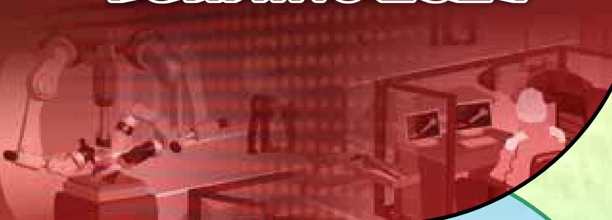
2nd World Congress on
ARTIFICIAL INTELLIGENCE IN MATERIALS & MANUFACTURING
AIM 2024

Symposium on
DIGITAL & ROBOTIC FORMING 2024



ACCELERATING DISCOVERY FOR MECHANICAL BEHAVIOR OF MATERIALS 2024

TMS SPECIALTY CONGRESS 2024

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Specialty Congress 2024: All-Congress Plenary Session All-Congress Plenary

Monday AM
June 17, 2024

Room: Hope Ballroom D
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

8:20 AM Introductory Comments

8:30 AM Plenary
Recovering Resources from the Past: How AI Can Enable a More Circular Future: *Emily Molstad*[1]; Caleb Ralphs[2]; Benjamin Longo[1]; Sean Kelly[3]; Diran Apelian[4]; [1]VALIS Insights, Inc.; [2]VALIS Insights Inc.; [3]Solvus Global, Llc; [4]University of Caliornia-Irvine

Discovery, design and fabrication of the latest and greatest materials have resulted in groundbreaking progress across every industry from medicine to transportation to energy. What happens when these materials reach their end of life? How can we ensure the valuable materials needed to support a modern society are available for future generations and are produced sustainably? The recycling industry is critical to keeping precious resources out of landfills and is essential in the fight against climate change as material demand continues to grow and natural reserves are increasingly depleted. Artificial intelligence, and broadly Industry 4.0 capabilities, presents a wealth of opportunities to enhance circularity and ensure the materials of yesterday are properly recovered for the demands of tomorrow. This talk will focus on the current and future impact of AI on recycling with a focus on major metals such as aluminum and copper.

9:10 AM Plenary
Thriving in the Digital Epoch of Materials and Manufacturing: *Charles Ward* [1]

In an era witnessing profound shifts in the generation, transfer, and application of information and knowledge used to develop, manufacture, and employ materials, a landscape of immense opportunities and challenges emerges for society. The synergy of global advocacy for open science, unprecedented insights into physical phenomena, a myriad of data-centric analysis techniques, the advent of digitally-native characterization and manufacturing equipment, and the widespread embrace of model-based engineering in industry are reshaping how we approach problems and innovate solutions. It is fitting that the three co-located meetings within this specialty congress represent exemplar topics that harness the full potential of these transformative changes. This talk will delve into the transformative journey we are undertaking, highlighting both the challenges that lie ahead and the abundant opportunities that await exploration in the rapidly evolving intersection of these advancements.

9:50 AM Break

10:20 AM Plenary
Navigating the Digital Transformation in Materials Science and Engineering and Your Role in Shaping Tomorrow: *Christoph Eberl*[1]; [1]Fraunhofer IWM / University of Freiburg

The digital transformation of Materials Science and Engineering represents a paradigm shift in how we conduct research and brings forth many opportunities as well as challenges. This evolution seeks to expedite materials development, processing, lifetime predictions, and the sustainable practices of reuse and recycling, paving the way for a circular economy. A cornerstone of this paradigm shift is the collaborative creation of a materials knowledge graph grounded in aligned ontologies, coupled with a distributed FAIR data research platform. In contrast to traditional text-based knowledge transmission, knowledge graphs provide a revolutionary approach by interconnecting diverse concepts—such as atomic bonds, chemical composition, crystal structure, grain boundaries, deformation, annealing processes, and mechanical properties—in a format comprehensible to both humans and machines. Especially in an interdisciplinary research environment as in MSE, this is a tremendous game changer, facilitating a seamless exchange of insights. Notably, knowledge graphs have been embraced by leading tech companies like Google, Facebook, Microsoft, Amazon, and LinkedIn, forming the technological backbone for search algorithms and AI applications. This lecture aims to sketch out how an ontology based de-centralized materials data infrastructure can capture the hierarchical dependencies between processes, microstructure, properties, and behavior for advanced materials. Furthermore, the opportunities of exponential growth in a digital infrastructure shall be described, alongside the risks associated with not actively participating and embracing data literacy. In the second part of the lecture, 'lessons learned' will be offered, outlining strategies for participation at various levels. How can individual scientists, research groups, and institutions reach low hanging fruits and become more productive will be discussed. Finally, this talk invites you to participate in this joined effort. Building up such a research infrastructure for us all is unprecedented and requires collaboration across borders. Hence, to guide the effort, several initiatives and hubs have been initiated (NFDI, NFDI-MatWerk since 2021 & MaterialDigital since 2019) or will be set in motion soon (Advance Materials Initiative 2025, EU).

11:00 AM Plenary
Advancing Materials Science: Intelligent Agents in Data-driven Discovery: *Ian Foster*[1]; [1]Argonne Nat Lab & University of Chicago

The convergence of enormous data, cloud services, supercomputers, robotic laboratories, and advanced simulation and machine learning promises unprecedented opportunities in materials design and discovery. However, harnessing these capabilities to tackle societal challenges, from energy to economic growth, demands nuanced orchestration beyond current norms. I propose that intelligent agents, working in tandem with human expertise, are pivotal for this quantum leap in materials science. These agents will not only automate routine tasks but also bring new capabilities: from synthesizing and interpreting vast literature to designing and managing complex experimental setups. Illustrating this, I will share insights from pioneering work at Argonne National Laboratory and other leading institutions. Finally, I will discuss emerging directions and the potential for new collaborations to shape the future of materials science.

11:40 AM Panel Discussion

Symposium on Digital & Robotic Forming 2024 Keynote

Monday PM
June 17, 2024

Room: Hope Ballroom D
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

1:40 PM Introductory Comments

1:50 PM Keynote
Evolution of Advanced Manufacturing Technologies in the Data Analytics and Computational Modeling Era: *David Furrer*[1]; [1]Pratt & Whitney

Traditional forging methods have evolved over many decades to enable development of unique microstructures and component capabilities. Introduction of Industry-4.0 approaches have driven a range of sensors and control technologies and methods to further enhanced material and component capabilities. Computer controls are becoming commonplace for many manufacturing methods including press and hammer forging methods. Computational modeling and simulation for location-specific component design and hybrid approaches are leading to increasingly efficient methods for future component design and manufacture. Traditional blacksmithing to modern computer-controlled deformation and hybrid processing will be discussed.

Accelerating Discovery for Mechanical Behavior of Materials 2024 Mechanical Behavior Keynote

Monday PM
June 17, 2024

Room: Hope Ballroom D
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

2:50 PM Introductory Comments

3:00 PM Keynote

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) High-Throughput Synthesis & Characterization

Monday PM
June 17, 2024

Room: Hope Ballroom A
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

1:40 PM Invited
High Performance Computing and Artificial Intelligence Enabled Materials Characterization and Experimental Automation: *Mathew Cherukara*[1]; [1]Argonne National Laboratory

The capabilities provided by next generation light sources along with the development of new characterization techniques and detector advances are revolutionizing materials characterization (metrology) by providing the ability to perform scale-bridging, multi-modal materials characterization under in-situ and operando conditions. For example, providing the ability to image in 3D large fields of view (~mm3) at high resolution (<10 nm), while simultaneously acquiring information about structure, strain, composition etc. However, these novel capabilities dramatically increase the complexity and volume of data generated. Conventional data processing and analysis methods become infeasible in the face of such large and varied data streams. The use of AI/ML methods is becoming indispensable for real-time analysis, data abstraction and decision making at advanced, high-data rate instruments. I will describe how high-performance computing (HPC) along with AI on edge devices enables real-time data analysis and self-driving experiments, creating the next generation of AI-powered materials characterization tools.

2:10 PM
AI-simulation Workflow to Accelerate Computational Screening of Metal-organic Framework Structures: *Xiaoli Yan*[1]; Hyun Park[2]; Logan Ward[3]; Eliu Huerta[3]; Ian Foster[3]; Emad Tajkhorshid[2]; Santanu Chaudhuri[1]; [1]University of Illinois at Chicago; [2]University of Illinois Urbana-Champaign; [3]Argonne National Laboratory

The challenge of designing novel metal-organic framework (MOF) structures with desired application performances lies in the chemical compositions' finite but vast search space. This search space usually consists of a constant list of metal secondary building units, organic ligands, and topologies. We present an open-source high-throughput workflow that combines generative AI models, regression AI models, and molecular dynamics simulations to screen MOF structures. The generative side of the workflow consists of a diffusion model and a generative adversarial network model. The two generative models can run independently to produce novel MOF candidates. With an array of AI and simulation screening methods with increasing time cost and level of accuracy. Each MOF candidate is evaluated for chemical validity, structure stability, and gas adsorption capacity. An open-source workflow manager, Colmena, is responsible for automatic job supervision, candidate filtering, and uncertainty quantification.

2:30 PM
Predicting Mechanical Behavior in Creep Conditions: High-Throughput Protocols With Unconventional Geometries and Digital Image Correlation: *Seyed Mohammad Ali Seyed Mahmoud*[1]; Samantha Mitra[1]; Raj Mahat[1]; Ali Khosravani[2]; Surya Kalidindi[1]; [1]Georgia Institute Of Technology; [2]Mutltiscale Technologies

Creep tests are fundamental for understanding the behavior of materials required to endure specific operational temperatures under load. Metals and alloys exhibit notable property variations at different temperatures. Our research focuses on developing high-throughput protocols employing unconventional sample geometries in tandem with digital image correlation to evaluate monotonic mechanical properties. These non-standard geometries induce stress heterogeneity during testing while maintaining controlled and consistent creep stress on samples. Utilizing finite element simulations and machine learning, we aim to construct a surrogate model predicting monotonic mechanical responses. By leveraging data from non-standard experiments and established standard properties of 6061 aluminum alloys, our methodology combines training and calibrating the model. The protocol's validity will be demonstrated through the analysis, establishing a pathway for understanding and predicting mechanical behaviors in materials subjected to varying stress conditions and temperatures.

2:50 PM
Leveraging Segmentation Models for Platinum Particle Identification on BWR Nuclear Reactor Components: *Txai Sibley*[1]; Elizabeth Hom[1]; Kevin Field[1]; [1]University of Michigan

This study delves into the application of advanced, AI-based image segmentation models to identify platinum particles on key components of Boiling Water Reactor (BWR) systems. These particles, introduced to mitigate radiation-induced cracking and stress corrosion, play a crucial role in reactor performance. Employing multiple segmentation models on small image datasets, our research aims to precisely characterize platinum particles adhering to reactor surfaces and to determine the application robustness of existing models. Both the characteristics of the image data and of the segmentation models are relevant to optimizing segmentation quality. By understanding how the models and data interact, we can select and apply a model to minimize the expense of data collection and annotation. This exploration provides a foundation for future insights into the interplay between platinum particle characteristics and their impact on BWR nuclear reactor functionality.

3:10 PM
High-throughput Approach to Support-free LPBF of Inconel 718 With In-situ High-speed Thermal Imaging: *Chun Kit Sit*[1]; Yunlong Tang[1]; Louis Chiu[1]; Aijun Huang[1]; [1]Monash University

Laser Powder Bed Fusion (LPBF) is a prominent Additive Manufacturing method to manufacture complex geometries in 3D space. However, the parameter optimization is complicated due to the complex and interconnected spatial scale and print parameter space. This presentation reveals a practical and iterative framework from first principle to support-free LPBF. In particular, we introduce not only the concept of parameter optimization on the 1st layer overhang basis, but a quantifiable metric using high-speed thermal imaging for IN718. Each pixel in the high-throughput imaging is further spatially calibrated using perspective transformation such that it can be used on different LPBF machines. Not only is the proposed framework material-agnostic but it allows for further print parameter refinement if necessary. This framework generates an extensive amount of data to optimize for printing 1st layer 0 degree overhang which will be the foundation for multi-layer overhang and process monitoring of support-free LPBF.

3:30 PM Networking Break

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) Image Processing I

Monday PM
June 17, 2024

Room: Hope Ballroom B
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

1:40 PM Invited
Development of a Machine Learning Based Tool for Defect Detection in Cold Spray Aluminum: *Joseph Indeck*[1]; Bruno Zamorano-Senderos[1]; [1]Boeing Research & Technology

In this work an in-situ method to monitor spray quality was developed to track where intentionally induced poor spray quality occurred. Cold spray plates were produced with and without intentional poor spray quality. Specimens were machined from both types of plates and tested under quasi-static uniaxial tension. This presentation will detail the development of a high throughput, automated method to detect the number of defects on the fracture surface of failed tensile specimens. First, a deep learning U-NET architecture was used to segment the images. Second, an unsupervised clustering approach was used to group different features of the fracture surface to isolate those that are characteristic of weak bonding due to the intentionally induced poor spray quality. It is anticipated that results from this work will be used to demonstrate that in-situ monitoring of the cold spray process can be used to supervise spray quality and part performance.

2:10 PM
Grain Segmentation Refinement Based on Perceptual Grouping Principles Using Conditional Random Fields: *Doruk Aksoy*[1]; Tim Rupert[1]; William Bowman[1]; [1]University of California, Irvine

Accurate segmentation of grains in electron microscopy images is key for high-throughput microstructure analyses that determine material properties. However, the task is challenging due to factors like intricate network connectivity influenced by crystallography and local atomic environments. Traditional post-processing of machine vision-generated segmentation masks is complex, especially when dealing with interconnected linear structures. Techniques like convolutional neural networks often miss fine details due to their large receptive fields. To address these issues, we introduce a generalizable post-processing approach that enhances segmentation masks in grain boundary networks. This approach uses conditional random fields and leverages perceptual grouping principles such as similarity, proximity, closure, and continuity. We validated the method's effectiveness using segmentation masks generated by a U-Net architecture on transmission electron microscopy images of an electrically conducting polycrystalline oxide. The approach demonstrated significant improvements in accuracy across multiple evaluation metrics, suggesting its utility for segmentation mask refinement in various application scenarios.

2:30 PM
A Unified Microstructure Segmentation Approach Through Incorporating Domain Knowledge Into Machine Learning: *Juwon Na*[1]; Se-Jong Kim[1]; Chang Dong Yim[1]; [1]Korea Institute of Materials Science

Microstructure segmentation, a technique for extracting structural statistics from microscopy images, is an essential step for establishing quantitative structure-property relationships. However, the task is challenging due to the morphological complexity and diversity of structural constituents as well as the low-contrast and non-illumination nature of microscopic imaging systems. While recent breakthroughs in deep learning have led to significant progress in microstructure segmentation, there remain two fundamental challenges: the need for extensive labeled data and the absence of incorporating domain knowledge into machine learning. In this work, we propose a unified framework for microstructure segmentation, which leverages the power of both weakly supervised learning and physics-inspired learning. The key idea behind our approach lies in the integration of human and machine capabilities to make accurate and reliable microstructure segmentation at minimal annotation costs. Extensive experiments demonstrate the versatility of our approach across different material classes, structural constituents, and microscopic imaging modalities.

2:50 PM
A Texture Synthesis Approach for Generating Synthetic Microstructural Images for Training ML Models in a Low-data Regime: *Martin Mueller*[1]; Frank Muecklich[2]; [1]Materials Engineering Center Saarland; [2]Saarland University

The more complex and elaborate annotations become, or the less frequently certain classes occur in a data set, the more costly the implementation of an ML evaluation becomes, and the more attractive the generation and use of synthetic training data becomes. This work adapts a texture synthesis approach from graphics design to the application to microstructural images. This approach can be assigned to the group of non-parametric example-based algorithms for image generation and allows the generation of new images by remixing from single or multiple examples. The applicability of this approach is assessed by the generation of macroscale defect structures and microscopic microstructural images. The quality of the synthetic data is determined by expert round robin tests as well as the application of appropriate image metrics. Furthermore, it is shown in which ways these synthetic data can be used for the training of a ML model.

3:10 PM
Boundary Monitoring for Optimized Sintering Processes: *Mohamed Boosiri Hassan Uvaise*[1]; [1]Lucideon

In-situ monitoring of shrinkage during sintering is a critical challenge for manufacturers of ceramic products. Lucideon Limited, a long-established materials development and commercialisation organisation, is developing a robust, non-invasive computer-vision based system, that harnesses Deep Learning and Image Processing. This system facilitates real-time monitoring of the specimen's boundaries during the sintering; minimising the risk of specimen's shape distortion within the kiln, a challenge often caused by poor visibility of the process. The approach has implemented and tested advanced deep learning models, such as U-Net and YOLO, alongside state-of-the-art unsupervised edge detection algorithms, facilitating boundary identification without dataset labelling. Also includes a robust image pre-processing module, all seamlessly integrated with a user-interface.The project not only stands out for its practical impact but also promises significant cost savings for industry by reducing material wastage and optimizing the sintering process, marking a promising advancement in both image processing and material science.

3:30 PM Networking Break

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) Machine Learning - Manufacturing I

Monday PM	**Room: Hope Ballroom C**
June 17, 2024	**Location: Hilton Cleveland Downtown**

Session Chair: To Be Announced

1:40 PM Invited
Machine Learning Assisted Discovery of Deposition Conditions for Binary Metallic Alloys: *Saaketh Desai*[1]; Manish Jain[1]; Sadhvikas Addamane[1]; Frank Rio[1]; Remi Dingreville[1]; Brad Boyce[1]; David Adams[1]; [1]Sandia National Laboratories

Designing thin films tailor-made for specific applications is challenging due to complex process-structure-property linkages. A powerful way of rapidly exploring the process-structure-property space is combinatorial deposition, allowing simultaneous fabrication of films with a wide range of compositions and properties. However, extracting insights from these high-throughput depositions to design films with specific properties is also challenging. In this work we combine high-throughput physical vapor deposition, multimodal characterization, and machine learning to identify deposition conditions that result in high hardness, high conductivity Pt-Au alloys. We train autoencoders to capture structural fingerprints in experimental X-ray diffraction patterns, and correlate the learnt fingerprints to electrical conductivity and hardness. Additionally, we correlate process conditions (energy/angle of incoming Pt/Au atoms) with structural fingerprints, and properties, discovering process conditions and compositions that yield properties beyond state-of-the-art nanocrystalline Pt-Au alloys. Our work demonstrates an approach to integrate combinatorial deposition with multimodal data analysis to design advanced thin films.

2:10 PM
Data Driven Modeling for Yield Improvement in Gas Atomization Process: *Michael Ridenhour*[1]; Shankarjee Krishnamoorthi[1]; David Bryan[1]; Darryl Glanton[1]; John Goetz[1]; [1]ATI Specialty Materials

Physics-based modeling is an invaluable tool for understanding the impact of process parameters on production quality and efficiency. However, in the case of gas atomization, physics-based modelling is immature and computationally impractical due to runtime and memory limitations. We offer an alternate approach utilizing machine learning techniques to identify critical process parameters as they relate to powder yield, which we define as the percentage of particles under a certain size, of Ni-based superalloys. We relax the problem and treat a deep-learning model trained to predict yield based on high-speed process data from our atomizer as a proxy for the physical process. We then analyze this model to determine which process parameters have the highest impact on our prediction values and offer that these parameters are similarly impactful in the physical process as well. The identified process parameters matched with parameters typically identified in literature and based on operator experience.

2:30 PM
Digital Twin for In-situ Process Monitoring and Control of Aerosol Jet Printing: *Vikash Kumar*[1]; Jianjing Zhang[1]; Pawan Tripathi[1]; Laura Bruckman[1]; Roger French[1]; Robert Gao[1]; [1]Case Western Reserve University

Aerosol jet printing (AJP) is a versatile additive manufacturing technology for flexible and hybrid electronics, offering precise feature dimensions and intricate structures under various functional inks. However, maintaining constant line width over time remains challenging due to variations in process parameters such as aerosol density and process disturbances. This work presents the development of a digital twin that coordinates the in-situ print quality monitoring and control of part line width based on a neural state space model (NSSM) and model predictive control (MPC). The process involves identifying critical control parameters for line width deviation, analyzing the printed part's image, quantifying line width, training NSSM over these parameters, and providing feedback on the AJP setup with the help of a controller to control line width according to quality requirements. Besides ink jet printing, the developed approach provides guidelines for a multivariate control approach for other additive manufacturing processes.

2:50 PM
Explainable Deep Learning Model for Defect Detection During Autoclave Composite Curing Process: Deepak Kumar[1]; Yongxin Liu[1]; *Sirish Namilae*[1]; [1]Embry Riddle Aeronautical University

Applications of artificial intelligence (AI) in manufacturing enable new opportunities for automated quality inspection. The practical application of AI in composite processing is currently constrained by the absence of real processing data and the deep learning approach's explainability. In this study, we have used a custom-built autoclave with viewports and an interior lighting setup to develop a novel dataset of the composite curing process using digital image correlation (DIC). Later, using a unique explainable AI technique, a zero-bias deep neural network (ZBDNN) model is developed by transforming the final dense layer of the standard DNN model into a dimensionality reduction layer and a similarity matching layer. This model is then used to identify defects during autoclave composite processing. Several visualization techniques, including Voronoi and t-SNE (t-distributed Stochastic Neighbor Embedding), are utilized to demonstrate that the ZBDNN model was able to identify composite processing defects with high accuracy.

3:10 PM
Integrating Machine Learning Into Constitutive Material Modeling for the Creep Age Forming Process: *Yo-Lun Yang*[1]; [1]National Taipei University of Technology

Machine learning (ML) has been implemented to refine constitutive models of aluminium alloys, enhancing the prediction and optimization of the creep age forming (CAF) process. ML algorithms have been utilized to fine-tune constitutive equations, improving the modeling of the relationship between creep-ageing conditions and yield strength based on data from creep ageing tests under various stresses at elevated temperatures. The use of ML accelerates the modeling of material behavior and decreases the labor involved in manually developing traditional constitutive equations. Experimental validation has shown the efficacy of ML in accurately modeling and predicting the mechanical properties during the CAF process. This method signals a shift towards more intelligent automation and optimization of constitutive equations in CAF operations.

3:30 PM Networking Break

Accelerating Discovery for Mechanical Behavior of Materials 2024 Accelerated Approaches I

Monday PM
June 17, 2024

Room: Center Street Room A
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

1:40 PM Invited
Automated Feature Extraction for Identifying Structure-property Relationships: William Frieden Templeton[1]; Justin Miner[1]; *Sneha Prabha Narra*[1]; [1]Carnegie Mellon University

Microstructural analysis is essential for establishing process-structure-property relationships in new materials and processes. However, the quantitative representation of sparse, complex, and spatially intertwined microstructural features in micrographs poses a challenge. In this work, we employ a variational autoencoder framework to encode micrographs into a latent space with minimal information loss. By analyzing the latent representation, we can identify certain dimensions that correlate with our property of interest, thus linking encoded features from micrographs to key properties. Further, visualizing these dimensions through the inverse transform enhances the interpretability of our analysis and enables us to understand the features that govern the property. Our results provide initial insights into the potential versatility of this approach for automated extraction of informative microstructural features that could help determine structure-property relationships.

