1]King Khalid University; [2]Northwestern Polytechnical University

An innovative design is proposed for a dissipative triatomic elastic metamaterial to obtain asymmetric wave transmission to realize asymmetric wave transmission in two low-frequency bands. These frequency bands can be analytically and experimentally predicted to realize two paths of wave propagation and wave attenuation along two different directions of transmission.

Enhanced Thermal Conductivity for Modified hBN and Epoxy Composite Using Electric Field: *Sidra Ajmal*[1]; Abul Arif[1]; [1]King Fahd University of Petroleum & Minerals

Hexagonal boron nitride (hBN) exhibits exceptional thermal and dielectric characteristics making it a suitable filler for enhancing thermal conductivity in high-temperature polymer matrix. In this study, hBN/epoxy composites were synthesised and their thermal conductivity was thoroughly examined. Furthermore, hBN particles were functionalizedusing plasma modification to improve the compatibility with the epoxy matrix. The composite fabrication involved compression molding, followed by drying in a vacuum oven at 70°C for 6 hours. An electric field was applied during the process to achieve directional alignment of the hBN particles, further enhancing thermal conductivity. The present work employs a representative volume element (RVE) approach and periodic boundary conditions (PBC) to accurately predict thermal conductivity (K), elastic modulus (E) and coefficient of thermal expansion () using 3D finite element (FE) simulations. The resulting composites exhibited significantly improved thermal properties, making them promising candidates for efficient heat dissipation in high-performance electronic devices.

Leveraging Advances in Additive Manufacturing Thermal Models to Predict Behavior During Laser Sheet Metal Forming: *Benjamin Begley*[1]; Zoe Lipton[1]; Daniel Bolden[1]; Tianchen Wei[1]; Nathan Fripp[1]; Victoria Miller[1]; [1]University of Florida

Laser sheet metal forming—along with additive manufacturing—is nearly unique in that it has been developed using an ICME-style research paradigm since its inception. Modeling both the thermal input and the mechanics of bending, then linking those processes together, is critical to realizing the full manufacturing process at an industrial scale. This work describes the development, validation, and application of an analytical, forward-stepping thermal model for laser forming in MATLAB, derived from computationally efficient models for additive manufacturing and welding. Small-scale, high-throughput laser forming experiments are used to link the thermal model outputs across laser forming parameter space with predictions of bending mechanism and extent. Finally, gaps in the current ICME approach are discussed, such as the changing absorptivity during multipass laser forming experiments.

Molecular Dynamics Simulation of Polyurea for Impact-Resistant Applications: *Tyler Collins*[1]; Sara Adibi[1]; [1]San Diego State University

Polyurea, a versatile block copolymer, is widely applied in impact-resistant applications like protective gear and structural reinforcements. Its unique molecular architecture, featuring hard segments for rigidity and soft segments for flexibility, provides remarkable elasticity and toughness. Additionally, polyurea dissipates stress from high-velocity impacts through the breaking of hydrogen bonds. This study employs molecular dynamics simulations in LAMMPS to investigate polyurea's nanoscale response to high-velocity impacts. We analyze temperature fluctuations, stress propagation, and failure mechanisms to better understand its performance under extreme conditions. These insights are valuable for designing enhanced materials for impact-resistant applications, such as body armor. By simulating scenarios difficult to replicate experimentally, this work highlights the utility of computational methods in advancing material design for high-performance and safety-critical applications.

Rapid Structure Prediction of Single-Phase High Entropy Alloys Using Graph Neural Network Based Surrogate Modelling: *Nicolas Beaver*[1]; Aniruddha Dive[1]; Marina Wong[1]; Keita Shimanuki[1]; Ananya Patil[1]; Anthony Ferrell[1]; Mohsen Kivy[1]; [1]California Polytechnic State University

In this study, we developed a rapid, reliable and cost-effective methodology via employing a Graph Neural Network based machine learning approach to effectively predict the crystal structures of single-phase high entropy alloys. Our novel approach searches through the enormous potential energy surface (PES) landscape with an aim to identify stable lowest energy crystal structure. Our approach was tested on 132 high entropy alloys, and the predictions were verified with the experimental data in literature. Overall, we achieved ~ 83 % accuracy in correctly predicting the stable crystal structures. Our prediction accuracy easily betters the prediction accuracy based on valence electron concentration (VEC) approach that is widely utilized for crystal structure prediction. Our proposed method was ultimately applied to predict the structure of a novel cobalt-free high-entropy alloy. Our predicted crystal structure of the alloy matched the one characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and X-ray fluorescence (XRF).

"Why Can't we Just use Excel?:" Lessons on Incorporating ICME in the Undergraduate Classroom: *Victoria Miller*[1]; [1]University of Florida

Developing a data literate workforce is crucial at every level, from K12 to PhD. However, undergraduate students are often resistant to learning basic data and coding skills. In other students, willingness to learn is eclipsed by a lack of basic computer literacy. In this presentation, lessons learned during the modernization of several individual classes and an undergraduate curriculum are discussed. Common pitfalls and strategies for overcoming them are presented.

A New Mathematical Model for Materials With Dissipating Properties: *Mathew Aibinu*[1]; [1]Durban University of Technology

A powerful tool to test hypotheses, confirm experiments and simulate the dynamics of complex systems is mathematical modelling. Using mathematical models can help to avoid the enormous costs of laboratory experiments and corresponding biological variations. Mathematical models simulate complex systems in a comparatively short time and can help to understand the basis of dynamical systems. The study proposes a mathematical model that is new and of more vitality and suitability for materials with dissipating properties. The study presents a method for the construction of solutions of the newly created mathematical model for materials with dissipating properties. Using a mathematical software package, the study presents the graphs of the solutions by choosing arbitrary values for the parameters for the graphical illustration of the processes.

The 7th International Congress on 3D Materials Science (3DMS 2025): Poster Session

Tuesday PM
June 17, 2025

Room: Poster Room
Location: Anaheim Marriott

Session Chair: To Be Announced

4D Multimodal Testing and Numerical Simulations Applied to the Study of Incipient Crystal Plasticity: *Clement Ribart*[1]; Aldo Marano[2]; Wolfgang Ludwig[3]; Henry Proudhon[1]; [1]Centre des Materiaux - Mines Paris; [2]ONERA; [3]ESRF

We present a multimodal analysis of incipient polycrystalline plasticity from a titanium tensile sample. The dataset was generated from experimental acquisitions involving synchrotron DCT and conventional EBSD at the initial and deformed state. The DCT allows to generate a 3D digital twin (1 cubic mm) on which a full field FFT simulation was performed with a finite strain continuum crystal plasticity formalism. Following a careful registration of the modalities, a detailed comparison was performed at the mesoscopic, intergranular and intragranular (1 cubic µm voxel resolution) scales. Results demonstrated the higher performance of DCT over EBSD to track orientations while revealing in bulk new sub-grains mechanisms from the computation of GND fields. In addition the numerical results show good agreement with experiment at every scale while offering extra information to interpret the link between disorientation fields and plastic slip activity.

A Novel Method for Microstructure Prediction of Austenitic Stainless Steel Based on Machine Learning: *Yuqing Du*[1]; Jun Sun[2]; Håkon W. Ånes[2]; Fei Chen[1]; [1]Shanghai Jiao Tong University; [2]Xnovo Technology ApS

The prediction of mixed grains is crucial for determining whether austenitic stainless steel achieves excellent mechanical properties after solution treatment. In this presentation, machine learning approach is adopted to predict the microstructure evolution of austenitic stainless steel during hot deformation and solution treatment. Five different machine learning models are compared, using experimental data from large-area EBSD measurements covering mixed grain areas. Shapley Additive exPlains (SHAP) method was found to be most accurate interpreting the model to find key factors affecting the formation of mixed grains in hot deformation and solid solution treatment. Moreover, a time series 3D grain data about these key factors was researched from lab-based diffraction contrast tomography (Lab-based DCT) characterizing the grain coarsening processing during solution treatment. Various aspects coupling 2D and 3D experimental data to machine learning will also be discussed.

Design Considerations for Printed Functional Prototypes: *Mark Patterson*[1]; Mathew Kuttolamado[2]; Carlos Mora Salcedo[2]; Herman Neid[3]; Chris Stricklan[4]; ANdy Bujanda[5]; Paul Allison[6]; Rachael Swinney[6]; Robert Amaro[1]; Paul Brune[1]; Madison Parks[1]; James Tucker[1]; Jason Benoit[7]; Victor Yun[8]; Grace Kim[8]; [1]Kratos SRE; [2]Texas A&M; [3]Lehigh University; [4]Kraetonics; [5]US Army DEVCOM; [6]Baylor University; [7]Sciperio; [8]3D Flexible

Additive manufacturing allows the printing of multi-material systems containing metals, polymers, ceramics and functional electrical circuits allowing the printing of fully functional prototypes. Design considerations are required to combine both interfaces between dissimilar materials and the use loads and environments that can introduce complex and directional loads. The design of polymer-metal and metal-ceramic interfaces has been investigated with respect to the load dependent failure mechanisms. The failure of printed electrical circuits has also been characterized highlighting the need for design improvements and process improvements based on the failures identified.