2:10 PM
Learning Full-rank Elastic Tensors With Equivariant Neural Networks: *Mingjian Wen*[1]; [1]University of Houston

The fourth-rank elastic tensor of a material provides a complete description of the response of the material to external load in the elastic limit. It has two unique characteristics regarding symmetry: first, it transforms equivariantly w.r.t. to the change of the frame of reference, and second, it must respect any symmetries that the material possesses. These requirements present significant challenges in effectively predicting elastic tensors with machine learning models.I will discuss a machine learning approach that automatically satisfies both symmetry requirements. Consequently, this model provides a universal treatment of elastic tensors for all crystal systems across diverse chemical spaces. Trained on a dataset of DFT reference values, the model performs very well in predicting the full tensor and derived elastic properties. It also enables rapid exploration of the anisotropic behavior of materials, which I will demonstrate via the search for new materials with extreme directional Young's modulus.

2:30 PM
Temperature and Dwell Hold Dependences of Fatigue Life by High-throughput High-resolution Digital Image Correlation: *J.C. Stinville*[1]; D. Anjaria[1]; C. Bean[1]; R.L. Black[1]; S. Sanandiya[1]; S. Hemery[2]; [1]University of Illinois Urbana-Champaign; [2]Institut PPrime

This study illustrates the connection between the characteristics of deformation events at the nanometer scale, which develop during early cycling, and the long-term performance of structural materials. Automated imaging inside the scanning electron microscope is used to perform high-resolution digital image correlation measurements over large fields of view. The characteristics of deformation events are then extracted using a computer vision algorithm. The characteristics of the deformation events that arise during the first loading cycle are found to inform long-term performance. Two material systems are investigated. First, the fatigue strength of a nickel-based superalloy and its dependency on temperature is rapidly evaluated using the proposed methodology. We identified the detrimental role of grain boundary sliding when temperature increases. Second, the reduction in lifetime of a titanium alloy subjected to different load hold periods is analyzed in light of the change in the intensity of deformation events during the first dwell-fatigue cycle.

2:50 PM Break (Keynote Session Occurs)

4:20 PM
Use of Indentation Plastometry for Inference of Stress-strain Behavior in Case-hardened Components: *Patrick Anderson*[1]; Mangesh Pantawane[1]; [1]Timken Company

Indentation plastometry is promoted as a fast, reliable method for gaining mechanical property data using less material than traditional mechanical testing. Through use of an instrumented indentation test in conjunction with inverse finite element analysis (FEA) modeling, engineering and true stress-strain curves are fit using an established model (Voce). Because of the relatively small indenter size (0.5 - 1.0 mm diameter ball), structured indent patterns can be used to fully interrogate deep case-hardened surfaces or as-tested mechanical test samples. Inferred stress-strain results can be used to validate and refine component design choices. Indentation plastometry results will be reviewed for deep case-hardened components, as well as comparison to tensile test data from equivalent component locations.

4:40 PM
Accelerated Discovery of Structural Materials for Harsh Environments: *Rameshwari Naorem*[1]; Hailong Huang[1]; Gaoyuan Ouyang[1]; Prashant Singh[1]; Duane Johnson[1]; Jun Cui[1]; Ryan Ott[1]; Iver Anderson[1]; Nicolas Argibay[1]; [1]Ames Natioanl Laboratory

Multi-principal-element alloys (MPEA) have emerged as a promising group of advanced materials with unprecedented combinations of mechanical properties compared to conventional alloys. Materials that can tolerate harsh environments and retain high strength at elevated temperatures are needed to enable greater efficiency in applications including nuclear reactors, hydrogen combustion turbines, bearings, and hypersonic vehicles. We will present results from materials design efforts focused on refractory alloys that rely on high-throughput synthesis and characterization methods like additive manufacturing, tribology-based mechanical testing, and electronic-structure modeling. Discussion topics will include rapid screening of thermomechanical properties using surface (scratch)-based techniques to assess hardness, fracture toughness, and tensile ductility. We will also present preliminary results from composition tailoring of MPEA to understand and control the impacts of hydrogen exposure on selected refractory MPEAs and to develop alloy design criteria for mitigating hydrogen embrittlement.

5:00 PM
An Experimental Investigation on the Tribological Behaviour of Electroless NiP-MoS_2-Gr Composite Coatings.: *Elayaperumal A*[1]; Subaash R[1]; Karthikeyan M[1]; Samrakshana E[2]; [1]Anna University; [2]Madras Institute of Technology, Anna University

The present work is focusing on the investigation of dry sliding wear behaviour of electroless NiP-MoS_2-Gr composite coating on carbon steel substrate. An electroless NiP-MoS_2-Gr coated carbon steel substrate was characterized using Scanning Electron Microscope [SEM], Energy Dispersive X-Ray Spectroscopy (EDS) and X-Ray Diffractometer (XRD). The surface hardness and roughness were evaluated using a vickers microhardness tester and contact-type surface profilometer. The tribological behaviour of the uncoated and coated substrate was determined at room temperature and high-temperature atmospheric conditions using a pin-on-disc tribometer and the worn surface analysis was carried out using SEM and EDS. A significant decrease in the wear mass loss, coefficient of friction and wear rate of the NiP-MoS_2-Gr composite coating was observed, this is due to the self-lubrication effect of MoS_2 and graphite particles added to the NiP matrix. The worn surface analysis results revealed that the coating has better adhesion with a substrate surface.

Accelerating Discovery for Mechanical Behavior of Materials 2024 Mechanics of Novel Materials I

Monday PM
June 17, 2024

Room: Center Street Room D
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

1:40 PM Invited
Mechanical Properties Assessment of AM Deposited Metallic Materials With the Use Miniaturized Samples: *Jan Dzugan*[1]; Daniel Melzer[1]; Ying Li[1]; Radek Prochazka[1]; Martin Rund[1]; John Lewandowski[2]; [1]Comtes Fht; [2]Case Western Reserve University

Additive manufacturing (AM) experiences dramatically increasing interest and in order to be successfully applied in the engineering structures, mechanical properties have to be well defined for considered specific cases. It is well known aspect of AM deposited structures that mechanical properties are very sensitive to deposition location, orientation, wall thickness and other crucial parameters in relation to which there can be quite significant variation of the properties achieved. Big issue in the case of AM deposited components is its size dependency, for which in many cases standard-sized samples are not applicable, and surface quality that are both strongly reflected in resulting mechanical properties. Standardization is being performed for mini-samples, which is mainly true for tensile, but fatigue, fracture toughness and potentially creep tests are still not addressed. This paper provides an overview on use of mini samples for above mentioned tests and standardization activities running in this field of interest.

2:10 PM
Scorpions and Goatheads Examined With Nanoindentation: *Stanislav Zak*[1]; Megan Cordill[1]; [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences

From the material science point of view, the materials occurring in different plant and animal species hold a plethora of secrets on how to improve their global mechanical properties by creative microstructure, hierarchical ordering, and chemistry. However, for further development of nature's ideas, a quantitative measurement of various properties is needed. A suitable way to asses material's mechanical properties is nanoindentation. Presented work consists of examples of nanoindentation of a plant seed pod (Tribulus terrestris, referred to as "goathead") and nanoindentation of two scorpion species' stingers (Buthidae Centruroides platnicki and Diplocentridae Nebo whitei). On the example sets, the issues regarding the sample preparation, testing and results analysis are summarized alongside the discoveries of clever microstructural designs. The scorpion stingers exhibited strong sensitivity on the sample preparation, but revealed interesting material properties gradients, regardless of chemical compositions. The goatheads showed expectable synergy of lightweight straw-like structures with columnar microstructural ordering.

2:30 PM
Dynamic Behavior of Smart Cellular Materials: *Marlini Simoes*[1]; [1]California Institute of Technology

The use of cellular materials in engineering applications has been hindered due to the challenges associated with the manufacture of such complex geometries. However, additive manufacturing (AM) technologies have enabled the fabrication of complicated structures. Nevertheless, the design optimization of AM cellular materials for impact loading scenarios remains underdeveloped. In this work, the opportunities created by Laser Powder Bed Fusion (LPBF) AM process have been explored by: (1) studying the process-geometry-mechanical property interactions of metallic cellular materials, and (2) manufacturing cellular structures which can exhibit a "self-healing" capacity through shape memory functional properties, after being mechanically deformed quasi-static and dynamically. From the first study, it was found that the geometry played a dominant role in the mechanical performance, relative to the AM parameters. Secondly, a newly designed diamond lattice and auxetic structures were successfully additively manufactured, and recovered up to 70% of their shape, after having been fully densified.

2:50 PM Break (Keynote Session Occurs)

4:20 PM
Uncovering Dislocation-precipitate Interactions During Tensile Loading of Wire Arc Additive Manufactured Nickel-Aluminum-Bronze: *Aeriel Murphy-Leonard*[1]; Veronika Mazanova[1]; [1]Ohio State University

Dislocation-precipitate interactions of a wire arc additive manufactured nickel-aluminum-bronze alloy subjected to uniaxial tensile loading were investigated in this study. A unique multi-scale methodology involving scanning transmission electron microscopy (S/TEM), electron back scatter diffraction (EBSD), and electron channeling contrast imaging (ECCI) was designed to uncover individual interactions with several -phase particles. A strong accumulation of dislocations along globular II and lamellar III particles were observed during loading. Shearing of small, coherent IV particles by dislocations was also observed within the matrix. These interactions provide insights into the processing parameters needed to enhance strength and the ductility of these complex microstructures.

4:40 PM
Improvement of the Mechanical Properties of M2 High-speed Steel With Tungsten Carbide: *Miroslav Urbanek*[1]; [1]COMTES FHT a.s.
High-speed molybdenum steel M2 has an excellent ratio between toughness, hardness, and wear. M2 steel is commonly used for cold work on tools such as punches, cutters, dies, etc. Tungsten carbide is most often found as a gray powder that is pressed and then sintered. Tungsten carbide has approximately twice the strength and stiffness of steel. Thanks to using additive manufacturing using direct energy deposition technology, the two materials can be mixed to create a new alloy of M2 steel with tungsten carbide hard balls. The investigated ratio of tungsten carbide in steel M2 was 5-20%.

5:00 PM
Research on the Microstructure and Properties of Ultralight Mg-Li-X Alloys: *Yan Yang*[1]; [1]Chongqing University
The engineering application of ultra-light Mg-Li alloys is seriously restricted because of their low strength, poor stability and high temperature performance. Ultralight Mg-Li-X alloys with high strength were designed and prepared via the introduction of alloying element and plastic deformation. Ultralight Mg-Li-Al-Sn, Mg-Li-Al-Mn and Mg-Li-Al-Ca alloys with high strength and good damping capacities have been developed in our research group. The microstructure, mechanical properties and damping property of Mg-Li-Al-X alloys were investigated systematically combing the usage of many advanced microstructure characterization methods and normal tensile tests, etc. The results from this research provide important technological support for the controlling of microstructure, mechanical properties and damping capacities of Mg-Li alloys.

Symposium on Digital & Robotic Forming 2024 Industry Applications I

Monday PM
June 17, 2024

Room: Center Street Room B&C
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

2:20 PM Invited
Technology Training Transfer for Advanced Manufacturing Technologies: *Lori Baukus*[1]; [1]Arctos Technology Solutions
It has become increasingly important to provide training that keeps pace with industry. The Smart Manufacturing Digital Thread (SMDT) project aims to define and implement processes to speed up process development and replication. The SMDT is an example of optimized Training Technology Transfer that can be applied to key technologies like robotic metal forming. The current SMDT project is currently focused on Automation and Robotics, Digital Thread, and Laser Materials Processing. The SMDT project showcases how to scale technology training to meet workforce demands. Key components include making the training accessible and flexible, and engaging a workforce that may never have considered advanced manufacturing as a career option.

2:50 PM Invited
In-space Manufacturing of Large Reticulated Structures via Deformation Processing: *Zachary Cordero*[1]; [1]Massachusetts Institute of Technology
Increasing the size of radio frequency (RF) reflectors in space can enhance gain and spatial resolution in space-based communication and remote sensing applications. The size of current passive deployable reflectors, such as the Northrop Grumman Astromesh, is limited by a tradeoff between diameter and surface precision, which causes surface precision to degrade as size increases. A promising approach to overcome this tradeoff combines a candidate in-space manufacturing process, termed Bend-Forming, with embedded actuation to correct for on-orbit disturbances. This talk will describe the principles of Bend-Forming, a deformation processing technique for forming net-shaped reticulated structures, and its application in a microgravity environment, where new challenges with attitude control arise. The present results highlight opportunities in new reflector technologies combining in-space manufacturing, which enables large structures, with distributed embedded actuation, which enables precise control over the reflector surface.

3:20 PM
Starting a Digital & Robotic Forming Company – Why, How, and the Role of Different Stakeholders: *Babak Raeisinia*[1]; Edward Mehr[1]; Glenn Daehn[2]; [1]Machina Labs, Inc.; [2]The Ohio State University
In this work we will look at how Digital & Robotic Forming can impact manufacturing across different sectors. We will examine what it takes to start a Digital & Robotic Forming company and accordingly, outline the general considerations in starting an advanced, software- and hardware-based manufacturing business. Special attention will be given to the journey of such a company from its early, so-called seed stage to its growth stage where factors such as maintaining a strong, healthy company culture will gain an equal footing to company's technical goals. Lastly, we will examine the role of different stakeholders, including public and private sector entities, in assuring a robust Digital & Robotic Forming manufacturing base can be established.

3:40 PM Networking Break

4:50 PM
Incremental Robotic Forging: An Initial Cyber-physical System: *Michael Groeber*[1]; Stephen Niezgoda[1]; Adam Buynak[1]; Brian Thurston[1]; Ben Turner[1]; Jared Glover[2]; [1]Ohio State University; [2]CapSen Robotics
Many entities tasked with sustaining systems face persistent challenges with rapidly sourcing replacement components. Many such components are custom to particular platforms or required in small numbers and supply chains are ill-equipped to deliver quickly. A collaborative team from academia, government, and industry is developing a disruptive and novel manufacturing technology to produce a part incrementally as opposed to all at once, similar to an artisan blacksmith. This kind of manufacturing can produce parts on demand with an on-site robotic work cell to yield parts of superior quality, with less material waste, and in record time. The first prototype system developed by the team consists of an industrial robot, small-scale forge press, induction furnace, and vision system, all easily obtainable off-the-shelf components and is driven by novel decision-making algorithms that mimic the choices of a human blacksmith. This talk will describe the system and its initial successes and challenges.

5:10 PM
Enabling Manufacturing of Next-gen Aerostructures Through Digital & Robotic Forming: *Babak Raeisinia*[1]; Glenn Daehn[2]; [1]Machina Labs, Inc.; [2]The Ohio State University
The aerospace industry as a whole is facing a number of manufacturing challenges as it looks to the future. Some of these challenges relate to the increased production rates that ought to be achieved to meet demand. Others, relate to new requirements imposed on emerging air vehicles (i.e., different to those defined for current platforms) that require new approaches to manufacturing. In this work, we will examine how leveraging Digital & Robotic Forming can help in achieving some of these manufacturing challenges. This includes assuring composite manufacturing rates can be achieved through agile fabrication of metal tooling for composites. By the same token combination with other emerging manufacturing technologies such as impact welding and localized heat treatment can enable manufacturing of novel, metallic aerostructures that were previously not possible.

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) Image Processing II

Tuesday AM
June 18, 2024

Room: Hope Ballroom B
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

8:30 AM Invited
Optimizing the Microstructure of Additively Manufactured Al Alloy Using Deep Learning: *Deepak Kumar*[1]; Quansheng Zha[1]; Sandeep Sahu[1]; Shuncai Wang[1]; Nong Gao[1]; [1]University of Southampton

Laser powder bed fusion (LPBF) has proven to be an exceptional technology for the manufacturing of complex and innovative design components. In this study, LPBF was used to manufacture AlSi10Mg alloy with varying laser distance. The microstructure of the samples was characterized using a combination of optical microscopy, SEM, and EBSD techniques. Additionally, image processing with CNN was used to assess the porosity, pore diameter, circularity, microstructure, and anisotropy of the samples. The deep learning techniques optimized melt pool features w.r.t. laser distance. The findings revealed that the printing parameter had a significant impact on the distribution of keyhole, lack of fusion, and gas porosities. Moreover, the CNN models provided a deeper understanding of the anisotropy of SDAS and its relationship with gas porosities. The study demonstrates the potential of LPBF technology and deep learning for the optimization of printing parameters to manufacture components with desired properties.

9:00 AM
A Materials Data Segmentation Garden for Benchmarking Segmentation Models: *Pawan Tripathi*[1]; Tommy Ciardi[1]; Mingjian Lu[1]; Kristen Hernandez[1]; Max Ligett[2]; Andrew Ballen[2]; Jean-Baptiste Forien[3]; Brian Giera[3]; Manyalibo Matthews[3]; Mengjie Li[2]; Kristopher Davis[2]; John Lewandowski[1]; Laura Bruckman[1]; Yinghui Wu[1]; Roger French[1]; Vipin Chaudhary[1]; [1]Case Western Reserve University; [2]University of Central Florida; [3]Lawrence Livermore National Laboratory

Segmentation of materials data is a critical task in various scientific and engineering fields, such as materials science, geology, and medical imaging. Accurate segmentation is essential for understanding the internal structure of materials, identifying defects, and optimizing material properties. To facilitate research and development in this domain, we propose the creation of a Materials Data Segmentation Model Garden (MDSMG). In conjunction with the Materials Data Segmentation Benchmark (MDSB), MDSMG will enable the research community to test their models uniformly and foster creation of better segmentation models. MDSMG will enable testing, evaluating, comparing and developing new materials data segmentation models. The MDSMG will establish standardized evaluation metrics and protocols to assess the performance of segmentation models. MDSL will be an open-source project, freely accessible to the research community. This will encourage innovation, democratize access to advanced segmentation tools, and accelerate the development of new materials analysis techniques.

9:20 AM
Semantic Segmentation of Scanning Electron Microscopy Images for Contact Degradation Analysis in Field-aged Photovoltaic Modules: Andrew Ballen[1]; *Max Liggett*[1]; Dylan Colvin[1]; Pawan Tripathi[2]; Roger French[2]; Kristopher Davis[1]; Mengjie Li[1]; Dana Kern[3]; [1]University of Central Florida; [2]Case Western Reserve University; [3]National Renewable Energy Laboratory

In the context of photovoltaics (PV) research, characterizing the front contact metallization is an integral part of understanding the performance, reliability, and durability of PV cells and modules. A common approach to evaluate PV front contacts is to obtain cross-sectional scanning electron microscopy (SEM) images and make qualitative observations on the quality of bulk, metal contact, interfacial glass fit, and the distribution of metal crystallites. We propose a novel way to objectively and quantitatively observe contact corrosion in silicon-based PV devices using cross-sectional SEM images. The approach uses semantic segmentation to isolate the various parts of the metal contact and its interface to the underlying semiconductor absorber. Then, a statistical analysis of the pixel intensity distribution is performed on specified regions known to correspond to contact corrosion. This approach is applied to various silicon-based PV devices at various states of disrepair due to different levels of exposure to environmental stressors.

9:40 AM
Identification of Binder Jet Spreading Anomalies Through Semantic Segmentation: *Alexander Gourley*[1]; Jonathan Kaufman[2]; Bashu Aman[1]; Edwin Schwalbach[3]; Jack Beuth[1]; Lisa Rueschhoff[3]; B. Reeja-Jayan[1]; [1]Carnegie Mellon University; [2]UES Inc.; [3]Air Force Research Lab

Binder jet additive manufacturing can achieve complex geometries with metal and ceramic materials, but low green densities and anomalies from powder spreading reduce final part performance. Exploring the multidimensional process parameter space is prohibitively expensive, so identifying and correcting problematic behaviors within a build is necessary for new materials. In this study, Dragonfly image processing software was utilized for the first time to segment additive manufacturing powder bed images. Photos were taken with 316 stainless steel and alumina and segmented using a U-Net convolutional neural network to identify spreading anomalies. The steel and alumina models trained on five print layers each achieved categorical accuracies of 95.4% and 92.3%, respectively. Trends in the number of pixels with each label reflected changes in conditions, including removing an anomaly type through parameter adjustments. Automated build monitoring for anomaly correction allows for improved part quality and the development of closed-loop additive manufacturing.

10:00 AM Break

10:20 AM
Optical to Scanning Electron Microscopy Style Transfer of Steel Micrograph Using Machine Learning: *Nicholas Amano*[1]; Bo Lei[2]; Martin Müller[3]; Dominik Britz[3]; Elizabeth Holm[1]; [1]University of Michigan; [2]Lawrence Livermore National Laboratory; [3]Steinbeis-Forschungzentrum Material Engineering Center Saarland

Observation and analysis of microstructure is fundamental to metallurgical science, hence significant resources are allocated towards preparing and imaging structured materials. We present two methods of generating scanning electron microscopy(SEM) images from optical micrographs to reduce imaging requirements and better understand microstructural behavior. This work is made possible by a unique dataset of optical and SEM micrographs collected at identical locations and length scales. We use generative adversarial networks(GANs) and diffusion-based models for style transfer of steel optical micrographs to SEM micrographs. This work reduces the etching and measurement times associated with SEM. Additionally, understanding how the models perform with differing amounts of prior SEM knowledge sheds light on indicators of microstructural outcomes. We demonstrate that both models produce plausible microstructures but share a difficulty with orientation specific recreations. GANs perform well on in-domain recreations, while diffusion models are better suited for generalized micrograph style transfer.

PRELIMINARY TECHNICAL PROGRAM

10:40 AM
Image Analysis of Fractography: Defect Feature Comparisons: *Kristen Hernandez*[1]; Austin Ngo[1]; Ayorinde Emmanuel Olatunde[1]; Thomas Ciardi[1]; Pawan Tripathi[1]; Anirban Mondal[1]; John Lewandowski[1]; Laura Bruckman[1]; Roger French[1]; [1]Case Western Reserve University

Fractography provides insight to defects below the resolution of traditional non-destructive testing (NDT) such as X-Ray Computed Tomography (XCT) or defects partially revealed during the preparation of metallography samples. In Additively Manufactured (AM) parts, defects in a printed material serve as the initiation site of failure. Defects such as lack-of-fusion (LoF), keyhole, or other morphological defects have measurable qualities that are unique. Samples fabricated under a range of speed-power combinations covering each defect regime were evaluated with Scanning Electron Microscopy (SEM) on the fracture surface. Traditional evaluation involves manual annotation of thousands of defect features on hundreds of images. Machine learning can accelerate this process by automatically segmenting features of interest given a subset of training samples. In this study we employ multiple feature extraction techniques: manual annotation, WEKA semi-supervised machine learning, and fully-supervised deep learning using U-Net to observe the distribution of detected features and compare time-accuracy tradeoffs.