Elucidating the 3D Morphology of Cicada Tymbals: A Multiscale X-Ray Microscopy Study: *Eshan Ganju*[1]; Pritam Ghoshal[1]; Richa Singh[1]; Hongcheng Tao[1]; James Gibert[1]; Anil Bajaj[1]; Nikhilesh Chawla[1]; [1]Purdue University

Cicadas are renowned for their loud, species-specific songs, produced by specialized vibrating organs called tymbals. This study leveraged lab-scale x-ray microcomputed tomography (XCT) to conduct a detailed, non-destructive analysis of the 3D tymbal morphology in Neotibicen canicularis (the dog-day Cicada). XCT allowed us to visualize and quantify internal tymbal structures, including the intricate rib arrangements, underlying support structures, and the morphology of the resonant cavity in three dimensions. A multimodal analysis of the relationship among tymbal structure, material characteristics, and acoustic emission yielded an in-depth multiscale understanding of the mechanisms via which cicadas produce their distinctive noises. This data will provide valuable insights into the evolution of sound production within this diverse insect group.

Extracting Grain Boundary Mobilities From 3D Data Using Convolutional Neural Networks: *Jules Dake*[1]; Leonard Lauber[1]; Thomas Wilhelm[1]; Lukas Petrich[1]; Orkun Furat[1]; Volker Schmidt[1]; Carl Krill[1]; [1]Ulm University

With the development and advancement of diffraction-based imaging techniques, an abundance of time-resolved 3D datasets of grain growth and other coarsening phenomena have recently become available. Large-scale 3D simulations of microstructural evolution are also now quite common thanks to progress in massively parallel computing architectures. These simulations rely on accurate values of grain boundary parameters (e.g., grain boundary energy and mobility) to return useful predictions; however, extracting these parameters from 3D experimental data, which is discretized in time and space, remains challenging. Here, we introduce a machine learning approach utilizing a convolutional neural network to directly extract grain boundary mobilities from sequential 3D mappings of grain growth in a single-phase aluminum alloy.

Getting More out of APT Mass Spectrum Analysis: *Ty Prosa*[1]; David Reinhard[1]; Robert Ulfig[1]; David Larson[1]; [1]Cameca Instruments Inc

Atom probe tomography (APT) provides unique spatial resolution and 3D compositional sensitivity at the nanoscale. Ultimately, the extractable information content from the measured mass spectra (MS) depends on both the quality of MS and the available analytical tools. CAMECA continues to work along multiple avenues to improve MS analysis. These include hardware improvements that result in background reduction and mass resolving power improvement, as well as collaborative software projects focused on creating tools for automatically segmenting chemically distinct regions within the 3D volume. Development of consistent, automated, user independent methods for 3DMS analysis directly impacts measurement accuracy, consistency, and time to knowledge. This presentation reports on CAMECA's recent advances in APT MS analysis.

Grain Structure Evolution During Heat Treatment of a Semisolid Al-Cu Alloy Studied With Lab-Based Diffraction Contrast Tomography: *Jun Sun*[1]; Jules Dake[2]; Jette Oddershede[1]; [1]Xnovo Technology; [2]Ulm University

3D experimental data of simultaneously high temporal and spatial resolution is key to validation of computational modelling of materials phenomena. In this study, we exploit lab-based X-ray imaging, combining absorption contrast tomography and diffraction contrast tomography, to capture the evolution of grain structure over a series of interrupted in-situ heat treatments of a semisolid Al-Cu alloy. Multiple aspects of the microstructure are characterised comprehensively on the meso-scopic scale, including grain coarsening driven by Ostwald ripening, grain rotation driven by grain boundary energy as well as grain boundary wetting. With the time resolved response of the selected Al-Cu model alloy system, the present work provides insights into the rearrangement, densification and coarsening of powder compacts at late-stage sintering, revealing the crucial impact of crystallography upon the microstructural evolution.