11:00 AM
Patch-wise Canonical Correlation Analysis in SEM: Advancing 3D Serial Sectioning Image Registration: *Zachary Varley*[1]; Marc De Graef[1]; Gregory Rohrer[1]; Megna Shah[1]; Michael Uchic[1]; [1]Carnegie Mellon University

While 3D serial sectioning experiments in a scanning electron microscope (SEM) with electron backscatter diffraction (EBSD) provide rich microstructure information, they present significant data collation challenges. Typically, electron backscatter diffraction (EBSD) maps are aligned with corresponding backscatter electron micrographs to eliminate distortions from any experimental factors or viewpoint changes. Existing registration metrics such as mutual information can fail to result in well aligned volumetric data, especially when applied to as-built 3D printed samples. Barrowing from recent advances in medical image registration, we propose using Patch-wise Canonical Correlation Analysis (PCCA) in conjunction with a pretrained Convolutional Neural Networks (CNN). Unlike mutual information, PCCA leverages local structure within images, conferring better accuracy at increased computational burden. This additional cost can be alleviated by approximating the PCCA metric with a CNN. This advancement demonstrates remains performant in challenging registration scenarios and shows potential for broader application across SEM imaging modalities.

11:20 AM
Microstructural Diffusional Variational Autencoder for Generation of Microstructure Ensembles: *Stephen Niezgoda*[1]; Maxwell Brown[1]; Simon Mason[1]; Dennis Dimiduk[2]; [1]Ohio State University; [2]BlueQuartz Software

Diffusion probabilistic models (DPMs) have been wildly successful at image generation across a variety of applications. One weakness of DPMs is the lack of a latent representation that is meaningful and decodable. Recently developed diffusion autoencoders have demonstrated a dual latent space that captures both the high-level semantics and stochastic variation separately. Current diffusion autoencoders are adept at producing multiple versions of an image with the same large scale features (e.g women's face) but very minor changes (position of individual strands of hair). They are not adept at producing multiple distinct realizations of a microstructure where each image is visually distinct but share common features (such as size and shape distributions). Here we present a novel microstructural diffusional variational autoencoder (MDVAE) with an architecture and latent space designed to properly capture and reproduce the full range of variability in realistic microstructure images.

11:40 AM
Modeling the Damage Healing of Self-healing Polymer Using Zero Bias Deep Learning Approach: Palvi FNU[1]; Deepak Kumar[1]; Foram Madiyar[1]; Yongxin Liu[1]; *Sirish Namilae*[1]; [1]Embry Riddle Aeronautical University

Intrinsic self-healing polymers are inherently self-repairing materials that do not require external stimuli such as heat or pressure. These materials find diverse applications in domains like aerospace and healthcare. In this study, we created a self-healing polymer recovery dataset using in-situ microscopic characterization of the damage healing process. Subsequently, an explainable AI approach, the zero-bias deep neural network (ZBDNN) model, is employed to analyze this data. ZB DNN modifies the final dense layer of the standard DNN model into a dimensionality reduction layer and a similarity-matching layer. This model provides a metric for characterizing the level of damage in each image based on the Mahalanobis distance between the feature vectors of healed and non-healed inputs. The model can be utilized to analyze and predict the temporal evolution of the healing process.

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) Machine Learning - Manufacturing II

Tuesday AM
June 18, 2024

Room: Hope Ballroom C
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

8:30 AM Invited

8:50 AM
Neural Networks as Surrogate Models for Real-time Optimization of Additive Manufacturing: *Devin Roach*[1]; Adam Cook[2]; Andrew Rohskopf[3]; [1]Oregon State University; [2]Sandia National Laboratories; [3]Apple Inc.

Direct ink write (DIW) additive manufacturing (AM) has enabled an elegant fabrication pathway for a vast material library. Nonetheless, each material requires optimization of printing parameters generally determined through significant trial-and-error testing. To eliminate arduous, iteration-based optimization approaches, we use machine learning (ML) algorithms such as neural networks (NNs) which provide opportunities for automated process optimization. In this talk, we highlight the use of computer vision (CV) measurements of DIW print parameters for NN training. By using trained NNs as surrogate models for the DIW process, inverse optimization problems could be solved and implemented in less than a second for real-time print optimization. The methods developed and presented in this talk eliminate user-intensive, time-consuming, and iterative parameter discovery approaches that currently limit accelerated implementation of AM processes. The approaches outlined in this talk can be generalized to provide real-time monitoring and optimization pathways for increasingly complex AM environments.

9:10 AM
Analyzing the Impact of Design Factors on Solar Module Thermomechanical Durability Using Interpretable Machine Learning: *Xin Chen*[1]; Todd Karin[2]; Anubhav Jain[1]; [1]Lawrence Berkeley National Laboratory; [2]PVEL

Solar modules in field are subject to cyclic thermomechanical loading, emphasizing the need for proper module design to resist thermal expansion incompatibility. However, isolating the impact of confounding components on overall durability remains a challenging task. In this work, we collected bill-of-materials data and thermal cycling power loss from over 250 distinct module designs. We developed a machine learning model to correlate design factors with the degradation and applied Shapley additive explanation to interpret the impacts of design factors. Our analysis reveals that the type of silicon cells predominantly influences the degradation, and monocrystalline cells present better durability. This finding was further substantiated by statistical testing. We also demonstrate the thickness of the encapsulant remains another important factor, with thicker encapsulants correlated with reduced degradation. The study here provides a blueprint for utilizing explainable machine learning in intricate material system and can potentially steer future optimization of solar module design.

9:30 AM
Application of Data-driven Digital Twins in Advanced Manufacturing: *Kristen Hernandez*[1]; Hein Htet Aung NA[1]; Alexander Bradley[1]; Thomas Cairdi[1]; Rachel Yamamoto[1]; Arafath Nihar[1]; Robert Gao[1]; Pawan Tripathi[1]; Laura Bruckman[1]; Roger French[1]; [1]Case Western Reserve University

Advanced manufacturing (AM) has seen large growth following the advancement of technology. Physics-based approaches and predictions have become increasingly infeasible with computation because considerations are multi-faceted. Digital twin is a virtual representation of a part using in-situ monitoring, ex-situ characterization or other data sources. This data-driven digital twin (dd-DTs) approach has shown promise and success in integrated systems by feeding real-world, data-driven information into simulations. Having a digital twin of a part can offer certainty of a print's outcome before using materials using spatio-temproal graph neural network model, in which each track is a graph node, and each node as a feature vector. This approach allows for the production of more reliable AM parts and the ability to apply quality metrics in-situ for informed problem solving. This study focuses on dd-DT of laser powder bed fusion (L-PBF) and direct ink write (DIW) printed parts.

9:50 AM Break

10:10 AM
Assessment of an Intelligent System for Additive Manufacturing Product Evaluation: *Sumaila Omeiza Jimoh*[1]; [1]Mechanical Engineering Department, Federal University of technology, Babura, Nig

Product policy is gear to the performance of additive manufacturing operations. It affect production time, cost and sale price and user acceptability. This paper, therefore aims to assess an intelligent system that will generate real time product quality information for AM technology based processes with emphasis on the production of industrial safety welding gogglers using AM technology based processes with emphasis on the design and asses an intelligent AM decision making support system with the goal of optimizing operations from a product evaluation perspective. The IAM system's information will enhance the pursuit of innovative works in product, quality development and management. It will support stakeholder's decision making during the design and development of tactical and strategic policies for product management.Keywords: Addictive, Manufacturing, Policy, Artificial Intelligence, Product, quality.

10:30 AM
Capturing AM Process Defects on Fatigue Fracture Surfaces Through Machine Learning Segmentation: *Austin Ngo*[1]; Kristen Hernandez[2]; Oluwatumininu Adeeko[1]; Ayorinde Olatunde[3]; Anirban Mondal[3]; Roger French[2]; John Lewandowski[1]; [1]Department of Materials Science and Engineering, Case Western Reserve University; [2]Materials Data Science for Stockpile Stewardship, Case Western Reserve University; [3]Department of Mathematics, Case Western Reserve University

While process defects arising in additive manufacturing (AM) may be quantified through several methods, only defects on fatigue fracture surfaces directly show the influence of defects on crack initiation and propagation. To quantify large defect populations on a fracture surface, machine learning algorithms for feature segmentation were utilized to characterize fracture surfaces of Ti-6Al-4V fatigue samples fabricated by powder bed AM. Process-induced defects were identified and quantified by feature training an image classification system using SEM images of fracture surfaces. Process defects were found to range in size, shape, and population due to variations in AM build process parameters. All process-induced defects across each fracture surface were quantified, with 'killer' fatigue crack initiating defects being identified. In addition, this computer vision method is compared to ground truth manual quantification of fracture surface defects. The advantages and challenges of implementing ML algorithms to streamline fracture surface defect quantification will be discussed.

10:50 AM
Pyrometry Mapping of Segmented Porosity in Computed Tomography: *Peter Pak*[1]; Francis Ogoke[1]; Andrew Polonsky[2]; Dan Bolintineanu[2]; Daniel Moser[2]; Anthony Garland[2]; Jesse Adamczyk[2]; Michael Heiden[2]; Amir Farimani[1]; [1]Carnegie Mellon University; [2]Sandia National Laboratories

Porosity in additively manufactured parts hinder the component's fatigue life and prevent its use in design critical areas and Machine Learning (ML) can help predict and prevent these defects. In-situ melt pool thermal image processing mapped to ex-situ porosity can improve production yield and minimize costs through waste reduction. This work shows a Swin Transformer fine-tuned on a thermal image dataset obtained using a two color pyrometry camera to map to Computed Tomography (CT) generated voxel space porosity. The dataset includes an input and label set of varying processing conditions which the model uses to generate its porosity predictions. This model displayed high accuracy in downstream prediction tasks such as layer-wise porosity classifications and volumetric porosity fractions from the processed input of thermal images. Furthermore, mapping of two-dimensional thermal images to a three-dimensional reconstruction of the sample and its corresponding porosity was investigated as well.

11:10 AM Cancelled
Automated Bulk Melt Pool Contour Data Acquisition From Micrographs Using Computer Vision: *Joshua Fody*[1]; [1]NASA Langley Research Center

PRELIMINARY TECHNICAL PROGRAM

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) Machine Learning - Modeling and Simulation

Tuesday AM
June 18, 2024

Room: Hope Ballroom A
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

8:30 AM Invited
Assessing the Performance of Machine Learning Universal Interatomic Potentials on Intermetallic Systems: *Giancarlo Trimarchi*[1]; Qing Chen[1]; [1]Thermo-Calc Software AB

A remarkable progress in the area of machine learning (ML) applied to materials modelling is the development of universal interatomic potentials such as M3GNet and CHGNet based on graph neural networks that can be applied to systems of any chemical composition. Here, we investigate whether these ML models predict the formation energies of structures typically found in intermetallic alloys with an accuracy comparable with that of DFT and thus could be viable sources of data for CALPHAD modelling. We take as test systems a wide range of binary structures formed by Al, Nb, Ti, and V, and give special attention to the performance of the models on configurations with the sigma-phase structure. Finally, we train new instances of these ML potentials on the original data sets augmented with DFT data on binary structures containing these elements and compare the performance of the original and custom-trained instances of the models.

9:00 AM
Accelerated Development of Materials Using High-throughput Strategies and AI/ML: *Surya Kalidindi*[1]; [1]Georgia Institute of Technology

This talk presents recent advances made in the presenter's research group, including: (i) a novel information gain-driven Bayesian ML framework that identifies the next best step in materials innovation (i.e., the next experiment and/or physics-based simulation to be performed) that maximizes the expected information gain towards a specified target (e.g., optimized combination of material properties, refinement of a material constitutive response), (ii) computationally efficient versatile material structure analyses and statistical quantification tools, and (iii) formulation of reduced-order process-structure-property models that enable comprehensive inverse solutions needed in materials design (e.g., identifying specific compositions and/or process histories that will produce a desired combination of material properties). These recent advances will be illustrated with case studies.

9:20 AM
Application of Graph Neural Network in Prediction of Mesoscale Structure in Dense Slurries: Joao Maia[1]; Armin Aminimajd[1]; *Abhinendra Singh*[1]; [1]Case Western Reserve University

Understanding the rheological response of particulate system is relevant to industry and nature. The mesoscale force chain network (FCN) structure holds the key for structure-property relationship in these disordered materials. While traditional simulation methods are expensive, recent deep learning techniques were found to be a powerful tool to predict properties of particulate systems. Herein, we train the deep graph convolutional neural network (GCNN) model using datasets obtained from lubrication flow discrete element modeling to accurately predict (above 98%) FCN in suspensions for different control variables. Our machine learning model goes beyond recent research on granular materials; it not only predicts FCN with higher accuracy but also interpolates and extrapolates to conditions far from control parameters. The method used in this study can be utilized for prediction of rheological and characterization of complex particulate systems in the future.

9:40 AM
Improved Methods to Predict the Mixing Enthalpy of Liquid Alloys for CALPHAD Databases With Artificial Neural Networks: Hai-Lin Chen[1]; Qing Chen[1]; *Paul Mason*[2]; [1]Thermo-Calc Software AB; [2]Thermo-Calc Software Inc.

When experimental data are unavailable, the semi-empirical Miedema model has historically been used during CALPHAD assessments to predict the mixing enthalpy of liquid alloys. The work described here aims to predict more accurately the mixing enthalpy using artificial neural networks (ANNs).Leveraging ANNs and selecting elemental properties from the Magpie Python module, nine elemental properties significant to mixing enthalpy were identified, some of which overlap with the Miedema model's parameters. Using CALPHAD thermodynamic databases, the mixing enthalpy of 1073 binary systems were analyzed. Data reliability was gauged using assessment deviations, and 220 binaries were initially chosen for model optimization. Through iterative evaluations and enhancements, the optimal model encompassed data from 853 binary systems (80% of the total). The final ensemble, comprising 100 ANNs models, achieved an average R2 score of 0.96, proving superior in accuracy and generalizability to the Miedema model for predicting the mixing enthalpy of liquid alloys.

10:00 AM Break

10:20 AM
Predicting Microstructure From Process Conditions Using Multi-modal Machine Learning: *Ankit Shrivastava*[1]; Matias Kalaswad[1]; Marta D'Elia[1]; Dave Adams[1]; Habib Najm[1]; [1]Sandia National Lab

We present a multimodal machine learning (ML) approach to build a process-structure mapping for molybdenum (Mo) thin films fabricated using physical vapor deposition (PVD). Optimizing thin films for semiconductor applications involves navigating many process conditions, making the approach inefficient. Data science models offer a more cost-effective solution. However, microstructure information comes from different sources of experiments in the form of multimodal datasets, for example, stress measurements, X-ray diffractograms, and scanning electron microscopy images. Predicting joint multimodal information of microstructure is a challenge. Our multimodal ML approach predicts joint structural information of microstructures from PVD process conditions. The construction employs multiple dimensional reduction algorithms to learn a joint latent representation of the multimodal microstructure data. Then, a deep learning model is used to learn the relationship between joint latent representation and process conditions. This approach can enhance our understanding of the complex interplay between process parameters and microstructure properties.

10:40 AM
Hybrid Denoising Diffusion Models for Statistically Conditioned Generation: *Andreas Robertson*[1]; Conlain Kelly[1]; Michael Buzzy[1]; Surya Kalidindi[1]; [1]Georgia Institute of Technology

Controllable generative models have emerged as a foundational cornerstone of modern Materials Informatics efforts. For example, these models allow researchers to systematically expand limited experimental datasets by injecting curated synthetic data into poorly represented regions of the microstructure statistics space. In this talk, we present the Local-Global Decomposition generative framework, a generative framework that provides 1- and 2-point statistical conditioning, can stably extrapolate, and requires (at most) only a single image for training. The framework utilizes statistical physics – specifically, a physics inspired decomposition – to stabilize the training and inference of a denoising diffusion model. In addition to presenting the proposed generative modelling framework, we present a series of examples – including both N-phase and polycrystalline systems – to explore its strengths and weaknesses. Finally, we discuss potential applications.

11:00 AM
Thermodynamically Consistent Neural Networks for Modeling of Inelastic Material Responses: *Liam Mackin*[1]; Bradley Davidson[1]; Rohan Patel[1]; Reed Kopp[1]; David Najera[1]; [1]ATA Engineering

The formulation of constitutive models for path-dependent materials is a well-known bottleneck for simulations of nonlinear material behavior, particularly for heterogeneous materials with distinct structures and behavior at different length scales We introduce an approach, inspired by deep recurrent neural networks, for automatic discovery of these unknown path-dependent constitutive models. The universal approximation properties of deep neural networks make them particularly well-suited for this purpose, and additional structure is imposed on the network to ensure that it learns a thermodynamically consistent set of internal state variables and state variable evolution laws. We show how the trained neural network can be embedded into a commercial Finite Element Solver and used to solve for stress and other state variables at each increment and integration point. Finally, we show how this approach can be used to homogenize RVEs at any length scale and enable efficient multi-scale modeling of advanced nonlinear path-dependent materials.

11:20 AM
Exploring Graph Neural Network Surrogates for Microstructure Analysis: *Kyle Farmer*[1]; Elizabeth Holm[1]; [1]University Of Michigan

Crystal deformation simulations offer a robust means of examining the anisotropic response of microstructures. This study evaluates the effectiveness of a versatile graph neural network (GNN) framework as a surrogate for capturing the dynamic evolution of microstructural phenomena. Traditional methods such as finite element analysis (FEA) and spectral methods have historically been applied to model deformation mechanisms, but they are often hindered by high computational demands and oversimplified deformation modes. In this investigation, we explore the training of a deep-learning-based GNN model using both 2D and 3D finite-element crystal elasticity data. Our model demonstrates commendable accuracy on unseen datasets, reliably extrapolates to larger systems, and the shows the potential to surpass traditional methods in terms of computational efficiency.

11:40 AM
Multiaxial Fatigue Life Prediction of Additively Manufactured Ti6Al4V Alloy Using Machine Learning Techniques: Raviraj Verma[1]; *Guru Shreyaas*[1]; Jayaganthan R.[1]; [1]Indian Institute of Technology Madras

The multiaxial fatigue behaviour of Ti6Al4V alloy fabricated by additive manufacturing is difficult to investigate experimentally. Machine learning (ML) can predict the dynamic mechanical behaviour, such as the multiaxial fatigue property, with less resources and more efficiency. This work uses three ML approaches: Support Vector Regression (SVR), Random Forest Regression (RFR) and Boosting Algorithms to predict the multiaxial fatigue life curve of Ti6Al4V alloy under different loading conditions. The test variables include stress ratio, laser powder bed fusion sample conditions, post-fabrication sample conditions, etc. The ML approaches are trained with experimental data from the literature. SVR handles nonlinear and complex data well, RFR processes small dataset efficiently, and Boosting Algorithms improve prediction accuracy by combining multiple models. These ML approaches capture the nonlinear characteristics of multiaxial fatigue behaviour of Ti6Al4V alloy and provide a reliable prediction of endurance limit.

Accelerating Discovery for Mechanical Behavior of Materials 2024 Accelerated Approaches II

Tuesday AM
June 18, 2024

Room: Center Street Room A
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

8:30 AM Invited
High-throughput Fatigue Behavior of Additively Manufactured Functionally-graded Metals: *Jason Carroll*[1]; Robert Rhein[1]; J.C. Stinville[2]; [1]Eaton Corporation; [2]University of Ilinois

Eaton envisions a future where highly differentiated and personalized products will be designed rapidly and entirely by computers through the unification of multiscale materials design & materials informatics, multi-physics engineering simulation & reduced order modeling, artificial intelligence-driven design & process automation, generative design, and additive manufacturing. In support of this vision, fatigue characterization of novel materials in the nanometer length scale, where the mechanics that control product life is highly stochastic, is needed. This study investigates the characteristics of the deformation and damage events at the nanometer scale during ultrasonic fatigue (very high-cycle fatigue, frequency of 20 kHz) on graded metallic specimens with a non-uniform distribution of defects fabricated via parameter changes during laser powder bed fusion (LPBF). Deformation and damage events are quantified using large-scale, high-resolution digital image correlation measurements during ultrasonic fatigue to rapidly extract the consequence of printing parameters on fatigue strength.

9:00 AM
Discovery of Hard and Conductive Pt-Au Thin Films Utilizing Multi-modal Large datasets and Machine Learning: *Manish Jain*[1]; Saaketh Desai[1]; David Adams[1]; Matias Kalaswad[1]; Sadhvikas Addamane[1]; Frank Delrio[1]; Remi Dingreville[1]; Brad Boyce[1]; [1]Sandia National Laboratories

The rapid progress in materials science, driven by remarkable technological advancements, finds its roots in the swift development of novel materials. This work is committed to the pursuit of new, durable materials, achieved through a combination of combinatorial strategies and machine learning (ML). By bridging experimental results with algorithmic approaches, we unveil intricate correlations between process, structure, and properties. Our research focuses on Pt-Au alloy films, synthesized using magnetron co-sputtering, covering the entire composition range via multiple combinatorial libraries. High-throughput methods were utilized to create large multi-model datasets encompassing processing variables and material characteristics. Leveraging machine learning and these vast datasets, we pinpoint the parameter space required to create hard and conductive Pt-Au coatings. This work exemplifies the potential to generate large datasets in high-throughput manner tailored for machine learning models, yielding invaluable insights. Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

9:20 AM
Transforming Materials Science With Ontologies, ELN, and LIMS: Semantic Web Solutions for Digitalization and Data Excellence: *Markus Schilling*[1]; Bernd Bayerlein[1]; Sebastian Bruns[2]; Matthias Grönewald[2]; Philipp von Hartrott[3]; Jörg Waitelonis[4]; Henk Birkholz[5]; June Lau[6]; Birgit Skrotzki[1]; [1]Federal Ministry of Materials Research and Testing; [2]TU Darmstadt; [3]Fraunhofer-Institut für Werkstoffmechanik (IWM); [4]FIZ – Leibniz Institute for Information Infrastructure; [5]Leibniz-Institut für Werkstofforientierte Technologien (IWT); [6]National Institute of Standards and Technology (NIST)

In the pursuit of advancing materials development and digitalization within materials sciences, ensuring quality assurance, interoperability, and adherence to FAIR principles is significant. To address these challenges, Semantic Web Technologies (SWT) are employed for storage, processing, and contextualization of data, offering machine-understandable and human-readable knowledge representations crucial for data management.The presentation delves into the 'platform MaterialDigital' (PMD) project, aiming to create a virtual material data space. Key focuses include developing data structure agreements, enhancing expressivity and interoperability through ontologies, and connecting data to these ontologies. Besides ontology development, a practical example involves semantically linking test data to an ontology through an electronic laboratory notebook, facilitating digitally integrated experiments. The presentation also discusses the seamless integration of this data pipeline into a laboratory information management system (LIMS) and the potential benefits of integrating semantic conceptualization and knowledge graphs into LIMS, providing a glimpse of the emerging SWT integration in LIMS.