In-Situ Characterization of Martensitic Phase Transformation Interfaces in CuAlNi During Mechanical Cycling Using Dark-Field X-Ray Microscopy: *E. Celeste Perez-Valenzuela*[1]; Adam Creuziger[2]; Sangwon Lee[1]; Evan Rust[2]; Raquel Rodriguez Lamas[3]; Albert Zelenika[3]; Can Yildirim[3]; Carsten Detlefs[3]; Ashley Bucsek[1]; [1]University of Michigan; [2]National Institute of Standards and Technology; [3]European Synchrotron Radiation Facility

A reversible martensitic phase transformation is the deformation mechanism behind the functional properties of many multiferroic materials including shape memory alloys. During forward and reverse transformation, interfacial stress fields emerge at phase interfaces, leading to a hysteresis and the formation of undesirable dislocations. Here, we use in-situ dark-field X-ray microscopy (DFXM) to characterize the nucleation and growth of these phase interfaces during mechanical cycling of a CuAlNi shape memory alloy. The results show the 3D emergence and evolution of individual phase interfaces and spatially-mapped orientation and elastic strain, including the interfacial elastic strain fields at the phase interfaces. These findings will contribute to an improved fundamental understanding of the origins of hysteresis and functional fatigue in functional materials that undergo reversible martensitic phase transformations.

In Situ Synchrotron-Tomographic and -Diffraction Investigation of the Effect of Tensile Load on Mg2Y1Zn(Gd, Ag, Ca): *Domonkos Tolnai*[1]; Dietmar Christian Florian Wieland[1]; Gabor Szakacs[1]; Daria Drozdenko[2]; Liam Perera[3]; Sharif Ahmed[3]; Kristian Mathis[4]; [1]Institute of Metallic Biomaterials, Helmholtz-Zentrum Hereon; [2] Charles University; [3]Diamond Light Source Ltd.; [4]Charles University

The addition of Y and Zn can substantially improve the mechanical properties of Mg. Further alloying elements modify the secondary phases formed by the former, enabling to tailor the properties. Samples of pure Mg1.8Y0.6Zn and modified with 1.6 wt.% Gd, 1 wt.% Ag or 0.4 wt.% of Ca, were subjected to in situ tensile testing at the Dual Imaging And Diffraction beamline, Diamond UK, with a strain rate of 10^{-3} s^{-1}, 10^{-4} s^{-1} and 10^{-5} s^{-1}. During testing, tomographies were acquired to follow the crack initiation and evolution in 3D and diffraction patterns alongside the acoustic emission signal from the samples were also recorded to track the microstructural changes, thus enabling a comprehensive description of the damage in the samples leading up to the failure. The results show that the additional alloying elements and the strain rate both have a significant effect on the damage process and the failure.

Multiscale Qualitative and Quantitative Assessment of Microstructural Elements in the IN718 Nickel-Base Superalloy After Various Annealing Durations at 760°C: Adam Kruk[1]; *Grzegorz Cempura*[1]; [1]AGH University of Krakow

Structural materials used in critical components in the energy and aerospace sectors operate under challenging environmental conditions, leading to gas corrosion and microstructural degradation due to high temperatures and complex stress states. Assessing the degree of microstructural degradation requires multiscale parameterization. 2D imaging using scanning and transmission electron microscopy enables phase composition identification based on TEM-SAED analysis, STEM-EDX, and high-resolution HRSTEM-HAADF imaging. To obtain information about the spatial distribution of specific microstructural elements, including their morphology, high-resolution 3D imaging techniques are required. One such technique is FIB-SEM tomography, which allows 3D reconstruction of microstructural elements with voxel resolution on the order of a few nanometers. These imaging methods and techniques enabled the analysis of microstructural changes caused by prolonged annealing at temperatures above the operating range of the IN718 alloy. Qualitative and quantitative changes in the microstructure were compared with data obtained through numerical simulations performed using Thermo-Calc 2024b software.

New Capabilities From the APS-Upgrade at the New 3D Micro/Nano Diffraction Station: *Jon Tischler*[1]; [1]Argonne National Laboratory

The recently completed upgrade of the Advanced Photon Source (APS) increases the brightness of the undulator sources by a factor of ~100. For micro-focusing/diffraction this provides a factor of 100 increase in the brightness of the focused spot. The improved instrument at the 3DMN station should thus have *both* more power *and* a smaller spot size of ~150 nm. In addition, using the newly developed technique to obtain depth resolution using a 1D coded aperture we expect data collection times to drop by and additional factor of ~5 with improved signal/noise. The combination of the coded aperture with the increased brightness should reduce collection times by more than a factor of 20 with an improved transverse resolution more than 2 times smaller. This talk will present examples of the first measurements and an appraisal of the improvements, as well as other improvements.