9:40 AM
Mechanical Properties Prediction of Functionally Graded Metallic Materials Through High-throughput Characterization and Machine Learning: *Christopher Bean*[1]; Dhruv Anjaria[1]; Rephayah Black[1]; Jackson Nie[1]; Marie Charpagne[1]; Jean-Charles Stinville[1]; [1]University of Illinois Urbana-Champaign

Advances in high-throughput material characterization, complemented by machine-learning techniques, have brought the longstanding goal of accelerating material discovery within grasp. With these advancements, materials of interest with favorable composition can be identified using computed approaches or combinatorial synthesis. However, mechanical characterization considerably hampers this material development cycle. High-fidelity macroscopic testing is time-consuming and remains the sole method for obtaining advanced mechanical properties. The present study presents an accelerated route for evaluating advanced mechanical properties by leveraging inverse analysis of large datasets of nanometer-scale plastic localization events collected through high-throughput, high-resolution digital image correlation correlated with electron backscattered diffraction measurement and analyzed by computer vision and graph neural network. We identified correlations between the characteristics of the plastic localization events (twinning and slip) and macroscopic properties. These correlations enabled a swift evaluation of advanced mechanical properties, including fatigue life, of stainless functionally graded materials.

10:00 AM Break

10:20 AM
High-throughput Characterization and Process-Structure-Property Optimization of LPBF SS316L: *Janith Wanni*[1]; Dan Thoma[1]; [1]Universiy of Wisconsin Madison

Understanding and predicting the processing-structure-property (PSP) relationships in additively manufactured metals is required for both design and qualification of components. This study uses high-throughput (HT) synthesis and characterization techniques to establish the PSP relationship in laser powder bed fusion (LPBF) of stainless steel 316L (SS316L). Dimensional analysis yielded dimensionless relationships that were used to identify a high-fidelity process parameter range capable of achieving a relative density of 99%. Samples were fabricated in a high-throughput manner for the design of experiments covering a large process parameter range. The HT characterization framework used advanced surface and imaging techniques to create a microstructural database. Finally, HT indentation is used to generate a mechanical property database. The PSP relationship between process parameters, grain size distribution, crystallographic texture, cellular subgrain structures, and the mechanical properties of LPBF SS316L has been established by integrating these databases, thus providing processing, microstructure, and property maps of LPBF SS316L.

10:40 AM
Accelerated Correlation of Microstructure-mechanical Property Relationships in Ni Based Superalloys: *Kevin Schmalbach*[1]; Toshio Osada[2]; Eric Hintsala[1]; Douglas Stauffer[1]; Takahito Ohmura[2]; [1]Bruker Nano; [2]National Institute for Materials Science

Rapid quantification of the mechanical properties of individual phases of multiphase materials can often be hindered by the slow process of aligning separately measured microstructure and mechanical property maps, especially for materials deformed at high temperatures or which undergo temperature-dependent phase transformations. Here, we discuss a novel system designed to streamline the process of correlating microstructure with mechanical properties using *in situ* nanoindentation testing. The system is a Bruker Hysitron PI89 Picoindenter system using a system of X, Y, rotation and tilt translations to directly target microstructures from EBSD with nanoindentation to assess site-specific material properties. This is coupled with a heating stage capable of attaining 1000 °C to directly assess the relationships between temperature, phase/orientation, and mechanical properties. We apply the new system to understand the phase- and temperature-specific mechanical properties in nickel-based superalloys.

11:00 AM
Crystal Plasticity Finite Element Method Accelerated by Efficient GPU-computing: *Fanglei Hu*[1]; Fan Chen[1]; Stephen Niezgoda[2]; Tianju Xue[3]; Jian Cao[1]; [1]Northwestern University; [2]The Ohio State University; [3]The Hong Kong University of Science and Technology

Crystal Plasticity Finite Element Method (CPFEM) has emerged as a powerful tool for establishing structure–property relationships. However, because of the need to handle the Newton iteration over the stress residual and calculate the Jacobian based on constitutive laws, CPFEM is computationally expensive. In this study, we propose the application of GPU to accelerate the three-dimensional CPFEM simulation, focusing on the mechanical response of metal polycrystals under different loading conditions while employing phenomenological constitutive models. The simulation code is developed based on our open-source code JAX-FEM, an affordable platform implemented with pure-Python while scalable to efficiently solve problems with moderate to large sizes (>100,000 degrees of freedom). Three simulation examples are performed for the cases of face-centered cubic (fcc) copper, body-centered cubic (bcc) tantalum, and bcc 316L steel. A thorough evaluation of the GPU implementation's acceleration performance in comparison to the fundamental CPU computations and Abaqus UMAT will be presented.

11:20 AM
Exploiting Metastable Phase Transformations to Achieve Low-cost High Room-temperature Strength Printable Al-alloys: *Benjamin Glaser*[1]; S. Mohadeseh Taheri-Mousavi[1]; [1]Carnegie Mellon University

Printable high-temperature aluminum alloys can be used in industries such as automotive, provided that their cost and sustainability metrics match the requirements of large-scale production. These metrics add additional constraints for the design of these alloys beyond printability and typical mechanical performance. We recently explored and experimentally validated a pathway to record high room-temperature strength by exploiting metastable phase development in an Al-Ni-Er-Zr-Y-Yb alloy. To adapt this design for high-demand industries, on data from CALPHAD-based ICME calculations we applied various unsupervised machine learning techniques and Bayesian optimization to efficiently explore high dimensional compositional and decipher influence of elements. We curated a complex objective function targeting high sustainability and low material cost, tailoring phase development to form at an opportune time. We discovered that changing the composition enables cost reductions of 20-30 percent and 10x the nanoprecipitation of metastable phase versus benchmark alloys, leading to 6x increase in room temperature strength.

11:40 AM
Eliminating Fatigue of Metals by Advanced Casting: *John Campbell*[1]; [1]University of Birmingham

Most of our engineering metals suffer from a dense population of preexisting cracks as proposed by Griffith. The cracks have been discovered to originate in the casting process, by the folding over of the oxide film on the surface of the liquid metal, top dry side to top dry side, so there is no bonding between the opposed surfaces. These unbonded double film cracks are formed mainly during the chaotic turbulence of pouring. The cracks, called 'bifilms', are often nm thin, but can be of large area. They are clear as 'quasi-cleavage' facets on fracture surfaces. They play a major role in fatigue, so that nearly all assumed fatigue failures in service applications are mainly preexisting bifilms, with a minor fatigue contribution which completes the failure. Castings techniques have now been developed to eliminate fatigue in components.

12:00 PM Mechnical Behavior Luncheon

Accelerating Discovery for Mechanical Behavior of Materials 2024 Mechanics of Novel Materials II

Tuesday AM
June 18, 2024

Room: Center Street Room D
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

8:30 AM Invited
Optimizing the Mechanical Performance of Interlocking Metamaterials for Extreme Environments: *Philip Noell*[1]; Brad Boyce[1]; Benjamin Young[1]; Ophelia Bolmin[1]; Nathan Brown[1]; [1]Sandia National Laboratories

Interlocking metasurfaces (ILMs), a newly developed class of joining technology, aim to overcome challenges inherent to conventional joining technologies and enable novel joint functionalities. ILMs are structural metamaterials that consist of autogenous latching features, similar to those observed cervid antlers. Because the mechanical performance ILMs is a strong function of unit cell topology and interaction, intelligent ILM design presents a significant challenge, particularly for complex environments. This work presents data-driven and machine-learning based design methodologies for ILMs that are widely applicable to metamaterial design. The mechanical performance of ILMs designed using both intuitive and data-driven techniques in a range of environments will also be discussed. Synergistic strengthening and frictional interactions between unit cells provide dampening of vibration, increased fracture toughness compared to the base material, and significant increases in strength compared to simple "snap-fit" joints. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

9:00 AM
Study on Mechanical Behavior of Serviced Material by Residual Stress Measurement: *Hariharan Sundaram*[1]; Raman Sankaranarayanan[2]; AlWaleed Alduaij[1]; [1]GE Kuwait Technology Center WLL; [2]National Institute of Technology Tiruchirappalli

Measuring the residual stress of a base material (hardware) in the as processed, heat treated and in the as serviced condition enables understanding of the mechanical property of material further. In this study two different material grades were used to evaluate the different effects on them after they were subjected to varying defects and processing. The stress relaxation behavior and relative stability were studied, after subjecting to heat treatment. Importance of x-ray elastic constants, high angle diffraction peaks and data interpretation were evaluated. Residual stress distribution along the depth direction and mapping of the measurements over the given size of the metal were performed. The equilibrium phase diagram and the corresponding temperature effect on the phases of interest were referred using CALPHAD. The mapping of stress zones on the hardware after processing and heat treatment, marking compressive stress conditions, finds application both in new make and repair of turbo-machinery components

9:20 AM
Computational Material Design and Performance Evaluation of Sintered SiALON/TiCN Tool Inserts: *Syed Sohail Akhtar*[1]; Muhammad Faizan[2]; Abba Abubakar[1]; [1]King Fahd University of Petroleum and Minerals; [2]Khalifa University

Novel SiAlON/TiCN composites are computationally designed and then synthesized intended for cutting tools followed by machining performance evaluation using the finite element method. The design and optimization of the volume fractions, the interfacial thermal resistance, and the sizes of the reinforcement particles are done using the effective medium theories and mean-field homogenization approaches, considering the impact of porosity on the effective thermomechanical properties of composites. The spark plasma sintering process is used to produce the designed composites followed by characterization. The stand-alone Al2O3 and designed SiALON/TiCN tools are then considered to quantitatively examine the thermomechanical behavior during the cutting simulation of superalloys. The simulated temperature distribution on the surfaces of the tool, workpiece, and chip are captured during cutting superalloys. It was found that the designed SiALON/TiCN tool resulted in lower temperature levels and improved mechanical response as compared to the commercially available Al2O3 tool.

9:40 AM
Coupling Effects of Grain Size and Dislocation Density on Stress-induced Martensitic Transformation of Nanocrystalline NiTi Alloys: A Molecular Dynamics Study: *Zhihao Zhao*[1]; [1]Tongji University

In this work, the coupling effects of grain size (GS: 5 nm–30 nm) and dislocation density (0–1 E16 m-2) on stress-induced martensitic transformation (MT) of nanocrystalline NiTi alloys were investigated quantitatively by molecular dynamics (MD) simulation. The forward transformation stress decreases with the increase of GS and dislocation density, which is attributed to the fact that the energy barrier of martensitic nucleation decreases with GS and dislocation density. The sensitivity of transformation stress to dislocation density increases with the increase of GS. We found that residual strain decreases with the GS but increases with dislocation density. The origins of residual strain are decoupled into (i) plastic deformation of grain boundaries and the disordered structure caused by dislocations, and (ii) the residual martensite. Plastic deformation is the main source of residual strain, except when residual martensite accumulates significantly (e.g., GS = 30 nm and dislocation density = 1 E16 m-2).

10:00 AM Break

10:20 AM

Key Aspects on Mechanical Properties for DED Deposited Functionally Graded Materials: *Jan Dzugan*[1]; Ying Li[1]; Daniel Melzer[1]; [1]Comtes Fht

Possibilities to create functionally graded multi-material components (FGM) by additive manufacturing (AM) techniques open new space for materials combinations and applications. This is a very new opportunity and challenge at the same time as AM makes formerly impossible things possible, however there some limits and some basis aspects that should be resolved and kept in mind when FGM components are going to be produced and designed. The work presented here is dealing with multi-material components deposition by laser powder blown Directed Energy Deposition process (LDED) for stainless steel 316 and Inconel 718. On these two relatively deposition friendly materials, basic aspects of materials deposition order, interface orientation and the interface quality (as deposited against machined) are demonstrated in relation to resulting mechanical properties. Also aspect of heat treatment is considered here as the considered materials are normally undergoing completely different heat treatment regimens due to their chemical composition.

10:40 AM

The Effect of Devulcanized (DR) and Non-devulcanized (NDR) Rubber in the Thermo-mechanical Behavior of Thermoplastic Polymer Blends: *Surafel Ashenafi Jemberu*[1]; [1]Ethiopian Quality Award Organization

This study explores the impact of devulcanized (DR) and non-devulcanized (NDR) rubber on the thermo-mechanical properties of thermoplastic polymer blends, utilizing polystyrene (PS) and thermoplastic polyurethane (TPU) as thermoplastic materials. The investigation involved compounding various rubber concentrations within the thermoplastic matrix. The influence of rubber concentration on the mechanical properties, thermal properties, and morphological behavior of thermoplastics was thoroughly examined.PS blends exhibited a decline in thermal degradation resistance upon DR/NDR introduction, while the glass transition temperature (Tg) of PS demonstrated a slight improvement. Tensile tests revealed a reduction in stiffness and stress at break upon DR/NDR addition, accompanied by an enhancement in elongation at break. In contrast, TPU/rubber blends exhibited a systematic decrease in both thermal degradation resistance and quasi-static tensile properties.

11:00 AM

Composition Dependence of the Thermoelastic Recovery in Additive Manufactured NiTi Shape Memory Alloys: *Arnab Chatterjee*[1]; Foster Feni[1]; Mique Gonzales[1]; Reginald Hamilton[1]; [1]Penn State

Shape Memory Alloys (SMAs) undergo a solid-state phase transformation under the application of stress or temperature enabling multifunctionality. The current work employs advanced thermal analysis to qualitatively and quantitatively investigate the extent to which SMAs exhibit thermoelastic transformations. SMA based Adaptive material system has matrix that begets a shape memory transformation within a host structural hierarchy through a reversible solid-state martensitic phase transformation (MT). In this work, we discuss thermoelastic reversibility of phase transformations in additively manufactured NiTi SMAs deposited with varying pre-blended ratio of elemental Ni and Ti powder feedstock. Standard differential scanning calorimetry (DSC) analysis is used for confirming the thermal-induced phase transformation occurs and establishing the temperature ranges for a material to exhibit shape memory effect (SME) or superelastic effect (SE). This work establishes an experimental and theoretical framework to evaluate the composition dependence of energetic variables to characterize underlying thermoelastic phase reversibility.

11:20 AM

Interpreting Strain Localizations in Ti-rich NiTi Alloys Fabricated Using Laser Directed Energy Deposition: *Mique Gonzales*[1]; Foster Feni[1]; Arnab Chatterjee[1]; Reginald Hamilton[1]; [1]The Pennsylvania State University

NiTi shape memory alloys (SMAs) are fabricated using the laser directed energy deposition (LDED) additive manufacturing (AM) technique using pre-blended elemental Ni and Ti powder. A Ti-rich composition is used which is reported to a significantly lesser extent than its near-equiatomic and Ni-rich counterparts. We report the mechanical strength properties and characterize the behavior resulting from the stress-assisted shape memory response. Due to the layer-/pass-wise build up and accompanying spatially varying melt/solidification histories, SMAs fabricated using AM techniques inherently exhibit microstructural features distinct from conventional processing. For benchmarking, we contrast the thermo-mechanical characterization of conventionally processed NiTi alloys whose compositions are equivalent to the AM NiTi SMAs. This work augments macro-scale mechanical experimentation with in-situ digital image correlation (DIC) analysis to study strain localizations. We use DIC to expound on structure-property relationships by interpreting the underlying MT pathway. Advancements for correlating the LDED structural hierarchy to the properties/behavior are highlighted.

11:40 AM

Thermal Stability and Wear Behaviour of TiCN-Co-Si3N4-Cr3C2 Based Cermets Modified by B4C: *Balasivanandha Prabu Shanmugavel*[1]; Anannya Murugan[1]; Jisha Raja[1]; [1]Anna University

This study evaluates the role of B4C -modified TiCN- Si3N4-Cr3C2-Co cermet for use in cutting tool applications. Three cermet compositions containing B4C at 5, 10, and 15 wt.% were developed using Vacuum Hot Pressing. Pin-on-disk wear testing was performed on the prepared cermet using EN31 steel as the disc material. The sliding velocities used for the wear testing were 0.31 m/s, 0.94 m/s, and 1.57 m/s, with a constant load of 30N. During wear testing, the cermet composition 60TiCN-15Si3N4-5Cr3C2-5Co-15 B4C (all in wt%) demonstrated the least mass loss. By conducting annealing studies on the prepared cermet at various temperatures, such as 600, 800, and 1000 ˚C for a constant time with soaking time of 4 hours, the thermal stability of the cermet was evaluated. Up to 800 ˚C, the prepared cermet exhibited excellent thermal stability. The composition 65TiCN-15Si3N4-5Cr3C2-5Co-10B4C displayed greater thermal stability than the other two cermet compositions.

12:00 PM Mechanical Behavior Luncheon

Symposium on Digital & Robotic Forming 2024 AI/ ML in Forming

Tuesday AM
June 18, 2024

Room: Center Street Room B&C
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

10:20 AM Invited
Toward Autonomous Research and Co-development of Alloys and Their Manufacturing: *Aaron Stebner*[1]; [1]Georgia Institute of Technology

Many different aspects of computational, materials, mechanical, and industrial science and engineering must converge to enable artificial intelligence to work with humans to perform research and development of new alloys and their manufacturing in ways we cannot achieve with human-only approaches. In this presentation, recent efforts in several different thrusts will be presented including high throughput experimentation, active machine learning across multiple design spaces, and machine learning process-structure-property modeling. Their connections will be shown to enable the design and construction of the AI Manufacturing Pilot Facility, to include a test bed that enables AI metamorphic manufacturing research and development.

10:50 AM
Application of Scientific Machine Learning for Robotic Forming: *Yeping Hu*[1]; Bo Lei[1]; Victor Castillo[1]; [1]Lawrence Livermore National Laboratory

We will discuss the development of fast-running reduced-order models (ROMs) based on thermomechanical simulations and graph neural networks (GNNs). We use Serac, a high-order nonlinear thermomechanical simulation code, to investigate robot/metal interaction under a variety of process conditions. These simulations are used to train GNNs, specifically MeshGraph networks, to replicate the results in a fraction of the time. Although the simulations and GNN training require large high-performance computing platforms, the ROMs can run on the edge to inform real-time path planning. We have used MeshGraphs to successfully solve complex fluid dynamics problems. Elastoplastic systems present additional complexities that will be discussed.

11:10 AM
Metamorphic Manufacturing (MM): Some Related Efforts Since the 2019 TMS Accelerator Study Report on MM: *George Spanos*[1]; Glenn Daehn[2]; [1]TMS; [2]Ohio State University

Since the 2019 TMS science and technology accelerator study on Metamorphic Manufacturing (MM), there have been many related efforts that can help accelerate the development and adoption of this potentially revolutionary manufacturing technology. After providing some brief background on the 2019 TMS MM accelerator study, this talk will briefly describe a few of these efforts to which TMS is connected, and discuss how they are related to MM. These activities include: (1) this TMS Specialty Congress 2024 event on Digital & Robotic Forming, (2) a new TMS accelerator study undertaken on behalf of the Office of Naval Research on A Revolution in Digital Manufacturing: Integration of Manufacturing Machines, Robotics, Artificial Intelligence and Forming Technologies, and (3) a relatively new National Science Foundation (NSF) Engineering Research Center (ERC) on Hybrid Autonomous Manufacturing, Moving from Evolution to Revolution (HAMMER), which is led by The Ohio State University.

11:30 AM
Metamorphic Manufacturing: a Tutorial Review: *Glenn Daehn*[1]; [1]Ohio State University

This presentation is a broad overview of metamorphic manufacturing. Dozens of creative people have been involved in this evolving conversation. A core question from the beginning is could we develop robotic systems that act like blacksmiths, but with more power, precision, reproducibility and a computational power or intelligence. This leads us to ask if we can develop autonomous systems that leverage artificial intelligence to demonstrate artificial skills? Building off the 2019 TMS study, can we better define and optimize the core elements of the metamorphic manufacturing (STARC) system of Sensors, Thermal control, Actuators, Robotics and Computation? What value could this bring, and in what applications? Further evolution to Hybrid Autonomous Manufacturing will be shown. We also see this as a physical manifestation of what is really a cyber system. This thinking leads us to new ways of assuring quality – through qualifying models, instead of parts.

Symposium on Digital & Robotic Forming 2024 Incremental Forming

Tuesday AM
June 18, 2024

Room: Center Street Room B&C
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

8:30 AM Invited
Metallurgy of Incremental Forming Processes: A Spin Forming Review: Melissa Thrun[1]; Alexandra Glover[2]; Matthew Zappulla[1]; Kayla Molnar[1]; *Paul Gibbs*[1]; [1]Los Alamos National Laboratory; [2]Michigan Technical University

Spin forming is a manufacturing technique for creating axi-symmetric geometries by iteratively shaping a metal blank to a mandrel. The success of spin forming methods relies on localized deformation initiated by one or more moving rollers: the degree and intensity of this localization are a function of process parameters and affect the macroscopic forming response. The use of CNC and hydraulically powered spinning machines allows for the forming of higher strength alloys and thicker section blanks at room temperature. Localized deformation challenges simplified assumptions about stress state and classic workability predictions that are traditionally used to guide process development. Here, we will review and consider the process parameter space for sub-techniques of spinning: namely spin, shear, and flow forming. Emphasis is placed on highlighting how microstructure and properties evolve, and tools for advancing process development through both analytical and computational techniques.

9:00 AM
Differences in Material Behavior and Limitations during Metal Spinning of 304 SS and 6061 Al: *Kayla Molnar*[1]; Melissa Thrun[1]; Matthew Zappulla[1]; Paul Gibbs[1]; [1]Los Alamos National Laboratory

Modern metal spinning is a CNC-controlled deformation process that is advantageous for its balance of process robustness and agility in comparison to traditional wrought processes. Additionally, metal spinning utilizes a very localized deformation area which poses advantages for traditionally difficult-to-form metals. In this processing study, physical challenges of spinning both 6061 aluminum and 304 stainless steel to the same geometry were explored. Ultimately, the process was not material agnostic; however, successful parts were made with both alloys. Differences arose in general deformation behavior, failure modes, attack angle response, starting stock dimensional changes, and edge preparation sensitivities

9:20 AM
Utilizing Strain Rate Jump Testing to Predict Flow Formability of Al Alloys Sensitive to Portevin-Le Chatelier Instabilities: *Mary Cecilia Mulvaney*[1]; David Stegall[1]; Stephen Hales[1]; James Fitz-Gerald[2]; Sean Agnew[2]; [1]NASA; [2]University of Virginia

Predicting the flow formability of Al alloys is challenging due to the incremental deformation, complex loading path, and wide range of strain rates characteristic of the process. State-of-the-art research efforts have primarily focused on formability metrics derived from ambient temperature, constant strain rate uniaxial tensile testing. However, Al alloys in formable tempers tend to exhibit serrated Portevin-Le Chatelier (PLC) flow. The appearance of PLC instabilities implies a negative strain rate sensitivity, loss of tensile area reduction capacity, and decreased formability. Elevated temperature and strain rate jump tensile tests of relevant Al alloys were conducted to investigate the effects of rapid changes in strain rate (analogous to a forming increment by a passing roller) on common formability metrics. Emphasis was placed on the character/extent of PLC instabilities using digital image correlation strain measurements. The outcome of this work highlights the possibility of predicting flow formability using strain rate jump testing.

9:40 AM
Integrated English Wheeling System: *Derick Suarez*[1]; Fan Chen[1]; Putong Kang[1]; Ben Forbes[1]; Margaret Gao[1]; Kevin Benton[2]; Nicholas Dewberry[2]; Balakrishna Gokaraju[2]; Kornel Ehmann[1]; Jian Cao[1]; [1]Northwestern University; [2]North Carolina Agricultural and Technical State University

The English wheel is a traditional metalworking tool allowing for flexible forming of compound curved sheet metal panels. Traditionally, the use of this process has been tied to a skilled craftsman/operator. With the advent of robot forming, the process has been reexamined. We present a framework for an integrated English wheeling system that leverages robots for forming, metrology for shape tracking, integrated sensors for real-time forming force control, computational modeling for toolpath generation and virtual reality (VR) integration, allowing the modern craftsman to seamlessly track the process. Fundamental mechanics of the English wheeling process are revealed through the integrated system. Representative parts are made through the integrated system to show its applicability.

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) AI Non-Destructive Evaluation

Tuesday PM
June 18, 2024

Room: Hope Ballroom C
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

1:40 PM Invited
Virtual Inspection of Advanced Manufacturing via Process-scale Digital Twins: *Brian Giera*[1]; [1]Lawrence Livermore National Laboratory

Inspection presents the largest bottleneck to advanced manufacturing (AM), costing as much as 4x fabrication itself. On top of this, there are no known methods to connect machine instructions to final part performance. Our work alleviated this issue via process- and part-scale digital twins: a framework that combines in situ process monitoring, data-driven prediction enhancement, virtual inspection, and virtual reality (VR) visualization. If successful, we can cut down the time and cost of inspection and, hence, of the overall production cycle. While we are using the Direct Ink Write AM as the initial demonstrator, the broader goal of is to instantiate a digital twin framework that applies to other AM processes and conventional manufacturing. This talk discusses our path towards a prototypical virtual environment that fundamentally changes the way multiple users (e.g. at production and design agencies) interact with all the data associated with a process and a part.

2:00 PM
Improved Deep Learning Image Classification of Rare Material Defects in Non-destructive-testing Processes by Utilizing Data Imbalance Methods and Synthetic Data: *Yann Schöbel*[1]; Martin Mueller[2]; [1]MTU Aero Engines AG; [2]Materials Engineering Center Saarland

Data Imbalance is a common problem in real world Machine-Learning datasets from industrial processes. Even more in Non-Destructive-Testing (NDT) applications, where some types of relevant material defects occur rarely. Therefore, effective measures against Data Imbalance are required to apply Deep Learning in this field. In this work, we evaluate the influence of increasing Data Imbalance on an Image Classification dataset of material defects sampled from macro etch testing on Nickel-Superalloy turbine disks. Furthermore, we investigate how conventional Data Imbalance approaches on the one hand and synthetic generated images on the other hand can reduce the influence of imbalance. We also compare human and machine perception to evaluate if such approaches can profit from manual filtering of the synthetic samples. Finally, we draw the conclusion if synthetic data generation is a valuable tool for highly imbalanced datasets in NDT applications and if it can outperform classic Data Imbalance countermeasures.

2:20 PM
High-throughput Microstructural-based Remnant Life Assessment of High-temperature Steels: *Johan Westraadt*[1]; Lindsay Westraadt[1]; [1]Nelson Mandela University

Small-punch creep (SPC) testing is currently used to evaluate the creep-rupture properties of steels used in the petrochemical industry. This study explores processing-microstructure-property relationships in service-exposed C-Mn steels using machine learning (ML). These reduced order models can be used to rank the different microstructural features in terms of their importance on the SPC-test and potentially be used to prioritize/reduce SPC testing requirements. A dataset consisting of 120 steel microstructures and their associated mechanical properties were collected. Large area mapping using secondary electron imaging of the etched surfaces yielded high-resolution data of the ferrite/pearlite phases in the C-Mn steels. These images were segmented and quantified using various traditional and deep-learning feature extraction methods, which were then used as inputs for training regression models using different ML techniques. The use of microstructure-property databases for microstructural-based remnant life assessments of high-temperature components will also be discussed.

2:40 PM
Realtime In-process Monitoring of Porosity via Convolutional Neural Networks During Additive Manufacturing and Laser Welding: Bin Zhang[1]; *Yung Shin*[1]; [1]Purdue University

This work describes in-process porosity monitoring for additive manufacturing and laser welding processes. A high-speed digital camera was mounted coaxially to the laser beam for in-process sensing of melt-pool data, and deep learning convolutional neural network models were designed to learn melt-pool features to predict the porosity attributes in specimens built by additive manufacturing and laser welding. The convolutional neural network (CNN) models with a compact architecture achieved a classification accuracy of 91.2% for porosity occurrence detection in the direct laser deposition of sponge Titanium powders and presented the predictive capacity for micropores below 100 µm. For local volume porosity prediction, the model also achieved a root mean square error of 1.32% and exhibited high fidelity for both high porosity and low porosity specimens. In laser welding of 6061 Aluminum alloy, the CNN-based monitoring model achieved a classification accuracy of 96.1% for porosity occurrence detection.

3:00 PM Networking Break

3:50 PM
PV-VISION: A Deep Learning Based Package for Automated Solar Module Inspection: *Xin Chen*[1]; Anubhav Jain[1]; [1]Lawrence Berkeley National Laboratory

Solar photovoltaic (PV) modules are susceptible to manufacturing defects, mishandling problems or extreme weather events that can limit energy production or cause early device failure. Trained professionals use electroluminescence (EL) images to identify defects in modules, however, field surveys or inline image acquisition can generate millions of EL images, which are infeasible to analyze by rote inspection. We developed an open-source computer vision package PV-VISION to automatically process the EL images using deep learning models, covering automatic image preprocessing, cell defect detection and crack feature extraction. We demonstrated the functions of PV-VISION on two tasks: investigating fire impacts on solar farms by inspecting 2.4 million cells and quantifying crack growth in solar modules under mechanical aging tests. We anticipate that PV-VISION can offer a supportive platform for researchers in the solar field, facilitating a more efficient and data-driven approach to EL image analysis.

4:10 PM
Generative Super-resolution for Inexpensive In-situ Layerwise Optical Imaging: *Odinakachukwu Ogoke*[1]; Sumesh Suresh[1]; Jesse Adamczyk[2]; Dan Bolintineanu[2]; Anthony Garland[2]; Michael Heiden[2]; Amir Barati Farimani[1]; [1]Carnegie Mellon University; [2]Sandia National Laboratories

The stochastic formation of defects during Laser Powder Bed Fusion (L-PBF) negatively impacts its adoption for high-precision use cases. Optical monitoring techniques can be used to identify defects based on layer-wise imaging, but these methods can be difficult to scale to high resolutions due to cost and memory constraints. Therefore, we implement generative deep learning models to link low-cost, low-resolution images of the build plate to detailed high-resolution images of the build plate, enabling cost-efficient process monitoring. To do so, a conditional probabilistic diffusion model is trained to produce realistic high-resolution images of the build plate from low-resolution webcam images, recovering the distribution of small-scale features and surface roughness. We evaluate the performance of the model by analyzing the statistical properties of the generated images, in addition to the similarity between the image anomalies detected by the high-resolution model to the generated samples.

4:30 PM
Classification of 2D Diffractograms Into "Spotty" and "Continuous" Patterns Using Deep Neural Networks Trained By ab-Initio Simulations: *Mohommad Redad Mehdi*[1]; Weiqi Yue[1]; Pawan Tripathi[1]; Matthew Willard[1]; Roger French[1]; Frank Ernst[1]; [1]Case Western Reserve University

The advances in current and next-generation synchrotrons for X-ray diffractometry has opened up a world of challenging data analysis opportunities. The short X-ray wavelength that can be achieved in synchrotrons can provide information about the atomistic structure and microstructure of the material to greater penetration depths and with higher spatial and temporal resolution. Since most of the detectors used in synchrotrons are area detectors, thus diffractograms and video sequences (movies) are 2D, we can use the tremendous power of deep neural networks (DNN) to extract detailed structural information from these diffractograms. We present a novel approach to classify sequences of diffractograms recorded during in-situ spatio-temporal investigations. Our approach uses deep learning, based on neural networks that are trained using ab-initio simulations of 2D diffractograms. These DNNs are capable of learning significant features from the simulated diffractograms, which allows them to classify the diffractograms as either "spotty" or "continuous."

4:50 PM
Federated Learning Approaches: Data-decentralized Analysis on Synchrotron X-ray Diffraction Data: *Weiqi Yue*[1]; Pawan Tripathi[1]; Roger French[1]; Vipin Chaudhary[1]; Donald Brown[1]; Erman Ayday[1]; [1]Case Western Reserve University

The remarkable growth and success of deep learning techniques have led to its widespread application across various scientific domains, including material science. However traditional centralized methods often raise privacy and security risks when handling sensitive materials, hindering data sharing between research facilities. Furthermore, not all institutions possess sufficient high-quality data for robust model training. To overcome these challenges, we introduce various federated learning algorithms, enabling collaborative model training among multiple clients without sharing raw data. In this study, we use data sets for four samples of Ti-6Al-4V generated by synchrotron X-ray diffraction experiments as our client data sets. We employ a convolutional neural network as a shared model to predict the volume-fraction of the beta phase within each diffraction pattern. Our experimental results show that federated learning models maintain a high degree of accuracy compared with the traditional centralized model.

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) Deep Learning for Materials Discovery

Tuesday PM
June 18, 2024

Room: Hope Ballroom B
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

1:40 PM Invited
Physics-constrained, Inverse Design of High-temperature, High-strength, Printable Al Alloys Using Machine Learning Methods: *S. Mohadeseh Taheri-Mousavi*[1]; [1]Carnegie Mellon University

Aluminum alloys that exhibit high strength and creep resistance at high temperatures can be our next-generation fan blades of jet engines and pistons of combustion engines. However, additive manufacturing (AM) or even welding of these alloys is traditionally challenging due to the presence of hot cracking. We demonstrate a physics-constrained, inverse design framework with data generated from integrated computational materials engineering (ICME) techniques to explore the compositional space of Al-Zr-Er-Y-Yb-Ni, and identify an optimal alloy composition achieving maximum predicted strength at a temperature of 250°C. Using only 40 sampling data with our most efficient machine learning algorithm (neural network), we predict a microstructure with 3.5X higher stability of nanoscale hardening phases than a state-of-the-art printable Al-alloy. Thetensile tests at different aging hours validated the predictions. The samples have non-textured equiaxed grains along the built direction and exhibit 400 MPa strength comparable to wrought Al7075.

2:10 PM
Unraveling the Mechanisms of Stability in CoMoFeNiCu High Entropy Alloys via Physically Interpretable Graph Neural Networks: Miguel Tenorio[1]; *James Chapman*[1]; [1]Boston University

High entropy alloys (HEA) have become a topic of significant interest due to their combinatorial nature. In particular, CoMoFeNiCu alloys have been studied extensively due to its reported superiority as a catalyst for ammonia decomposition. However, such reactions take place at elevated temperatures, leading to phase separation of the HEA. Here, we aim to understand the structural features of these HEA that are responsible for stability within the catalyst operational temperature range. To this end, we combine density functional theory (DFT) calculations with physics-inspired graph neural networks (GNN), to predict HEA stability. We show that by learning the mixing free energy with our GNN framework we can rank geometric HEA descriptors based on their importance towards stability. This work showcases the power of combining DFT with interpretable GNN to uncover design rules for complex materials with targeted properties, bridging the gap between simulations and experiments.

2:30 PM
Machine Learning Customized Novel Metals for Energy-efficient 4D Printing: *Chaolin Tan*[1]; [1]Singapore Institute of Manufacturing Technology(SIMTech), A*STAR

Existing commercial powders for laser additive manufacturing (LAM) were designed for traditional manufacturing methods requiring post heat treatments (PHT). LAM's unique cyclic thermal history induces intrinsic heat treatment (IHT) on materials during deposition, which offers an opportunity to develop LAM-customized new materials. This work customised a novel Fe-Ni-Ti-Al maraging steel assisted by machine learning to leverage the IHT effect for in-situ forming massive precipitates during LAM without PHT. Fast precipitation kinetics of steel, tailored intermittent deposition strategy, and the IHT effect facilitate the in-situ Ni3Ti precipitation in the martensitic matrix via heterogeneous nucleation on high-density dislocations. The as-built steel achieves a tensile strength of 1538 MPa and a uniform elongation of 8.1%, which is superior to a wide range of as-LAM-processed high-strength steel. This work highlights in-situ 4D printing via the synchronous integration of time-dependent precipitation hardening with 3D geometry shaping, which shows high energy efficiency and sustainability.

2:50 PM
High-throughput In-silico Multi-objective Materials Screening for Accelerated Polymer Design and Discovery: *Joydeep Munshi*[1]; Ghanshyam Pilania[1]; Jonathan Doll[1]; Dung-Yi (Jackson) Wu[1]; Paul Smigelski[1]; Vipul Gupta[1]; Kareem Aggour[1]; [1]GE Research

The vast chemical universe of polymer materials poses a significant challenge to design and synthesis of novel candidates. Polymer informatics strives to address the daunting challenge of materials discovery, utilizing state-of-the-art statistical and AI/ML methods. In this presentation, we discuss a high-throughput informatics framework to discover potential candidate polymers with enhanced material properties. We designed a generic formalism of material discovery for a variety of industry-wide applications. A deep learning model for effective chemical fingerprinting from one-dimensional chemical representations, such as SMILES, is used and neural network models are trained to predict material properties. The framework is extended to a multi-objective optimization paradigm, using evolutionary algorithms to attain a Pareto frontier for a variety of properties desired for aerospace components. Utilizing such a high-throughput framework, in a close coupling with domain expert feedback, extends recent efforts to effectively explore the vast polymer space towards accelerating industry-relevant materials design and discovery.

3:10 PM Networking Break

4:00 PM
Predicting Interfacial Solute Segregation in Nanocrystalline Alloys Using Advanced Atomic Descriptors and Machine Learning Schemes: Jacob Tavenner[1]; Ankit Gupta[2]; *Garritt Tucker*[2]; [1]KBR, Inc, Intelligent Systems Division, NASA Ames Research Center; [2]Department of Physics, Baylor University

It is well known that alloying elements can drastically improve the stability and strength of interfaces (i.e., grain boundaries (GBs)) in nanocrystalline materials. However, the underlying relationships between interfacial atomic environments and their segregation tendencies are complex and not fully understood. In this study, the interfacial solute segregation behavior of P in nanocrystalline Ni alloys is investigated. It is shown that the solute segregation behavior of GBs, especially in nanocrystalline structures, cannot be properly captured with average measures such as GB misorientation and energy. A set of higher-order atomic descriptors is leveraged to efficiently quantify disordered atomic environments. Machine learning techniques are utilized in concert with these atomic descriptors to predict segregation tendencies and elucidate complex relationships relating segregation potential to changes in the local Gaussian density. This effort elucidates the role that artificial intelligence can potentially play in accelerating materials discovery such as designing alloys with exceptional thermo-mechanical stability.

4:20 PM
AI-driven Topology Optimization of Photonic Structures With Manufacturing Constraints: *Alok Sutradhar*[1]; Fariha Haque[1]; [1]The Ohio State University

Machine learning and AI have seen tremendous adoption in design and manufacturing in recent years. We aim to utilize machine learning and AI to obtain optimum designs for multi-functional photonic structures governed by electromagnetics coupled with manufacturing constraints. Machine learning-generated designs enable a new optimization approach that is less prone to falling in local minima than gradient-based optimization. Inverse design tools and topology optimization often yield complex structures in the electromagnetic domain that can pose a learning challenge for the neural network. To remedy this issue, we demonstrate an efficient optimization technique that reduces the training samples' complexity and enables higher-quality predictions from the neural network. Additionally, by training a neural network over a large pool of multi-physics parameters and manufacturing constraints, we can demonstrate a rapid design exploration environment for complex designs that would otherwise be computationally expensive to carry out using traditional gradient optimization and design tools.

4:40 PM
Designing a Castable Aluminum-based Multicomponent Concentrated Alloy using a Hybrid Approach of CALPHAD Modeling and Machine Learning: Jianyue Zhang[1]; Deepak Soman[1]; Jiashi Miao[2]; Sushil Mishra[2]; *Alan Luo*[1]; [1]Ohio State University; [2]Indian Institute of Technology Bombay

Lightweight multicomponent concentrated alloys are of great interest due to their potential mechanical and physical properties. It is challenging to design such alloys to achieve a synergistic combination of density, strength, ductility and manufacturability, due to the large composition space and complex property requirements. In this presentation, a hybrid approach is developed to design lightweight multicomponent concentrated alloys with improved ductility and castability. This novel alloy design approach combines CALPHAD-based modeling with machine learning (ML) to select suitable compositions. A high-throughput Scheil solidification calculation was set up with CALPHAD to explore solidification path of aluminum-based compositions with favorable phases. The results were used as input for a ML algorithm to predict ductility (tensile elongation) with corresponding uncertainty. New alloy compositions with good castability were then selected for casting trials and mechanical property testing. This hybrid approach of CALPHAD modeling and machine learning shows promise in designing new materials.

5:00 PM

Electronic Structure Prediction of Multi-million Atom Systems Through Uncertainty Quantification Enabled Transfer Learning: *Shashank Pathrudkar*[1]; Ponkrshnan Thiagarajan[1]; Shivang Agarwal[1]; Amartya Banerjee[1]; Susanta Ghosh[1]; [1]Shashank Pathrudkar

The ground state electron density obtainable using Kohn-Sham Density Functional Theory (KS-DFT) simulations - contains a wealth of material information, making its prediction via machine learning (ML) models attractive. However, the computational expense of KS-DFT scales cubically with system size which tends to stymie training data generation, making it difficult to develop accurate ML models that are applicable across many scales and system configurations. Here, we address this fundamental challenge by employing transfer learning to leverage the multi-scale nature of the data. Our ML models employ descriptors involving scalar products, comprehensively sample system configurations through thermalization, and quantify uncertainty in electron density predictions using Bayesian neural networks. We show that our models incur significantly lower data generation costs while allowing confident - and when verifiable, accurate - predictions for a wide variety of bulk systems well beyond training, including systems with defects, different alloy compositions, and at unprecedented, multi-million-atom scales.

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) Machine Learning - Processing I

Tuesday PM
June 18, 2024

Room: Hope Ballroom A
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

1:40 PM Invited

Rethinking Materials Simulations: Blending Direct Numerical Simulations With Neural Operators: *Vivek Oommen*[1]; Khemraj Shukla[1]; Saaketh Desai[2]; Remi Dingreville[2]; George Karniadakis[1]; [1]Brown University; [2]Sandia National Laboratories

Direct numerical simulations (DNS) are accurate but computationally expensive for predicting materials evolution across timescales, due to the nature of spatiotemporal interactions across scales, and the need to reach long-time integration. We develop a new method that blends numerical solvers with neural operators to accelerate such simulations. Specifically, we integrate a community numerical solver (MEMPHIS) with a U-Net enhanced by temporal conditioning mechanism that enables accurate extrapolation and efficient time-to-solution predictions of the dynamics. We demonstrate the effectiveness of this framework on simulations of microstructure evolution during physical vapor deposition modeled via the phase-field method. These simulations exhibit high spatial gradients due to the co-evolution of different material phases with simultaneous slow and fast materials dynamics. We establish accurate extrapolation of the coupled solver with 16.5x speed-up compared to DNS. This methodology is generalizable to a broad range of evolutionary models, from solid mechanics, to fluid dynamics, climate, and more.

2:10 PM

Deep Material Network Trained With Local Field Information: Predictions of Homogenized and Local Field Distribution: *Dongil Shin*[1]; Remi Dingreville[1]; [1]Sandia National Laboratories

In recent years, the Deep Material Network (DMN) has emerged as a powerful method for developing reduced order models in composite modeling. Unlike other machine-learning approaches for reduced order models, the DMN focuses on learning microstructure interactions rather than material behavior under specific loading paths. This unique feature allows for extrapolating to other constitutive behaviors without the need for retraining. Traditionally, DMNs have been trained using linear homogenized material properties, making use of low-cost direct numerical simulation data. However, a critical question arises: Why restrict ourselves to homogenized material properties when we have access to a wealth of information gathered during direct numerical simulations? In this study, we have expanded the capabilities of the DMN by training it with homogenized and local field information. We have updated the DMN architecture to incorporate linear local information during training, and our results demonstrate how this novel approach enhances the performance of DMNs.

2:30 PM

Intelligent Data Sampling for Autonomous Parameterization: A Gaussian-Process-Ensemble Approach: *Erick Braham*[1]; Marshall Johnson[2]; Andrew Fassler[1]; Surya Kalidindi[2]; James Hardin[3]; [1]UES / Air Force Research Laboratory; [2]Georgia Institute of Technology; [3]Air Force Research Laboratory

Can machines efficiently build an “intuition” that will guide autonomous decision making? Leveraging a knowledge base that provides necessary relevant information such as historical data, expert heuristics, simulation data, or exploratory presampling, we hypothesize automated decision making can be informed enough to adapt to a diversity of challenges. Building this knowledge can often be prohibitively expensive or require expert human knowledge that may be impossible to obtain or translate to machine intelligence. Our approach is to develop an automated rapid exploration protocol using an ensemble of gaussian-process models to target specific desirable information while efficiently building a high-value dataset. We demonstrate this method by building a knowledge base for an automated parameterization protocol for direct ink write 3D printing of various freestanding structures. Ideally, automated training of machine intuition will enable more agile manufacturing, high-throughput screening of materials and geometries, and more efficient collaboration across systems.

2:50 PM

Bayesian SegNet for Semantic Segmentation With Improved Interpretation of Microstructural Evolution During Irradiation of Materials: *Marjolein Oostrom*[1]; Karl Pazdernik[1]; Alexander Hagen[1]; Nicole Lahaye[1]; [1]Pacific Northwest National Laboratory

Understanding the relationship between the evolution of microstructures of irradiated pellets and tritium release could improve predictions of tritium release and production. Given expert-labeled segmented images of irradiated and unirradiated pellets, we trained Deep Convolutional Neural Networks to segment these images into defects, backgrounds, and boundaries. Qualitative microstructural information was obtained from these segmented images to facilitate the comparison of unirradiated and irradiated pellets. We tested modifications to improve the sensitivity of the model, including incorporating meta-data into the model and utilizing uncertainty quantification. The predicted segmentation was similar to the expert-labeled segmentation for microstructural qualification, including pixel proportion, defect area, defect density, and the proportion of defects on boundaries. Overall, the high performance metrics for the best models for both irradiated and unirradiated images shows that utilizing neural network models is a viable alternative to expert-labeled images.

3:10 PM Networking Break

4:00 PM
Unsupervised Physics-informed Disentanglement of Multimodal Materials Data: Nathaniel Trask[1]; Carianne Martinez[2]; Troy Shilt[2]; *Elise Walker*[2]; Kookjin Lee[3]; Anthony Garland[2]; David Adams[2]; John Curry[2]; Michael Dugger[2]; Steven Larson[2]; Brad Boyce[2]; [1]University of Pennsylvania; [2]Sandia National Laboratories; [3]Arizona State University

Materials are often characterized by a variety of experimental modalities, e.g. process parameters, material properties, microstructure, chemistries, and performance. Typically, subject matter experts are tasked with making sense of this onslaught of disparate data. In contrast, representation learning algorithms may provide an alternate way of parsing these large, multimodal datasets. We thereby present physics-informed multimodal autoencoders (PIMA): a variational inference framework for discovering shared information in multimodal datasets. This framework also enables the incorporation of physics-based models to constrain the model and aid in disentanglement. Due to its variational construction, PIMA admits closed-form uncertainty quantification computations for cross-modal predictions. Tested against three multimodal materials datasets, we demonstrate that PIMA can discover fingerprints in high-dimensional datasets and perform informative cross-modal inference.