Observation of Damage and Fracture in Al-5Mg-2Si Cast Alloy by Means of Synchrotron Radiation Multi-Scale Tomography: *Masakazu Kobayashi*[1]; Shogo Furuta[1]; Pei Loon Khoo[1]; Yojiro Oba[1]; Hiromi Miura[1]; [1]Toyohashi University of Technology

Hypoeutectic Al-Mg-Si cast alloy has a good balance of strength and ductility. However, coarse block-shaped Mg2Si surrounded by plate-shaped ones are formed depending on cooling rate and chemical composition. This characteristic shape of the particle might control ductility. In-situ observation of damage and fracture process during tensile deformation was conducted by means of synchrotron radiation multi-scale tomography to understand the role of coarse block-shaped Mg2Si particle on fracture in Al-5Mg-2Si casting alloy. It revealed that a block-shaped part that is in the center is definitely fractured when a plate in horizontal spread cracks, because plate-shape parts spread radially surrounding a block-shaped part. It is concluded that block-shaped parts were not the origin of cracking, though they can be frequently observed on fracture surfaces.

Quantitative Elemental Mapping of Bimetallic Nanoparticles From Atomic Scale STEM-HAADF Images: *Adrien Moncomble*[1]; Damien Alloyeau[1]; Maxime Moreaud[2]; Guillaume Wang[1]; Nathaly Ortiz-Peña[1]; Hakim Amara[3]; Riccardo Gatti[3]; Romain Moreau[3]; Christian Ricolleau[1]; Jaysen Nelayah[1]; [1]Université Paris Cité, Laboratoire Matériaux et Phénomènes Quantiques, CNRS, F-75013; [2]IFP Energies Nouvelles, 69360; [3]Université Paris-Saclay, ONERA-CNRS, Laboratoire d'Etude des Microstructures, 92020

We propose a deep-learning method for quantifying atomic column composition in bimetallic nanoparticles (NPs) using high-angle annular dark field scanning TEM (HAADF-STEM). When traditional EDX techniques require high-brightness electron sources and are limited by noise at atomic resolution, HAADF-STEM images are promising alternative to get access to the chemical composition of NPs. In this approach, elemental composition is retrieved from HAADF signal intensities using a U-Net like deep-learning model trained on multislice-simulated images and corresponding elemental maps. Multislice simulations reveal that HAADF-STEM intensity is influenced by atomic column composition, configuration, and thickness, requiring a sophisticated model to capture these interactions. Our approach disentangles these parameters, allowing accurate predictions at atomic resolution and providing robust, high-throughput in situ quantification of elemental composition. This method offers a significant advantage over EDX by achieving non-destructive, contamination-free composition analysis, making it highly suitable for real-time experimental conditions.

Time-Resolved Measurement Capabilities at the Forming and Shaping Technology Beamline: *Katherine Shanks*[1]; Amlan Das[1]; [1]Cornell University

The Forming and Shaping Technology (FAST) beamline at the Cornell High Energy Synchrotron Source (CHESS) provides high-flux, high-energy (20-88 keV) x-rays and experimental infrastructure for the structural materials community. In particular, the beamline focuses on in-situ measurements probing material microstructure during thermomechanical loading and processing. The energy range covered by FAST allows for characterization of materials over a wide range of density and atomic weight, from lightweight composites to steels and nickel-based alloys, while the use of transmission geometry techniques (e.g. powder diffraction, absorption- and phase-contrast radiography) gives insight into the material state through the bulk of millimeter-scale specimens. Here, we describe recent developments focused on deployment of instrumentation tailored to time-resolved experiments, including high-frame rate area detectors and emerging techniques for real-time data monitoring to guide data collection strategy.

Unsupervised Learning for Structure Detection in Plastically Deformed Crystals: *Armand Barbot*[1]; Riccardo Gatti[2]; [1]ONERA; [2]CNRS

Molecular Dynamics is a powerful method allowing to simulate different materials at the particle scale such as glassy materials or metallic nanocrystals. To determine the local structure at the particle-scale, several approaches were developed, mainly relying on local order parameters to describe the surrounding environment of each particle. However, they are mostly relying on hand chosen criteria and thus only works for already known structures. In this study, we present an unsupervised learning method to automatically study and detect the different substructures appearing at the atomistic scale within a crystal under plastic deformation. This approach combines autoencoder, clustering and classification methods.By applying our method on a Nickel FCC nanocrystal plastically deformed under uniaxial compression, we were able to detect more sub-structures associated with plasticity and with a higher degree of precision than traditional hand-made criteria. This study was published on Computational Materials Science.