4:20 PM
Training Requirements of a Deep Learning Network With Physics-based Regularization Functions Enforcing Stress Equilibrium: Ashley Lenau[1]; Dennis Dimmiduk[2]; *Stephen Niezgoda*[1]; [1]Ohio State University; [2]BlueQuartz Software LLC

Incorporating scientific knowledge into deep learning (DL) models is becoming common practice due to the likely increase in accuracy of a materials-based simulations. Altering the loss function or adding a physics-based regularization term to reflect the physics of the material system informs the network about the physical boundaries the simulated material should obey. The training and tuning process of a DL network greatly affects the quality of the model, but how this process differs when using physics-based loss functions or regularization terms is not commonly discussed. In this presentation, several physics-based regularization methods are implemented to enforce stress equilibrium on a network predicting the stress fields of a high elastic contrast composite. Hyperparameters, like learning rate and loss weight, were tuned separately for each method. The amount of time to train each implementation is discussed, as well as the model performance when the training dataset size is reduced.

4:40 PM
A Manufacturing Technology Roadmap for AI-enhanced Multimodal Sensing of Materials and Processes for Complete Product Lifecycle Performance: *John Lewandowski*[1]; Nick Barendt[1]; Robert Gao[1]; Ken Loparo[1]; [1]Case Western Reserve University

Digital manufacturing technologies are critical to accelerating product development and commercialization, enhancing sustainability, and optimizing manufacturing processes, enabling new products and revenue streams, and boosting economic productivity. Advancements in distributed sensing, imaging, closed-loop controls, and Edge Computing are enabling artificial intelligence/machine learning (AI/ML) to integrate with physical domain knowledge for to integrate multiscale, multimodal data streams over entire product lifecycles. This talk provides an overview of a National Institute of Standards and Technology (NIST) funded manufacturing technology roadmap on developing a comprehensive approach to future manufacturing and advanced materials by integrating sensing, data analytics, and AI/ML tools with traditional process domain knowledge over entire product lifecycles. This integrative approach has the potential to achieve shorter time-to-markets; improved sustainability with lower environmental impact; greater resource efficiency; higher product yield; longer product lifespans; higher product quality; optimized manufacturing processes; and better supply chain visibility of product data.

5:00 PM
A Surrogate-assisted Uncertainty Quantification and Sensitivity Analysis of a Ni-base Superalloy Hot Isostatic Pressing Finite Element Mode: *Alon Mazor*[1]; Swapnil Patil[1]; Ryan Jacobs[1]; Vipul Gupta[1]; Timothy Hanlon[1]; [1]GE Aerospace Research

Modeling of hot isostatic pressing (HIP) holds significant potential for enhancing performance while reducing costs in industries such as aviation, power generation, and additive manufacturing. The ability to virtually optimize HIP parameters for achieving complete densification in components of varying sizes and intricate geometries is crucial for expediting process development. However, the success of this modeling approach may depend on addressing various sources of uncertainty, particularly in material behavior.To address these uncertainties, we conducted a sensitivity analysis to examine how variations in material properties impact the densification model. Our research incorporates General Electric's proprietary tools, including bayesian hybrid modeling (BHM) and intelligent design and analysis of computer experiments (IDACE), in both metamodeling and intelligent sampling frameworks. The results highlight the significant influence of material properties on the densification process in HIP, both as independent main effects and in their interactions, whether second-order or higher.

Accelerating Discovery for Mechanical Behavior of Materials 2024 Accelerated Approaches III

Tuesday PM
June 18, 2024

Room: Center Street Room A
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

1:40 PM Invited
Autonomous Design of Tough Structures Using Self-driving Labs: *Keith Brown*[1]; [1]Boston University

Tough materials are ubiquitous in protective equipment and structural elements. The more energy they can absorb per unit weight or volume translates to additional safety, cost effectiveness, or sustainability. However, measuring toughness requires physical testing, making design cycles slow and costly. To accelerate this process, we develop a self-driving lab (SDL) that combines additive manufacturing and mechanical testing to study the toughness of 3D printed components in a high-throughput and autonomous fashion. First, we benchmark the acceleration afforded by this SDL and it to be ~60 times faster than grid-based searching, which comprised the first experimental benchmarking of SDLs. Subsequently, we incorporate finite element analysis into this SDL to search in a physics-aware fashion. We also use the resulting databases to identify structures with superlative impact performance using transfer learning. Finally, we conduct an extensive experimental campaign in which we find structures that have superlative energy absorbing efficiency.

2:10 PM
Towards a Fatigue-based Process Window: Influence of LPBF Build Parameters on Process Defect Characteristics and Mechanical Properties in Ti-6Al-4V: *Austin Ngo*[1]; David Scannapieco[1]; Tharun Reddy[2]; Oluwatumininu Adeeko[1]; Christian Gobert[2]; Justin Miner[2]; Sneha Narra[2]; Jack Beuth[2]; Anthony Rollett[2]; John Lewandowski[1]; [1]Case Western Reserve University; [2]Carnegie Mellon University

To characterize process-induced defect characteristics across LPBF power-velocity space, we have conducted tensile and high-throughput fatigue testing on Ti-6Al-4V specimens built under varied process parameters. Specimen fracture surfaces were further imaged via SEM, and process-induced defects on fracture surfaces were quantified, with the critical 'killer' fatigue crack initiating defects being identified. Process-induced defects were found to range in size, shape, and population due to variations in AM build process parameters. Fracture surface defect characteristics are compared to the corresponding mechanical properties and S-N fatigue data to evaluate the influence of LPBF build parameters on process-induced defect formation and the resulting mechanical performance and reliability. In addition, we compare identification and quantification of defect features as conducted both by manual quantification and by feature training a machine learning image classification system using SEM images of fatigue fracture surfaces. Defect quantification and fatigue performance will be discussed following Kitagawa-type modeling.

2:30 PM
Applications Driven High Throughput Analytical 4D-STEM for Multimodal Nanoscale Materials Characterization: *Robert Stroud*[1]; [1]Tescan USA

The methodology and automation behind a fully integrated, precession-assisted, Analytical 4D-STEM will be explained as the solution of choice for high-throughput characterization at the nanoscale. The power of Analytical 4D-STEM lies in its ability to acquire complete image, crystallographic and compositional information at nanometer-scale spatial resolution. Historically researchers although aware of the potential benefits of S/TEM were generally turned off by the perceived operational difficulty, time required, and effort needed to produce results with conventional approaches.Multimodal characterization of a nickel based superalloy, following Vickers indentation induced plastic deformation, and a nanocrystalline Cu-Ta alloy, following shock loading, will be used to demonstrate the automation of complicated, repetitive, and time-consuming tasks. Furthermore, it will be shown how knowledge about the instrument and the techniques can be encapsulated in software to minimize the number of decisions the user needs to make, which will allow them to focus on their specimen and results.

2:50 PM
Accelerated Alloy Design Workflow Through Laser-scanning of Arc-melted Al Alloys: Are They Representative of Additively Manufactured Ones?: *Zhaoxuan Ge*[1]; S. Mohadeseh Taheri-Mousavi[1]; [1]Carnegie Mellon University

Additive manufacturing (AM) enables various advantages such as complex geometry and short supply chain. We have recently designed an additive-manufactured Al alloy with strength even higher than cast Al7075 at ambient and elevated temperatures. With gas-atomization being the major time-consuming and costly step for further enhancement of the mechanical properties of AMed products, we propose to mimic the rapid solidification during AM by laser scanning arc-melted samples. We ask the following three questions: (1) to what extent do the laser-scanned microstructures resemble the AMed ones? (2) Does laser scanning manage to realize the conceived strength? (3) What are the critical factors that govern the microstructure-property relationship during laser scanning? These questions will be explored in greater depth with the aid of multi-scale SEM, TEM, and STEM characterization. Broad revelations for AM Al alloy design will also be discussed.

3:10 PM Networking Break

4:00 PM
Investigating High Throughput Structure-property Relationships in Compositionally Graded Transitions From Ni-base Superalloy to Nb-base Refractory Alloy: David Collins[1]; Marcus Hansen[2]; James Haley[1]; Brian Jordan[1]; Yousub Lee[1]; *Soumya Nag*[1]; [1]Oak Ridge National Laboratory; [2]Texas A&M University

To make additive manufacturing (AM) a substantial manufacturing strategy, one must incorporate its unique attributes of optimizing alloy composition, design and manufacturing modalities to fit site-specific performance needs, by tailoring metal-metal or metal-ceramic compositional transitions. The current work highlights phase transformations and deformation mechanisms in AM Ni-based superalloy (IN718) graded to Nb-based refractory alloy (C103), specifically, successfully achieved via a third transition alloy to avoid regions of brittle phases. Thus, ex-situ DIC assisted tensile testing of monolithic and FGM builds were conducted at room temperature from as-built and heat treated specimens. Micro and nanoindentation studies across the graded transition zones were also performed on these specimens to obtain localized microstructure-property relationships. Overall, this effort is directed towards synergistic coupling of experimental and modeling tools to design pathways for compositional gradation and understand the thermal response on phase/stress evolution of additive builds in a spatio-temporal manner.

4:20 PM
High-throughput Vibration-based Fatigue Testing to Produce S-N Curves of HCF Life in an Afternoon: Brandon Furman[1]; Jeffrey Wagner[1]; Jacob Rigby[1]; Jacob Heninger[1]; Tate Adams[1]; Sam Mulhall[1]; *Ryan Berke*[1]; [1]Utah State University

High cycle fatigue testing is slow and expensive -- for example, a load frame cycling at 40 Hz requires about 70 hours to complete 10^7 cycles, producing only one datapoint on an S-N curve. Consequently, designers of fatigue-sensitive systems often resort to outdated materials that have been qualified by regulators and cannot take full advantage of new advances in material science. As an alternative to axial testing, vibration-based methods operate on the order of kHz, completing the same 10^7 cycles in about 2-3 hours. This can be further accelerated by shaking multiple specimens simultaneously and incorporating Digital Image Correlation to monitor strains independently in each specimen. The DIC data additionally monitors fatigue crack growth in each specimen. Under this approach, a fatigue testing campaign that would previously have taken months of effort to execute can now complete in an afternoon, which will greatly accelerate the development of fatigue-resistant alloys.

4:40 PM
Fundamental Design of Alloys Resistant to H-embrittlement: Nanoscale H-defect Interactions Using Large Scale Simulations: *Matthew Melfi*[1]; S. Mohadeseh Taheri-Mousavi[1]; [1]Carnegie Mellon University

Revealing Hydrogen-defect interactions provides insights on significant ductility loss due to the particular strain partitioning in H-charged structural alloys. Experimental investigation of these interactions are extremely difficult, labor-intensive, and costly. This limitation motivates the development of simulation models to study nanoscale interactions. Using hybridization and parallelization of molecular dynamics and grand canonical Monte Carlo, polycrystalline scale atomistic models of H-diffusion deformation can be simulated with high efficiency. To study H-grain boundary interactions at various concentrations, we developed a model containing various randomly oriented grains and studied the characteristics of H-segregated sites with respect to H-free ones, acting as high-throughput calculations. We analyzed the dislocation activities, e.g., dislocation type, length, distribution in two scenarios. To study H-crack surface interactions, large pillars including all possible sites from different angles of free-surfaces were modeled. We will discuss how H significantly changes the dislocation activities of these defects leading to ductility loss.

Accelerating Discovery for Mechanical Behavior of Materials 2024 Mechanics of Novel Materials III

Tuesday PM
June 18, 2024

Room: Center Street Room D
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

1:40 PM Invited
Characterizing and Tuning the Mechanical Properties of Nanoparticle Assemblies: *Gang Feng*[1]; [1]Villanova University

Nanoparticle assemblies (NPAs) have emerging applications. Tuning the interparticle interaction is shown to be essential to reinforce NPAs, and three feasible ways of tuning are (1) establishing interparticle bonding, (2) developing local configurational confinement, and (3) adjusting the particle size. Interparticle bonding may be established through introducing a gluing-phase, e.g., through atomic layer deposition (ALD). ALD enables us to tone the interparticle interaction by depositing a reinforcing layer around all NPs. The ALD-treated silica NPA is drastically stiffened up to 30 times and hardened up to 200 times. We would also discuss the interparticle-interaction reinforcement through developing local configurational confinement, e.g., introducing shape-anisotropic NPs into NPAs greatly toughen NPAs without sacrificing their strength. Finally, we found that with decreasing the particle size from 300 nm to 10 nm, the NPAs become drastically harder (39×), stiffer (15×), and tougher (>3.5×).

2:10 PM
Thermal-induced Transformation in Additive Manufactured Ti-rich NiTi Shape Memory Alloys: *Foster Feni*[1]; Blake Miller[1]; Arnab Chatterjee[1]; Mique Gonzales[1]; Reginald Hamilton[1]; [1]Pennsylvania State University

The functional characteristics inherent to NiTi shape memory alloys arise from the reversibility of the shape memory transformation mechanism, known as martensitic transformation. Additive manufacturing (AM) is an emerging technology, offering a means to finely tailor the shape memory properties and overall performance of the alloy. In this work, laser directed energy deposition (LDED) and powder bed fusion (PBF) AM were used with NiTi powder feedstock to manufacture NiTi SMAs with Ti-rich compositions. NiTi with Ti-rich compositions are reported to significantly lesser extent than their near-equiatomic and Ni-rich counterparts. Due to the layer-/pass-wise build up and complex thermal history, SMAs fabricated using AM techniques are expected to cause spatial variation in properties. Differential scanning calorimetry (DSC) was employed to spatially characterize the transformation temperatures of specimens sectioned at different locations within builds. DSC results were also augmented to provide advanced metrics for insight into the thermoelastic nature of deposited parts.

2:30 PM
Optimized Microstructure for Enhanced Properties of Novel Ecofriendly Green Plants Wastes Hybridized Ultrafine Grained Al7Si2Cu0.5Ni Eco-composite Inoculated by Al-Nb-V-Zr Master Alloy: *Kingsley Nnakwo*[1]; [1]Nnamdi Azikiwe University

The utilization of eco-friendly green plant waste materials as reinforcing agents in aluminium alloy-based composites represents a sustainable and environmentally responsible approach to material development. The primary objective of this research is to explore the reinforcing characteristics of Irvingia wombolu shell nanoparticulates (IWSNp)/carbon nanotubes (CNTs) hybrid on the electrical and thermo-mechanical properties of Al-7Si-2Cu-0.5Ni eco-composite. The CNTs were synthesis from Rice Husk. The IWSNp and CNTs were prepared using a sol-gel technique. The IWSNp and CNTs hybrid were in the ratio 2:0.5, 2:1, 2:2, 0.5:2, and 1:2. The eco-composites were inoculated by Al-Nb-V-Zr master alloy and subjected to thermo-mechanical treatment (cold worked/homogenized/hot worked/aged at 450oC and 480oC for 2-12h) to produce a high strength, super electrical and thermal conductivity ultrafine-grained Al7SiCu0.5Ni/IWSNp/CNTs eco-composite. The microstructure evolution and Phase compositions of the eco-composites were analyzed using Optical Microscope, Scanning Electron Microscope (SEM), X-ray Diffractometer (XRD), and Energy Dispersive Spectroscopy (EDS).

2:50 PM
Microstructure, Texture, and Tensile Properties of the 50% Hot-rolled and Subsequent Heat treated Ti6Al4V-5Cu Alloy: *Solomon Yeshanew*[1]; [1]Dire Dawa University

In order to investigate the influence of 50% hot-rolling on the microstructure, textural evolution, and tensile properties in Ti6Al4V-5Cu alloy, an electron backscattered diffraction (EBSD) was used. The results show that hot-rolling at high temperature significantly promote the transformation of phases to a fully -phase structure and lamellar microstructure with different grains structure starting from elongated to coarsened appearance was produced. Using tensile testing experiment by considering 0.02 strain offset method, the yield strength of the alloy were estimated. Using specimen sectioned in rolling direction (90°), the true stress-strain curve revealed that the strength at which the alloy has significant plastic deformation under 0.02 offset yield strength method. The alloy revealed 35 MPa yield strength at 800 °C and its area reduction reached 168.5%, and elongation reached up to 83%.

3:10 PM Networking Break

4:00 PM
The Influence of Alloying Elements on the Mechanical Properties and Microstructure of Nickel-based Alloys: *Elyorjon Jumaev*[1]; Orifjon Mikhliev[1]; Sarvar Rozikhodjaev[1]; Dilshodbek Usmonov[1]; [1]FDI UZLITI Engineering LLC

The medium entropy alloys based on Ni were created using Thermocalc software and produced through arc suction casting, with Ti-guttering in an argon environment. The impact of adding Cu on phase development, microstructure, and mechanical properties was examined. A detailed analysis revealed that the alloys demonstrate a dual microstructure, comprising BCC dendrites and FCC interdendrites in the N4 alloy, whereas the Cu-added N6 alloy exhibits a rectangular morphology with + phases. Mechanical property tests indicated exceptional strength at high temperatures compared to Inconel 713C, coupled with excellent ductility in the presence of the + phase microstructure. Various alloy design methods, including composition-based models and predictive techniques, aim to find suitable compositions. Certain non-equiatomic multi-component Medium Entropy Alloys (MEAs) show uncomplicated solid structures and impressive strength, similar to equiatomic quaternary and quinary alloys.

4:20 PM
Study on the Changes in Microstructure and the Mechanical Characteristics of the Quaternary High Entropy Alloys: *Orifjon Mikhliev*[1]; Elyorjon Jumaev[1]; Khasanjon Shanazarov[1]; Dilshodbek Usmonov[1]; Mukhammadjon Usmonov[1]; Sarvar Rozikhodjaev[1]; Azizbek Norov[2]; [1]FDI UZLITI Engineering LLC; [2]Enter Engineering Pte Ltd

This study investigates the microstructure and mechanical properties of the quaternary AlCoCrNi high-entropy alloy, prepared through the arc melting method. The alloy exhibits a microstructure with two phases: dendritic and inter-dendritic areas. After annealing at various durations, grain growth in the inter-dendritic area and phase transformation in the dendritic area were observed. The composition of alloys revealed a good distribution of elements, with Al and Ni concentrated in dark regions and Cr-rich regions in bright areas. Mechanical tests conducted on both as-cast and annealed samples at room temperature showed a significant increase in yield strength after annealing, ranging between 1,8 and 2,9 GPa. This comprehensive analysis of the crystal structure, microstructure, and mechanical properties delves into the quaternary AlCoCrNi alloy using the high-entropy concept.

4:40 PM
Micromechanics-based Framework for Understanding the Magneto-mechanical Behavior of Hard-magnetic Shape Memory Polymers: *Prathik Narayanan*[1]; [1]Indian Institute of Technology, Madras

Shape memory polymers (SMPs) exhibit the capacity to recover a predetermined configuration when exposed to specific stimuli, rendering them suitable for diverse engineering applications. These materials, characterized by rapid, reversible shape transformations, secure locking, and reprogrammability, offer substantial advantages across various domains. To achieve this, they are augmented with multifunctional external fillers, such as hard-magnetic particles, giving rise to hard-magnetic shape memory polymers (h-MSMPs). This infusion introduces inherent complexity, resulting from the interplay of multiple physical phenomena encompassing magnetics, solid dynamics, geometric, and material nonlinearities. This complexity necessitates a rigorous mathematical framework for comprehending their behavior under magneto-mechanical loads. Here, a micromechanics-based framework to study these materials has been proposed, aiming for an in-depth understanding of the physics underpinning their mechanical behavior. The model incorporates a novel double-yield function to account for material plasticity, further enhancing the understanding of these materials' large deformation behavior under various load conditions.

5:00 PM
Fabrication and Characterization of a Strong Aluminum Foam Using Al-Si-Cu Alloy as a Matrix and Cermet Hollow Spheres as Pores-creating Agents: *Fisseha Zewdie Weldemariam*[1]; [1]Indian Institute of Technology, Delhi

This study investigated that compared to steel hollow spheres, cermet hollow spheres (CHS) became more important as pore-creating agents in improving the mechanical performance of closed-cell aluminum foam, especially compression strength and energy absorption capacity. The CHSs were used as reinforcement in molten Al-Si-Cu (LM24) alloy to develop the foam samples using infiltration casting process. At the same time, the CHSs were fabricated from a mixture of SiC and stainless-steel powders at a ratio of 0%, 5%, 10% and 15% SiC in the steel. The CHS reinforcement significantly improved the foam's performance. The LM24-CHS foam samples were tested and characterized for their strength, density, energy absorption, and potential applications. Compared to aluminum foam reinforced with steel hollow spheres, the LM24-foam reinforced with CHS has a higher energy absorption capacity of 88 MJ/m3. Its density, compressive strength, densification strain and porosity were found as 1.5g/cm3, 400MPa, 34% and 67%, respectively.

Symposium on Digital & Robotic Forming 2024
Control in Incremental Forming

Tuesday PM	**Room: Center Street Room B&C**
June 18, 2024	**Location: Hilton Cleveland Downtown**

Session Chair: To Be Announced

1:40 PM Invited
Toward Achieving Autonomy in Incremental Forming: *Mihaela Banu*[1]; [1]University of Michigan

The autonomy revolution in manufacturing requires that traditional mass production can be transformed into personalized production. Personalization involves low volume production of high-value, smart parts with embedded sensors and software, and requires highly-flexible manufacturing processes. Thus, flexible forming such as incremental forming gained interest in the last decade due to its dominant advantages over the conventional processes in customization and personalization. This variability is driven by novel parameterization methods of the designs resulted from utilization of topology optimizations. Incremental sheet forming is a suitable technology for adapting these continuous changes with a fast and cost-effective turn around. Moreover, there is a growing interest in data-driven methods to assist forming processes for in-situ corrections of errors. Highly accurate methods requires large data-sets training through either physical testing or high-fidelity simulations. In this context, we will discuss data-driven hybrid algorithms for defect predictions in incremental forming and their significance in attaining autonomy.

2:10 PM
Control of Part Geometry in Incremental Profile Forming – Challenges and Solution Strategies: *Krishnaswamy Srinivasan*[1]; Satyanarayana Seetharaman[1]; Erman Tekkaya[2]; [1]Ohio State University; [2]Technical University Dortmund

Incremental profile forming is a cold forming process for varying the cross-section of tubular structural elements. It has limited accuracy because of inability to compensate for the effect of post-process phenomena such as springback. A multi-loop control hierarchy suitable for general profile geometries is proposed here with provisions for updating the initial programmed tool trajectory based on two forms of part geometry feedback, during and after the forming of each part. Challenges in implementing some components of the control hierarchy are examined here, for an example process of forming steady axial grooves of uniform depth on a tube moving axially while multiple indenters are moved in radially and held at constant depth. Experimental results on on-line sensing of the groove geometry are presented, along with simulation results on the use of mechanics-based neural network process models to update the programmed depth after the forming of each part.