3D Mapping of Intragranular Strain and Microstructure in Recrystallized Iron Using Dark-Field X-Ray Microscopy: *Virginia Sanna*[1]; Yubin Zhang[2]; Wolfgang Ludwig[1]; James Ball[1]; Abderrahmane Benhadjira[1]; Marilyn Sarkis[1]; Carsten Detlefs[1]; Can Yildirim[1]; [1]ESRF; [2]DTU

This study examines intragranular residual strain and orientation distributions in fully recrystallized pure iron grains, using Dark-Field X-ray Microscopy (DFXM) for high-resolution, non-destructive imaging at the submicron level. Our findings reveal uneven strain distributions within grains, with localized values up to 3 × 10, and visualize individual dislocations, highlighting microstructural complexity even after full recrystallization. Simulations of DFXM dislocation contrast offers insights into Burgers vectors. Complementary 3D X-ray Diffraction (3DXRD) analysis using a box beam adds context on overall texture and grain size distribution, enhancing our grasp of grain-level heterogeneity. By combining the two techniques, we relate DFXM strain and orientation data to 3D grain structures, providing a clear view of residual strain landscapes. This combined approach underscores the role of residual strain effects in recrystallized grains and advances our understanding of microstructural evolution in polycrystalline materials.

A High-Efficiency Laser Powder Bed Fusion Additive Manufacturing Simulation Method: *Gregory Wong*[1]; Gregory Rohrer[1]; Anthony Rollett[1]; [1]Carnegie Mellon University

There is a need to simulate the linkage between processing parameters and microstructure in the laser powder bed fusion metals additive manufacturing process. Additionally, it is important that these models be efficient to fit well into simulation pipelines to predict the process, structure, and properties relationship without creating bottlenecks. Presented here is a low-cost model that simultaneously simulates entire laser passes. This "Pass Scale Model" utilizes <100> type preferred growth to inform both the morphology of the 3D microstructure and include texture information in the output. These synthetic microstructures extend hundreds of microns in each direction with model run times of a few hours. Of note is the introduction of a modified Rosenthal thermal model to calculate the shape of non-conduction mode melt pools. The model method and validation against experimental results for both grain morphology and texture via the Wasserstein Distance will be shown.

High-Fidelity 3D Microstructural Characterization of ZrB2 During Hot-Pressing: *Randi Swanson*[1]; Darko Kosanovic[2]; Michael Chapman[3]; Ashley Hilmas[3]; Lisa Rueschhoff[3]; Michael Uchic[3]; Wei Xiong[4]; Hessam Babaee[4]; William Fahrenholtz[2]; Scott McCormack[1]; [1]University of California Davis; [2]Missouri Science and Technology; [3]Air Force Research Laboratory; [4]University of Pittsburgh

Standard ultra-high temperature ceramic (UHTC) manufacturing results in components with large differences in properties due to variability in microstructural "critical flaw" distributions. Critical flaws can be any irregularity in a component, such as a secondary phase, cracks, pores, etc. This is problematic when designing reproducible UHTC components. The goal of this project is to understand how these critical flaws evolve during hot pressing of ZrB2 (a UHTC) by examining them in 3D. This study incorporates 3D imaging such as: (i) ex-situ X-ray μ-CT and (ii) 3D electron imaging and backscattered diffraction data collected at different stages of densification. 3D microstructure statistics along with unique observations of individual pore and secondary phase evolution will be presented. This data is brought together to give a holistic view of the densification of ZrB2 during hot pressing at multiple length scales.

High Accurate Modelling and Large-Scale Simulation of Melt Pool Dynamics in Metal Additive Manufacturing Using Phase-Field Lattice Boltzmann Method: *Konosuke Ikeda*[1]; Shinji Sakane[1]; Takayuki Aoki[2]; Tomohiro Takaki[1]; [1]Kyoto Institute of Technology; [2]Institute of Science Tokyo

Material structures in metal additive manufacturing are formed through melting and solidification in laser scanning. The melt pool flow plays important role for the formation of the solidification structures. In this study, a phase-field lattice Boltzmann (PF-LB) model was developed to numerically reproduce the melt pool flow with high accuracy. In addition, since high-resolution is required for the high-accurate melt pool flow simulation, we implemented multiple GPU parallel computing to achieve large-scale simulations. Then, we validated the developed simulation method by comparing the results with experimental results, such as melt pool and keyhole shapes.

In-Situ Characterization of Supercritical Martensitic Phase Transformations in NiFeGaCo Single Crystals Using High-Energy Diffraction Microscopy: *Timothy Thompson*[1]; Abdulhamit Sarac[1]; Sangwon Lee[1]; Amlan Das[1]; Fei Xiao[1]; [1]University of Michigan

Superelastic behavior, enabled by reversible martensitic phase transformations, has been observed in many multiferroic materials like shape memory alloys. Typically, martensitic phase transformations involve the formation and migration of interfacial stress fields at phase interfaces, causing hysteresis and degradation of superelastic behavior. However, recent research indicates that above a critical temperature (in a supercritical thermodynamic state), the transformation occurs with exceptional cyclic stability and no hysteresis. This study uses high-energy diffraction microscopy (HEDM) to characterize martensitic phase transformations below ("subcritical") and above ("supercritical") the critical temperature during compression of NiFeGaCo ferromagnetic shape memory alloys. In-situ HEDM experiments are supported by in-situ differential interference contrast (DIC) optical microscopy. Results reveal the evolution of martensite within single crystals and changes in phase interfaces. These findings will enhance the fundamental understanding of supercritical martensitic phase transformations.

In Situ Measurement of Three-Dimensional Intergranular Stress Localizations and Grain Yielding Under Elastoplastic Axial-torsional Loading: *Yaozhong Zhang*[1]; [1]University of Michigan

The three-dimensional grain-scale elastoplastic response of solid bar samples during non-proportional (NP) axial-torsional loading was investigated using in situ high energy diffraction microscopy (HEDM) and companion crystal plasticity finite element (CPFE) modeling. Important stress metrics were tracked for ~ 300 grains under two different loading conditions: (i) Torsion-dominated loading (low NP) and (ii) Tension-torsion loading (high NP) in equiatomic NiCoCr, a representative multicomponent face-centered cubic (FCC) alloy. NP boundary conditions led to a complex interplay between stress components resulting in grain yielding near the sample surface largely driven by shear stress, whereas internal grain yielding largely accommodated by axial stress. Overall, grain-resolved stress localization trends were well-captured by the CPFE model, although some discrepancies in magnitude occurred due to initial type II residual stress distributions which were overcome via the superposition of initial residual stress states onto CPFE grain-resolved data.

Incorporating Experimental Data Into Molecular Dynamics: A Method for Voxel-Atomic Structure Conversion: *Meizhong Lyu*[1]; Zipeng Xu[2]; Gregory Rohrer[2]; Elizabeth Holm[1]; [1]University of Michigan; [2]Carnegie Mellon University

Many studies on three-dimensional grain growth depend on computer simulations due to the inherent challenges of experimental methods, such as limitations in characterization resolution and impurities. Computer simulations can model grain boundary motion in pure materials and capture detailed microstructural features. Unlike other mesoscale methods, molecular dynamics (MD) simulations do not rely on assumptions about grain boundary migration mechanisms. The existing methods of constructing computational microstructures from experimental data typically involve defining a surface mesh. However, the construction of a surface mesh from data points introduces a certain level of error, which may have an impact on the precision of the constructed atomic-scale microstructure. In this study, we developed a method to convert voxel-based structures from experimental data into atom-based structures for initial configurations in MD simulations. When comparing the MD simulation results with experimental data, we observed typical features of grain growth in nickel polycrystals.

Large-Scale 3D Multi-Phase-Field Sintering Simulation of Texture Development by Templated Grain Growth: *Aoi Nakazawa*[1]; Shinji Sakane[1]; Tomohiro Takaki[1]; [1]Kyoto Institute of Technology

It is well known that the properties of ceramics can be improved by tailoring the texture. For example, lamellar textured ceramics have high thermal conductivity along the lamella and good mechanical properties in the perpendicular direction. Templated grain growth (TGG) is a powerful texturing method. However, as microstructure evolution is strongly affected by various factors, such as matrix particle size, template particle size, and aspect ratio, it is difficult to experimentally determine these parameters to obtain an optimal microstructure. Multi-phase-field sintering (MPFS) simulator [Nakazawa et al. 2025], which can continuously reproduce from powder compaction to sintering for arbitrarily shaped particles, is a powerful tool to investigate effect of those parameters on TGG. Using the MPFS, we performed large-scale 3D TGG simulations by changing size and shape of matrix and template particles systematically, and investigated what is the dominant effect on the formation of texture microstructure.