2:30 PM
Digital Incremental Forming System: *Robert Landers*[1]; Zongze Li[1]; Balark Tiwari[1]; Cindy Huang[1]; David Akinsanya[1]; [1]University of Notre Dame

Digital incremental forming is a numerically controlled process to form parts with complex morphologies and tailored engineering properties. This process does not require custom tools and dies, substantially decreasing cost and lead time. This paper describes the design and application of a digital incremental forming system. The current system consists of a ram rated to one ton, a linear axis to change dies, a robot to manipulate the part position, and a line scanner to measure part morphology. In addition, a video camera and a force sensor are used for in process measurement and control. Operations will be presented where force control and simple part morphology control are implemented in-situ. Other operations will demonstrate the system's capability to do incremental control, namely, the part will be measured between forming steps and the subsequent forming step will be automatically modified based on these measurements.

2:50 PM Networking Break

4:00 PM
Control System Problem Formulation of Robotic Forming, With Robotic Plate Forming as a Case Study: *Yixue Chen*[1]; Tyler Babinec[2]; Brian Thurston[2]; Javier Vasquez-Armendariz[2]; Luis Olivas-Alanis[2]; Ciro Rodriquez[3]; Kornel Ehmann[4]; David Dean[2]; Kenneth Loparo[1]; Robert Gao[1]; David Hoelzle[2]; [1]Case Western Reserve University; [2]Ohio State University; [3]Tecnologico de Monterrey; [4]Northwestern University

Robotic forming is a process where a metallic alloy is sequentially and locally deformed to incrementally change the shape and material properties from an initial state to a goal state. This process enables both part complexity and part customizability, whilst maintaining the fine-grained microstructures inherent to hot and cold forging processes. Autonomous control of the incremental forming process is a formidable challenge. Most current robotic forming is an open-loop process, with the exception of a few examples of incremental sheet forming. The field of control systems has a mature suite of techniques that enable robotic forming control. This paper proposes a general formulation of robotic forming processes as a state-space dynamic system that facilitates the application of the established techniques. Based on this formulation, we study the incremental plate forming process as a case study to demonstrate control formulation, controllability and observability analysis, and control design synthesis.

4:20 PM
Constitutive Law Selection for Finite Element Modeling of Incremental Rotary Forming: *Elizabeth Urig*[1]; David Stegall[2]; Leonid Zhigilei[3]; [1]Analytical Mechanics Associates; [2]NASA Langley Research Center; [3]University of Virginia

Incremental spin and flow forming are promising manufacturing methods for aerospace Al alloys, though computational modeling of the deformation process is still in the developmental phase. The selection of a constitutive law, within existing finite element models, to describe the underlying material behavior affects prediction of final residual stresses, plastic strains, and part geometries. The large thermal gradients, varied strain rates, and oscillating loading characteristic of spin and flow forming require a constitutive law that accounts for thermal profile, deformation history, and work hardening behavior. This study evaluated the modified Hollomon, Johnson-Cook, and Kocks-Mecking constitutive models for accuracy and predictive capability for AA6061 in the O temper condition. Rolling mill and spin forming experiments were employed for model validation and calibration by monitoring plastic strain through hardness measurements and part geometry scanning. The results suggest that the Kocks-Mecking constitutive model, with inherent path-dependency, most accurately captures the progressive mechanical response.

4:40 PM Invited
A Paradigm Change in Metal Forming: From Formability to Usability: *Erman Tekkaya*[1]; [1]TU Dortmund University

Traditionally, metal forming is shaping metals with the ultimate goal to manufacture complicated components without material failure such as necking, fracture and/or surface defects. The dependency of the component performance under service loads on the forming process is rarely considered. This leads to a design of formed components with no failure but with large safety margins and results too large mass of the parts. This presentation will reveal the close relationship of component performance and the parameters of the forming process creating the component giving the opportunity to reduce the mass of the product by simply controlling the forming process. This perception of metal forming process design will require new actuators and processes (such as incremental processes) to boost the component performance. Ductile damage, residual stresses and anisotropic hardening will be discussed as three basic properties of formed workpieces that affect significantly the performance of the component.

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) Data Management - Materials Science I

Wednesday AM
June 19, 2024

Room: Hope Ballroom B
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

8:30 AM Invited
A Materials Data Segmentation Benchmark (MDSB): Pawan Tripathi[1]; Kristen Hernandez[1]; Tommy Ciardi[1]; Mingjian Lu[1]; Max Liggett[2]; Andrew Ballen[2]; Jean-Baptiste Forien[3]; Brian Giera[3]; Manyalibo Matthews[3]; Mengjie Li[2]; Kristopher Davis[2]; John Lewandowski[1]; Laura Bruckman[1]; Yinghui Wu[1]; Roger French[1]; *Vipin Chaudhary*[1]; [1]Case Western Reserve University; [2]University of Central Florida; [3]Lawrence Livermore National Laboratory

This work focuses on creating Materials Data Segmentation Benchmark (MDSB), designed to provide diverse materials datasets, ground truth, and metrics for evaluation of models for benchmarking purposes. The MDSB library will serve as a centralized directory/repository of diverse materials datasets, containing various imaging modalities and representing a wide range of materials. It provides rich collection of data encompassing materials from metals and alloys to polymers. The repository ensures that segmentation models can be rigorously evaluated on a diverse range of materials and imaging techniques. MDSB will curate a wide array of materials datasets, including 2D and 3D data, along with various imaging techniques such as microscopy, tomography, and radiography with the annotated ground truth/gold standard. MDSB will be an open-source project, freely accessible to the research community. This will encourage innovation, democratize access to advanced segmentation tools, and accelerate the development of new materials analysis techniques.

9:00 AM
FAIRification of Data-centric AI: Programmatic JSON-LD Creation and OWL Generation: *Balashanmuga Priyan Rajamohan*[1]; Alexander Harding Bradley[1]; Erika Barcelos[1]; Hayden Caldwell[1]; Arafath Nihar[1]; Laura Bruckman[1]; Yinghui Wu[1]; Roger French[1]; [1]Case Western Reserve University/SDLE

In the realm of AI in Materials & Manufacturing, achieving FAIR (Findable, Accessible, Interoperable, Reusable) data is vital for transformative advancements. Our Python package streamlines FAIRification by seamlessly transforming CSV data into JSON-LD and generating OWL files. Integrated JSON-LD validation ensures high-quality standards, expediting the integration of materials and manufacturing data into FAIR standards, accelerating research processes. This automated approach fosters collaboration, propelling the field towards a future where intelligent systems leverage FAIR data for rapid advancements. Beyond JSON-LD creation, our methodology identifies key data relationships, organized into an RDFLib graph, and transformed into OWL, seamlessly integrating with knowledge frameworks. The package not only aligns user data with FAIR standards but also provides a graphical representation, marking a pivotal step towards FAIR materials and manufacturing data, fostering more efficient and collaborative research endeavors.

9:20 AM
A FAIR-framework for Integrating Advanced Manufacturing Multimodal Data Sets: *Hein Htet Aung*[1]; Kristen Hernandez[1]; Erika Barcelos[1]; Balashanmuga Priyan Rajamohan[1]; Alexander Harding Bradley[1]; Arafath Nihar[1]; Laura Bruckman[1]; Yinghui Wu[1]; Roger French[1]; [1]Case Western Reserve University

Monitoring an Advanced Manufacturing (AM) process often requires a multimodal approach given the diverse and rich data generated from ex-situ and in-situ characterization tools for AM. Despite the richness and high-fidelity quality, data obtained in a process is disparate and integration is unintuitive. The lack of reproducibility and quality controls of manufactured parts also bottlenecks the scalability of AM. Therefore, a systematic data management workflow integrating multimodal and historical data is necessary to prepare high-quality datasets to analyze part reproducibility and reliability. In this study, we propose the application of our data management framework based on FAIR (Findable, Accessible, Interoperable, and Reusable) principles using laser powder bed fusion (L-PBF) and direct ink write (DIW) data as case studies. A FAIR-guided data management framework for seamless multimodal data integration and scalability of robust data analytics and modeling will lead toward the possibility of automated FAIR analytics in AM.

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) Large Language Models for Materials

Wednesday AM
June 19, 2024

Room: Hope Ballroom A
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

8:30 AM Invited
MatGPT™ - Accelerated Alloy Development by Combining LLMs, Machine Learning, Simulation & Validation: *Achim Tappe*[1]; Rüdiger Franke[2]; Golnar Geramifard[2]; Jun-Gyu Kim[1]; Sebastian Jäger[1]; Yiwen Wen[1]; Shameem Ebna Hai[1]; Arnab Mukherjee[1]; Taylor Sparks[3]; Hasan Sayeed[3]; [1]Fehrmann MaterialsX; [2]Fehrmann Materials; [3]University of Utah

This work offers insights into AI-driven rapid alloy development methods, aimed at enhancing alloy properties and resource efficiency. A pivotal strategy involves GenAI-driven materials development, incorporating LLMs, machine learning, simulation, and comprehensive validation. The rising demand for advanced alloys, exemplified by the automotive industry's shift from combustion engines to electric motors, underscores the imperative for agile and eco-friendly alloy innovations. Such transitions drive reductions in CO2 emissions and fossil fuel dependency. Our study vividly illustrates how validated GenAI-driven materials development translates into tangible benefits: improved alloy properties, weight reduction, and a more eco-conscious approach. We also introduce the integration of LLMs and natural language processing techniques, further expediting knowledge extraction from various sources. This inclusive process fosters enhanced accessibility and interpretability of materials data, contributing to the acceleration of advanced material development. This streamlined approach combines AI, LLMs, and validation, addressing industrial alloy challenges more swiftly, efficiently, and sustainably.

9:00 AM
Using Large Language Models to Aid Materials Design Workflows: *James Saal*[1]; [1]Citrine Informatics

Large language models (LLMs) are a unique and powerful foundation for building general purpose tools and there is great promise in their use for materials applications. Citrine has been integrating LLM technology in our cloud-based materials informatics Citrine Platform for customer use and experimenting with novel methods to use LLMs for aiding in materials design workflows. In this talk, Citrine's LLM experience and products will be described, including perspectives on how the materials science community can best leverage these exciting new technologies.

9:20 AM
AI for Science: Data-centric AI by Utilizing D/HPC and FAIRified Scientific Analysis Workflows: *Roger French*[1]; Arafath Nihar[1]; Thomas Ciardi[1]; Rachel Yamamoto[1]; Erika Barcelos[1]; Priyan Rajamohan[1]; Alexander Harding[1]; Rounak Chawla[1]; Pawan Tripathi[1]; Vipin Chaudhary[1]; Laura Bruckman[1]; Yinghui Wu[1]; [1]Case Western Reserve University

Model-centric AI has made strides by focusing on algorithmic design of models often neglecting challenges associated with heterogeneous datasets. This myopic focus limits the role of data to merely fuel the model training, potentially leading to unpredictable and negative consequences in downstream AI deployments. The Center of Excellence in Materials Data Science for Stockpile Stewardship (MDS3:COE) is dedicated to advancing the forefront of artificial intelligence in science, we prioritize data and generalizing AI models for use in larger scientific domains. We use an integrated distributed and high performance computing (D/HPC) environment focusing on a data-centric AI approach based on FAIRified scientific workflows that make data and models findable, accessible, interoperable and reusable facilitating seamless integration with AI systems. This integration not only improves data analysis through scalability (utilizing a scaled-out computing architecture) but also enhances performance (leveraging parallelism), ensures resilience (via redundancy), and promotes cost-effectiveness (utilizing low-cost commodity hardware).

Accelerating Discovery for Mechanical Behavior of Materials 2024 Design I

Wednesday AM
June 19, 2024

Room: Center Street Room D
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

8:30 AM Invited
Bulk Rare Earth Free Permanent Magnets by Severe Plastic Deformation: *Andrea Bachmaier*[1]; Lukas Weissitsch[1]; Stefan Wurster[1]; Heinz Krenn[2]; [1]Erich Schmid Institute, Austrian Academy of Sciences; [2]Institute of Physics, University of Graz

High-performance permanent magnets, which are usually based on rare earth elements (NdFeB and SmCo), are critical parts in energy conversion technologies such as electric motors or power generators. However, the U.S. Department of Energy and the European Commission listed several rare-earth elements as critical materials, as supply shortages will be a crucial problem for future economic development.The ferromagnetic -MnBi phase is a promising alternative magnetic material, but synthesis of large volumes containing a significant amount of -MnBi is still challenging. To overcome current processing limitations, we use (multistep) high-pressure torsion, a method of severe plastic deformation in combination with magnetic field assisted thermal treatment. Annealing induced changes are monitored by in-situ synchrotron X-ray diffraction and the -MnBi phase formation is correlated with different HPT-deformation grades. Results obtained by means of electron microscopy and SQUID magnetometry emphasize a positive influence of HPT-deformation and annealing on -MnBi phase formation.

9:00 AM
Impact of Microstructure on Mechanical Property and Multi-property Optimization in Porous Materials: *Longsheng Feng*[1]; Bo Wang[1]; Sourav Chatterjee[1]; Donglin Li[2]; Natalie Hwee[1]; Sijia Huang[1]; Jianchao Ye[1]; Sangil Kim[2]; Tae Wook Heo[1]; Juergen Biener[1]; [1]Lawrence Livermore National Lab; [2]University of Illinois at Chicago

In the quest to enhance the performance of porous materials, understanding the intricate link between their microstructure and mechanical properties is crucial. Utilizing phase field simulations, we generate bicontinuous porous structures, coupled with a spectra-based perturbation method to evaluate their effective modulus. We identify key microstructural features that play a significant role in dictating local stress hotspots and overall mechanical performance. Further, an advanced machine learning model is developed to enable accurate prediction of these properties. Design methodologies are proposed to augment the mechanical characteristics of these materials. Our study also investigates multi-property co-optimization, which includes a thorough exploration of the interdependencies between mechanical and transport properties, underlining our commitment to the integrated design of multifunctional porous materials for targeted innovative applications. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

9:20 AM
Multiscale Modelling-based Polycrystalline Alloy Design Framework: Akash Gupta[1]; Sumit Maurya[1]; *Surya Ardham*[1]; Srimannarayana Pusuluri[1]; Gerald Tennyson[1]; [1]Tata Consultancy Services (TCS), Research

Meeting original equipment manufacturer specified mechanical property by designing polycrystalline alloys is challenging. Such model-based designs are done for specific alloy considering cost and time for experiments. Here, we present a novel atomistically assisted microstructure and crystallographic texture-based accelerated alloy design framework based on multiscale modelling. We demonstrate its capability for automotive applications by improving formability of aluminium 5xxx series alloy through tailoring of chemistry and process parameters. In this framework, mobilities and activation energies calculated using molecular dynamics simulation are passed to cellular automata model of static recrystallization during annealing along with cold rolled microstructure and texture. Post annealed microstructure and texture is input to crystal plasticity based forming limit diagram (CP-FLD) prediction model and predicted FLD is used in finite element method based stamping simulation. This framework can guide designers for optimization of microstructure during cold rolling, annealing and stamping processes for meeting formability requirements for sheet metal.

Accelerating Discovery for Mechanical Behavior of Materials 2024 ML Applications and Accelerated Approaches

Wednesday AM
June 19, 2024

Room: Center Street Room A
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

8:30 AM Invited
Mesoscale Investigations of Dislocation-grain Boundary Interactions in Metals and Alloys: *Abigail Hunter*[1]; [1]Los Alamos National Laboratory

"Microstructure" refers to the large number of crystal grains and their boundaries that make up metals and alloys. A material's ability to accommodate stress induced through mechanical loads is dependent on the ease with which dislocations can move through the microstructure to relieve accumulated stress. Grain boundaries (GBs) are the largest impediment to this motion. For example, dislocations can pile-up against GBs, building localized internal stress regions that work-harden the material, and are precursors to damage nucleation. Understanding and predicting dislocation-GB interactions are key for capturing mechanical response, but they are also incredibly complex in part due to the vast number of possible GBs and corresponding dislocation interactions. This talk will focus on recent multiscale modeling efforts addressing dislocation-GB interactions, with particular focus on a mesoscale approach called phase field dislocation dynamics. Connections to atomistic efforts will also be discussed, along with methods/approaches that can be used to scale information.

9:00 AM
High Dimensional Fatigue Life Process Window Modeling of Ti-6Al-4V Laser Powder Bed Fusion, Enabled by Graph-based Data Fusion: *Alex Gonzalez*[1]; [1]Colorado School of Mines

Effective process windows require rigorous statistical context. Process stability regions for the fatigue life of laser powder bed fusion (PBF-LB)-produced Ti-6Al-4V are identified via high statistical power, nested extreme value distribution parameter estimation. Specific focus is given on simultaneous variable screening and confounding analysis for numerous independent, physics-informed, and feature-engineered variables. Such variable breadth is enabled by explicit retention of data heritage/lineage from a simple, extensible, and robust data collection, alignment, and cleaning system. This system successfully structured data for a multi-year, multi-university NASA ULI program across multiple machines and participants, despite personnel churn and asynchronous data generation. The resulting model yields expected life trends with respect to laser power and laser velocity, however, also includes simultaneous interactions in multiple other variables that would otherwise distort a two-dimensional view of the process window for any given stress level. Discussion on life prediction maps with practical implications for operations is included.

9:20 AM
Determination of Intrinsic Mechanical Properties of Polycrystalline Nickel-based Superalloy Using Spherical Indentation and Bayesian Inference: *Hyung Kim*[1]; Michael Buzzy[1]; Camilla Johnson[1]; Surya Kalidindi[1]; [1]Georgia Institute of Technology

Extracting the intrinsic mechanical properties of polycrystalline materials poses a significant challenge in materials science due to the absence of straightforward mechanical testing methods. Furthermore, when such materials contain second-phase precipitates, conventional mechanical tests become unfeasible. In this study, we introduce a novel approach that utilizes spherical indentation coupled with Bayesian inference techniques, specifically Gaussian Process Regression (GPR) and Markov Chain Monte Carlo (MCMC) sampling. Through this methodology, we demonstrate a solution to overcome both challenges on a polycrystalline nickel-based superalloy which contains a relatively high volume fraction of second-phase precipitates. Our results indicate that spherical indentation, in conjunction with advanced statistical tools, offers a promising avenue for accurately characterizing the intrinsic mechanical properties of complex polycrystalline materials. This research contributes to the advancement of materials characterization techniques, enhancing our understanding of critical mechanical properties in high-performance materials like nickel-based superalloys.

Symposium on Digital & Robotic Forming 2024 Industry Application II

Wednesday AM
June 19, 2024

Room: Center Street Room B&C
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

8:30 AM Invited
Architectural Applications and Workflows for Robotic Incremental Forming: *Paul William Nicholas*[1]; [1]Royal Danish Academy, School of Architecture

Formed thin sheet metal enables lightweight structures that integrate ornament, structure and skin - a trajectory of architectural and structural opportunity initialized in the design of buildings by Prouve, Junkers, and LeRicolais. Where previously the need for a mold has limited design approaches to the contexts of mass production, mold-less Robotic Incremental Sheet Forming (RISF) provides new opportunities for customized and bespoke architectural panels and structures. This presentation will describe the computational design and fabrication approaches developed across three prototypical architectural structures: an arch, a bridge and a façade, and how incremental forming has been leveraged within the design process to achieve structural optimization and architectural expression. Central concerns include the use of incremental forming to achieve extremely lightweight high performance structures, the integration of customized rigidization geometries informed by structural optimization, and the incorporation of material property changes induced by the forming process into the design and optimization workflow.

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) Data Management - Materials Science II

Wednesday PM
June 19, 2024

Room: Hope Ballroom B
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

1:40 PM Invited
MICRO2D: Statistically Conditioned Deep Generative Models for Curating Big Microstructure Datasets: *Andreas Robertson*[1]; Adam Generale[1]; Conlain Kelly[1]; Michael Buzzy[1]; Surya Kalidindi[1]; [1]Georgia Institute of Technology

Researchers have demonstrated that data scientific and machine learning techniques, trained using available large datasets, can be used to rapidly accelerate the pace of technical innovation. Unfortunately, the lack of inexpensive data sources in Materials Informatics means that collecting datasets composed of statistically diverse material microstructures is extremely challenging. Here, we will demonstrate that statistically conditioned microstructure generative models provide a natural pathway to overcome this challenge. We propose a framework expanding on our recently proposed statistically conditioned Local-Global Decomposition generative models. The crux of the proposed framework is a novel suite of algorithms for generating salient 2-point statistics – without needing prior examples – for conditioning. We provide two demonstrations. First, we address the general dataset generation problem; we generate a general statistically diverse microstructure dataset of 2-phase composite microstructures. Second, we briefly discuss how dataset generation algorithms play a critical role in accelerating the extraction of process-structure models.

2:10 PM
Ontology-based Digital Representations of Materials Testing in the MaterialDigital Initiative: *Hossein Beygi Nasrabadi*[1]; Birgit Skrotzki[1]; [1]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). The PMD-funded KupferDigital project is developing a data ecosystem for digital materials research. The fundament of the data ecosystem is ontology-based digital representations of copper materials. In the current research, we present the methodology and toolchains for the development of domain-level ontologies for materials testing that address the requirements of materials testing standards. The collection of the required terminology from the testing standard, the semantic representation of the process graphs, the conversion of the ontology files, their integration with the upper-level ontologies, and the data mapping processes were presented for the Brinell hardness testing use case.

2:30 PM
Dataset Generation and Verification for Additive Manufacturing Using Explainable AI: *Jennifer Ruddock*[1]; Robert Weeks[2]; James Hardin[1]; Jennifer Lewis[2]; [1]AFRL; [2]Harvard University

Machine learning shows promise for helping automate manufacturing processes, but suffers from a lack of data and poor explainability. The generation of high-quality datasets is important for overcoming both these challenges. To that end, we have generated a dataset using additive manufacturing as a prototypical process, because it is an accessible and controllable process that is governed by the complex physics connecting process parameters to printed outcomes. Our dataset includes processed and segmented images of test print patterns, print process parameters, and rheological data of 15 inks from two different material sets. We created a schema so an end user can access the processed data while also having access to relevant source files and processing code. We have used this dataset to train a convolutional neural net to predict rheological properties using the test print pattern and subsequently created an explainable AI tool for model and dataset verification.

2:50 PM
Not as Simple as We thought: A Rigorous Examination of Data Aggregation in Materials Informatics: *Taylor Sparks*[1]; Federico Ottomano[2]; Giovanni De Felice[2]; Vladimir Gusev[2]; [1]University of Utah; [2]University of Liverpool

Recent machine learning developments have opened new possibilities for materials research. However, due to the underlying statistical nature, the performance of machine learning estimators is heavily affected by the quality of training datasets, which are severely limited and fragmented in the case of materials informatics. Here, we investigate whether state-of-the-art machine learning models for property predictions can benefit from aggregation of different datasets. We probe three different aggregation strategies in which we prioritize training size, element diversity, and composition diversity by using novelty scores from the DiSCoVeR algorithm. Surprisingly, our results consistently show that both simple and refined data aggregation strategies lead to a reduction in performance. This suggests caution when merging different experimental data sources. To guide the size increment, we compare the use of DiSCoVeR, which prioritizes chemical diversity, with a random selection. Our results show that targeting novel chemistries is not beneficial in building a training dataset.