Numerical Simulations of the Wire-Arc Additive Manufacturing (WAAM) Process: *Fernando Valiente Dies*[1]; [1]ANSTO & The University of Sydney

Wire Arc Additive Manufacturing (WAAM) is a direct energy deposition additive manufacturing process that uses well-established welding technology. It consists of a sequential deposition of weld passes and layers to form engineering components. The WAAM process is characterised by high heat input, high deposition rate, high surface roughness and the anisotropy of material properties.In this project, the WAAM process has been employed to manufacture multipass, multilayer walls made using 316L Stainless Steel. An array of thermocouples on the base plate has been used to monitor the transient temperature field during the WAAM manufacturing of test specimens. The thermocouple readings are used to calibrate the thermal model, which we then used in a phase-field model capturing the solidification process and formation of weld-like microstructure. Furthermore, the same thermal model was used in the mechanical model capturing material response to the heat source, thus predicting the macroscopic distortion and residual stresses.

Study of Three-Dimensional Granular Matter Using Tomography and Far-Field High-Energy Diffraction Microscopy: Will Hobson-Rhoades[1]; *Yuefeng Jin*[1]; Iñigo De Gracia[1]; Wenxi Li[1]; Janice Moya[1]; Amlan Das[2]; Katherine Shanks[2]; Ashley Bucsek[1]; Hongyi Xiao[1]; [1]University of Michigan; [2]Cornell High Energy Synchrotron Source

The general goal of this work is to understand force distributions within three-dimensional (3D) disordered contact networks of frictional granular materials. The advancement of 3D in-situ experimental techniques has made it possible to characterize the packing configurations and forces in 3D frictional stiff granular media. This study leverages X-ray tomography and far-field high-energy diffraction microscopy (ff-HEDM) to investigate different granular material topics: (1) the effect of different confinement geometries on the force and contact networks of monocrystalline ruby spheres under uniaxial compression; (2) the validation of Janssen's law in a uniaxial compression test on monocrystalline ruby spheres; (3) the packing geometry of silicon cubes, rods, and plates under uniaxial compression. Discrete element method (DEM) simulations are conducted to supplement the experimental results. The findings from this work will enhance the understanding of force distribution and contact networks in 3D granular materials and help improve the modeling of 3D granular systems.

Investigating the Influence of Strain Rate on Hydrogen Embrittlement in Steel Sub-size Tensile Specimens Using 3D X-Ray Tomography: *Luciano Santana*[1]; Victor Okumko[2]; Andrew King[2]; Thilo Morgeneyer[1]; Jacques Besson[1]; Yazid Madi[1]; [1]Mines Paris PSL - Centre des Matériaux; [2]Synchrotron SOLEIL

This study investigates the effect of strain rate on hydrogen embrittlement in ferritic-pearlitic E355 steel using sub-size tensile specimens and micrometer-scale 3D X-ray tomography. Tests were conducted in air and 100 bar hydrogen at varying strain rates, with some interrupted before rupture to capture damage evolution. Hydrogen reduces ductility, with losses reaching up to 62.8% at lower strain rates.3D X-ray tomography enabled the quantification of damage and the determination of its shape and orientation at different strain rates. At 5 × 10 s^{1}, brittle surface cracks appear as flat ellipsoids perpendicular to the tensile axis, while ductile bulk damage consists of prolate voids aligned along it. Hydrogen-enhanced shearing promotes coalescence through slant fracture. At 1 × 10 s^{1}, deeper hydrogen diffusion increases embrittlement, causing both surface and bulk damage to adopt a brittle, flat ellipsoidal morphology perpendicular to the tensile axis.

The Dynamics of Grain Growth in Thin Specimens: The Role of Free Surfaces: *Varun Srinivas Venkatesh*[1]; Marcel Chlupsa[1]; Hrishikesh Bale[2]; Ashwin Shahani[1]; [1]University of Michigan; [2]Zeiss Research Microscopy Solutions

Optimizing the properties of polycrystalline materials requires significant microstructural design, driven by our understanding of grain growth. Studies on grain growth have focused mostly on system-wide properties like grain size and growth rate, often overlooking local geometric, topological, crystallographic, and network effects, factors that require reliable 3D measurement. Developments in laboratory-based X-ray diffraction contrast tomography (DCT) have enabled us to study the temporal evolution of an unprecedented 10,000 grains in a thin aluminum disc upon annealing, where the sample thickness is ~5x the initial grain diameter. With this data, we test the validity of the Lewis, von Neumann-Mullins, and the Aboav-Weaire laws for the ensemble of interior and surface-touching grains. Our analysis of surface and bulk grain boundary planes over time explores how curvature, crystallography, and free surface effects influence and constrain grain and grain boundary evolution. These insights deepen our understanding of microstructure evolution in thin samples.

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