3:10 PM Networking Break

4:00 PM
Managing Scientific Data in Characterization Investigations With FAIR: *Erika Barcelos*[1]; Alexander Bradley[1]; Balashanmuga Rajamohan[1]; Hayden Caldwell[1]; Mengjie Li[1]; Leean Jo[1]; Laura Bruckman[1]; Yinghui Wu[1]; Roger French[1]; [1]Case Western Reserve University

Scientific investigations enable new discoveries, improvement of existing technologies, and advancement in science. Experimental investigations generate substantial amounts of data. A large proportion of metadata is either not recorded or stored in lab notebooks, which poses several challenges for sharing and reusing these assets across different groups and organizations. In this work, we showcase different applications of our FAIR framework in scientific investigations focusing on chemical and materials characterizations. The proposed framework enables metadata and data to be easily findable, accessible, interoperable and reusable, which is fundamental to guarantee an efficient and robust data management system enabling reproducibility, reliability and efficiency in the research.

4:20 PM
Spatiotemporal Scene Graph Representations for Terabyte Scale X-ray Computed Tomography Datasets of AlMg: *Thomas Ciardi*[1]; Pawan Tripathi[1]; John Lewandowski[1]; Roger French[1]; [1]Case Western Reserve University

X-ray computed tomography (XCT) enables non-destructive 3D characterization of material microstructures and defects. The Terabyte-scale dynamic XCT datasets output from these imaging modalities, however, remain a challenge to analyze. To solve this, we developed a spatiotemporal scene graph representation to encode objects, relationships, and evolution in large-scale 4D XCT data of AlMg undergoing stress corrosion cracking (SCC). The graph nodes represent segmented cracks, precipitates, and pitting, with attributes capturing morphological metrics. Edges encode spatial relationships between defects and microstructural features. Dynamic edges connect defect instances across time steps, explicitly modeling crack growth and microstructural evolution. The graph formulation further allows integration of deep learning techniques and relational reasoning between defects and microstructure. This establishes scene graphs as a flexible and powerful representation for exploiting structure in massive tomographic imaging data.

4:40 PM
A FAIRification Framework for Synchrotron High Energy X-ray Diffraction Datasets: *Pawan Tripathi*[1]; Weiqi Yue[1]; Mohammad Mehdi[1]; Erika Barcelos[1]; Balashanmuga Rajamohan[1]; Alexander Bradley[1]; Dan Savage[2]; Don Brown[2]; Laura Bruckman[1]; Yinghui Wu[1]; Roger French[1]; [1]Case Western Reserve University; [2]Los Alamos National Laboratory

The scale of synchrotron High-energy X-ray diffraction datasets poses significant challenges in data management, processing, and standardization. The intricate metadata associated with experimental conditions and instrument settings often hinders machine decipherability, limiting both machine and human reusability of the dataset. Our proposed FAIRification approach, based on Findability, Accessibility, Interoperability, and Reusability (FAIR) principles, transforms synchrotron datasets' metadata into JSON-LD using a Python package. This package employs an object-oriented programming paradigm to convert varied formats, like CSV, into JSON-LD (version 1.1), enhancing data utility for semantic queries. The approach also generates ontologies in OWL files, adhering to the Basic Formal Ontology standard (2020) and ISO/IEC 21838-1 standard, providing semantic context and enabling graphical visualization of data relationships. By addressing challenges in data management, sharing, and long-term preservation, we aim to promote wider adoption and reuse of these valuable datasets through FAIR principles, standardization, and enhanced data lifecycle practices.

5:00 PM
Overcoming Integration Barriers for Multivariate Big Geospatiotemporal Data: *Olatunde Akanbi*[1]; Deepa Bhuvanagiri[1]; Erika Barcelos[1]; Jeffrey Yarus[1]; Yinghui Wu[1]; Roger French[1]; [1]Case Western Reserve University

Harnessing the potential of massive, heterogeneous geospatiotemporal datasets requires robust data management capabilities. This research presents an integrated framework for agricultural monitoring that applies state-of-the-art practices for ingesting, processing, and analyzing massive agricultural data assets. Open access satellite imagery, soil data, hydrological measurements, and land use classifications are synthesized. Kriging and conditional simulation techniques model and predict spatial distributions of key soil nutrients like nitrogen. Custom extraction, transformation, and loading pipelines ingest and process the multivariate data assets. Distributed computing infrastructure enables storing, accessing, and analyzing the big data. Spatiotemporal analytics reveal connections between crop growth dynamics, edaphic factors, and nutrient transport. The methodology underscores the critical role of data management in fully leveraging emerging geospatiotemporal big data to address real-world agricultural and environmental challenges. Advanced data curation, geospatial modeling, and quality verification techniques help overcome integration barriers and extract actionable insights from complex, multimodal datasets.

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) Machine Learning - Processing II

Wednesday PM **June 19, 2024**	**Room: Hope Ballroom A** **Location: Hilton Cleveland Downtown**

Session Chair: To Be Announced

1:40 PM Invited
Autonomous Learning of Atomistic Structural Transitions via Physics-inspired Graph Neural Networks: Bamidele Aroboto[1]; Shaohua Chen[2]; Tim Hsu[3]; Brandon Wood[3]; Yang Jiao[2]; *James Chapman*[1]; [1]Boston University; [2]Arizona State University; [3]Livermore National Laboratory

Materials processing often occurs under extreme dynamic conditions leading to a multitude of unique structural environments. These structural environments generally occur at high temperatures and/or high pressures, often under non-equilibrium conditions, which results in drastic changes in the material's structure over time. Computational techniques such as molecular dynamics simulations can probe the atomic regime under these extreme conditions. However, characterizing the resulting atomistic structures has proved challenging due to the intrinsic levels of disorder present. Here, we introduce SODAS++, a universal and interpretable graph neural network framework that can accurately and intuitively quantify the transition between any two arbitrary phases. The SODAS++ framework also quantifies local atomic environments, providing one with the power to encode global state information at the atomic level. We showcase SODAS++ for both solid-solid and solid-liquid transitions for systems of increasing geometric and chemical complexity such as elemental metals, oxides, and ternary alloys.

2:10 PM
Fracture Toughness and Fatigue Life Prediction of Additively Manufactured Al 2024 Alloy Using Machine Learning Models: Saurabh Gairola[1]; Sneha Jayaganthan[2]; *R. Jayaganthan*[1]; [1]Indian Institute of Technology Madras; [2]Stanford University

The present study focuses on the fatigue life and fracture toughness behaviour of the additively manufactured Al 2024 alloy. The mechanical properties were investigated for different build orientations (horizontal (0°), and vertical (90°)). The test variables such as stress amplitude, build orientation, stress ratio, and post-processing condition (T6 ageing heat treatment) were considered for machine learning (ML) prediction. The experimental data were used to train the ML models such as Support Vector machine, Random Forest, Decision trees, and CNN and the trained models were used as predictive models for fatigue life estimation in Al 204 alloy. The pre-processed data set were used for training the ML models and the hyperparameters tuning were made using kernel function to ensure close match with experimental data. The predictive accuracy of these ML models was compared and discussed the hidden pattern of fatigue life influenced by process and dynamical loading conditions.

2:30 PM
Intrinsic Dimensionality Estimates for Microstructural Data: Veera Sundararaghavan[1]; *Megna Shah*[2]; Jeff Simmons[2]; [1]University of Michigan; [2]Air Force Research Laboratory

We hypothesize that there are regions of processing space that are homeomoprhic to microstructure space. That is, the domains are continuous, invertible and one-to-one. The continuity assumption implies that small changes in the processing domain result in small changes in the microstructure domain, and vice-versa. The invertibility assumption means that microstructure can be inverted to find the process. And both of these assumptions mean the mapping is one-to-one. We know that not all microstructures are homeomorphic to processing, but finding regions where this is true will enable autonomous materials design. A key property of homeomorphism that both domains have the same intrinsic dimensionality. Here we use an approach for non-linear data, to measure the intrinsic dimensionality of microstructure data. The approach, its modifications and the results will be described here.

2:50 PM
HotSpotNet: A Deep Learning Approach to Predicting Stress Hot Spots in Materials Based on Microstructural Features: Karthik Narayanan Giriprasad[1]; *Michael Groeber*[1]; Steve Niezgoda[1]; [1]The Ohio State University

Failure in materials often arises due to localized stress or strain concentrations, referred to as "stress hot spots". The likelihood of these hot spots forming is influenced by microstructural factors like local features, misorientations, among others, in relation to the applied load. Since these hot spots may lead to failure, it is advantageous to develop techniques to predict their formation based on the initial microstructural images. We describe a Convolutional Encoder-Decoder based approach to first model the elastic response in the form of stress fields simulated using Fourier transforms which can then be used to determine high-stress regions. The model is trained on local patches from synthetic microstructures generated using DREAM.3D and the results show that the Encoder-Decoder based approach can effectively learn spatial relations that may lead to hot spots.

3:10 PM Networking Break

4:00 PM
Reinforcement Learning Approaches to Developing Policies for Incremental Robotic Forging: *Michael Groeber*[1]; Stephen Niezgoda[1]; Josh Groves[1]; Anahita Khojandi[2]; Sam St. John[2]; [1]Ohio State University; [2]University of Tennessee - Knoxville

This work aims to establish the foundation for an AI-driven, learning-based control system for a robotically integrated incremental metal forming. We will present and discuss different ML and optimization approaches to learn a generalized policy for selecting incremental deformation actions with the goal of matching a desired component geometry. The target is not a minimization of total deformation, instead the minimization of the Wasserstein distance between the workpiece and the target geometry. We will discuss approaches for using physics-based simulations, data-driven reduced-order models, and physical experiments to train the policy, as well as how to incorporate expert knowledge. We will also present initial results of using the AI-learned policies to control a physical forging system.

4:20 PM
Space Launch System Weld Process Optimization Using Informatics and Machine Learning: *Joshua Stuckner*[1]; [1]NASA Glenn Research Center

The Artemis core stage fuel tank welding process was optimized, significantly reducing process variation and improving weld strength. Machine learning models were used to establish process structure property relationships and identify an improved process window after model selection. A space filling experimental design was used to explore the design space and capture non-linear effects. A data pipeline was built to automatically ingest, verify, and clean complex data types including fracture surface images, sequential weld tool sensor data, and tabular processing and property data from test labs. Fracture surface defects were quantified using ConvNets for segmentation and traditional computer vision for featurization. Sequence data was analyzed using Long-Short Term Memory neural networks and activation maps were used to provide model interpretability. This presentation will discuss how machine learning, experimental design, and informatics were used to propose and validate hypothesis to improve Artemis fuel tank weld quality.

4:40 PM
Unveiling Metal Additive Manufacturing Microstructure Through Data-driven Unsupervised Clustering of Crystallographic Texture: *Aashique Rezwan*[1]; David Montes de Oca Zapiain[1]; Daniel Moser[1]; Michael Heiden[1]; Theron Rodgers[1]; [1]Sandia National Laboratories

Metal additive manufacturing (AM) parts often have microstructural features that are not well described by traditional quantification metric and have variations within an AM part that are challenging to quantify. This work presents a data-driven approach to quantifying microstructures that incorporates grain morphology, crystallographic orientation and phase information. A combination of generalized spherical harmonics (GSH), spatial correlation, and a dimensionality reduction technique (i.e., Principal Component/Auto-encoder) is used to perceive the complex microstructural data into human-readable results for comparison. The method shows sensitivity to minor microstructural differences within specimens created with nominally identical processing parameters, when applied to an experimental dataset of AM 316L-SS. The method can identify different build batches, orientation and outliers present in the process and can potentially serve as a tool in detecting AM process changes for quality control applications.SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

5:00 PM
A Data-driven Laplacian-penalized Non-rigid iterative Closest Point Reverse Deformation Model for Net-shape Investment Castings: *Jiayu Cui*[1]; Jun Wang[1]; Donghong Wang[1]; Da Shu[1]; Baode Sun[1]; [1]Shanghai Jiao Tong University

In the realm of industrial manufacturing, dimensional distortions frequently occur. This is particularly evident in investment castings where the underlying mechanisms are complex and ambiguous. Despite intensive studies, maintaining precise dimensions remains elusive. This research introduces a cutting-edge Laplacian-penalized non-rigid iterative closest point reverse deformation model to address this challenge. The learnable approach is able to provide the ideal mold design for investment castings using just one mold trial data. With more data supplied, the model can provide more accurate descriptions of deformation patterns and better reverse deformation design. Utilizing blue light scanning, 8 test reverse deformed castings from three production batches were assessed, all adhering to the stipulated dimensional standards of ±0.5 angular error limit and CT2 linear dimension specifications. This breakthrough offers significant advancements in the precise dimensional control of investment castings as well as other manufacturing processes.

Accelerating Discovery for Mechanical Behavior of Materials 2024 Design II

Wednesday PM
June 19, 2024

Room: Center Street Room D
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

1:40 PM Invited
Modeling Location-specific Material Behavior in Polycrystalline Ti Alloys With Material Design Implications: *Somnath Ghosh*[1]; [1]Johns Hopkins University

Location-specific property distribution, through differential material distributions, is a desirable attribute for structural components. For polycrystalline metals and alloys, this translates into location-specific distributions of grain size, crystallographic orientations, micro-texture, etc. that can be harnessed to deliver optimal mechanical behavior and failure/life response. A necessary ingredient for material design is multiscale models of deformation, fatigue, and failure, that explicitly incorporate lower-scale material descriptors in higher-scale material constitutive models. This talk will discuss a parametrically upscaled constitutive and crack nucleation modeling (PUCM/PUCNM) platform for predicting structural-scale fatigue crack nucleation inTi alloys. The thermodynamically consistent PUCM/PUCNMs incorporate a parametric representation of lower-scale microstructural descriptors in higher-scale constitutive coefficients. These coefficients are expressed as functions of Representative Aggregated Microstructural Parameters (RAMPs), representing descriptors of local microstructural morphology and crystallography in lower-scale statistically equivalent representative volume elements. The talk will discuss the effect of the local microstructural variabilities on the fatigue crack nucleation.

2:10 PM
Maximizing Tensile Properties Through Partially Active Grain Boundary Segregation in Nanocrystalline Sterling Silver Alloys: *Pavel Nikitin*[1]; Frederic Sansoz[1]; [1]The University of Vermont

Enhancing thermal stability and tensile mechanical behavior in nanocrystalline alloys by grain-boundary (GB) solute segregation is a critical but challenging problem, due to the complexity of relationships between solute segregation and deformation mechanisms at GBs. Notably, understanding the nature of GB strengthening and softening mechanisms in nanocrystalline alloys requires the integration of multiscale experimental and theoretical studies. This talk presents an integrated experimental and atomistic simulation study focused on the effects of Cu solute concentration on the tensile behavior of nanocrystalline Ag alloys produced by DC magnetron sputtering technique. We support our experiments by large scale hybrid Monte-Carlo and Molecular-Dynamics simulations and present a systematic study where three concentration-dependent regimes of plasticity are investigated: (1) Classical segregation strengthening behavior at low solute contents, (2) shear band-induced softening at high contents, and (3) maximum strengthening in nanocrystalline Sterling silver (8 at.% Cu) governed by partially active segregation from GB solute clustering.

2:30 PM
Obtaining Auxetic and Isotropic Metamaterials in Counterintuitive Design Spaces: An Automated Optimization Approach and Experimental Characterization: *Timon Meier*[1]; [1]UC Berkeley

Recent advancements in manufacturing, finite element analysis (FEA), and optimization techniques have expanded the design possibilities for metamaterials, including isotropic and auxetic structures, known for applications like energy absorption due to their unique deformation mechanism and consistent behavior under varying loads. However, achieving simultaneous control of multiple properties, such as optimal isotropic and auxetic characteristics, remains challenging. This paper introduces a systematic design approach that combines modeling, FEA, and optimization to create targeted mechanical behavior in metamaterials. Through strategically arranging 8 distinct neither isotropic nor auxetic unit cell states, the stiffness tensor in a 5 × 5 × 5 cubic symmetric lattice structure is controlled. Employing the NSGA-II genetic algorithm and automated modeling, we yield metamaterial lattice structures possessing both, desired isotropic and auxetic properties. Multiphoton lithography fabrication and experimental characterization of the optimized metamaterial highlights a practical real-world use and confirms close correlation between theoretical and experimental data.

2:50 PM
Discovering Superhard High-entropy Diboride Ceramics via a Hybrid Data-driven and Knowledge-enabled Model: *Jiaqi Lu*[1]; William Yi Wang[1]; [1]Northwestern Polytechnical University

Materials descriptors with multivariate, multiphase, and multiscale of a complex system have been treated as the remarkable materials genome, addressing the composition–processing–structure–property–performance relationships during the development of advanced materials. With the aid of high-performance computations, big-data, and artificial intelligence technologies, this work derive an explainable model of composition–property–performance relationships via a hybrid data-driven and knowledge-enabled model, and designing 14 potential superhard high-entropy diboride ceramics with a cost-effective approach. Five dominate features and optimal model were screened out from 149 features and nine algorithms by machine learning and validated in first-principles calculations. The HEBs component electronic-property influence trend and mechanism has been analysis effectively from the atomic and electronic bottom layer. Moreover, this electron work function-machine learning model not only has better capability to distinguish the differences of solutes in same group of periodic table but is also a more effective method for material design than that of valence electron concentration.

3:10 PM Networking Break

4:00 PM
Enhanced Strength of Additively Manufactured Inconel 718 Through a Simplified Heat Treatment Strategy: Jake Benzing[1]; Nicholas Derimow[1]; Orion Kafka[1]; Nikolas Hrabe[1]; Philipp Schumacher[2]; Donald Godfrey[2]; Chad Beamer[3]; Priya Pathare[4]; Jay Carroll[4]; Ping Lu[4]; Isaiah Trujillo[4]; *Frank DelRio*[4]; [1]National Institute of Standards and Technology; [2]SLM Solutions; [3]Quintus Technologies; [4]Sandia National Laboratories

This study abridged the heat treatment route and reduced the post-processing time for additively manufactured Inconel 718. The implementation of an experimental heat-treatment process with a single pre-aging step and a single aging treatment resulted in a total heat treatment time of 15 hr, far shorter than the baseline five-step strategy of 42 hr. Grain structure, pore size, and tensile properties were measured for parts from the as-built condition and with the two heat treatment processes. Unique findings in the experimental heat treatment process included the generation of localized micro-scale recrystallization throughout the retained columnar grain and sub-grain structures, internal pore closure, incomplete dissolution of the Laves phase, and the absence of delta phase. Moreover, the experimental process improved strength, decreased total elongation, and exceeded properties outlined in ASTM F3055-14a. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

4:20 PM
Improved Corrosion Resistance of Additively Manufactured 316L Stainless Steel via Tailored Porosity, Roughness, and Passive Film Morphology: *Frank DelRio*[1]; Ryan Khan[1]; Michael Heiden[1]; Paul Kotula[1]; Peter Renner[1]; Erin Karasz[1]; Michael Melia[1]; [1]Sandia National Laboratories

The development of additively-manufactured (AM) 316L stainless steel (SS) using laser powder bed fusion (LPBF) has enabled near net shape components from a corrosion-resistant structural material. In this talk, we investigate the effects of processing parameters on the corrosion behavior of as-printed surfaces of AM 316L SS formed via LPBF. Laser power and speed were varied across the instrument range to produce parts with > 99% density, and the macroscale corrosion trends were interpreted via small-scale measurements of porosity, roughness, microstructure, and chemistry. In general, samples with smaller porosity and roughness values and larger work function homogeneity exhibited larger breakdown potentials. The porosity and roughness effects stemmed from an increase to the overall number of initiation sites for pitting, and the oxide contributed to passive film breakdown by acting as a crevice former or creating a galvanic couple. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

4:40 PM
Defect Populations and Their Linkage to Strength Distribution Parameters in Additively Manufactured Alumina: Sarah Boardman[1]; *Corinne Packard*[1]; [1]Colorado School of Mines

Optimizing microstructure of additively manufactured ceramics first requires knowledge of the strength-controlling defects, which may or may not be the same defects in conventionally processed ceramics even within the same material system. We use a combination of designed experiments, statistical methods, and extensive fractographic examination to measure the 4-point flexural strength and defect distributions in high purity, Lithography-based Ceramic Manufacturing alumina. We find that the characteristic strengths of fully dense bars are near or above that of conventionally processed alumina for all print conditions, but the Weibull modulus varies greatly ($m = 3.8$–19.5) depending on print parameters. The dominant strength-controlling defect populations all have a printing-based origin, but the specific defect type varies with print orientation. Lowest performance results from alignment of the print axis along the bar length, yielding a low Weibull modulus arising from weak delamination flaws. Results point towards slurry reformulation as a potential design solution.

5:00 PM
Mechanical Behavior and Microstructural Evolution of Additively Manufactured Ti Modified Al 2024 Alloy: Saurabh Gairola[1]; *R. Jayaganthan*[1]; [1]Indian Institute of Technology Madras

The current study investigates the effects of built orientation and T6 ageing heat treatment on mechanical properties and microstructural evolution of Ti-modified Al 2024 alloy. The additive manufacturing of high-strength Al alloys such as Al 2024 alloy, suffers from high solidification cracking. Therefore, the present work has attempted to incorporate Ti to promote the columnar to equiaxed transformation and reduce the solidification cracking. The mechanical properties such as tensile, hardness, fracture toughness, and fatigue life were measured experimentally for different orientations in as fabricated and aged samples, and the corresponding strengthening mechanisms were explored in detail. The ultrafine grains (of average grain size 0.4 µm) produced due to Ti addition, along with the strengthening precipitates such as Al2Cu and Al2CuMg, characterized through SEM/EBSD & TEM, were observed to be the primary strengthening mechanism contributing to the high mechanical properties, which are comparable to their conventional wrought counterparts.

Accelerating Discovery for Mechanical Behavior of Materials 2024 ML Applications and Extreme Environments

Wednesday PM **June 19, 2024**	**Room: Center Street Room A** **Location: Hilton Cleveland Downtown**

Session Chair: To Be Announced

1:40 PM Invited
Understanding and Mitigating Bias in Autonomous Materials Characterization and Discovery: *Jason Hattrick-Simpers*[1]; [1]University of Toronto

Since the publication of the Mission Innovation Materials Acceleration Platform, AI is increasingly responsible for driving automated experimental and computational campaigns. There have been multiple case studies for which autonomy was demonstrated to successfully drive materials optimization or discovery and the world of scientific robots has moved from science fiction to reality. However, within the AI community it is recongized that AI's carry with them their creators' biases which has serious implications for model deployment. Using specific case studies, I will illustrate how these biases arise in materials science and specific steps that can be taken to remove them. Specifically, I will discuss some of our recent work in (1) reducing human bias in label generation by applying robust statistics to spectroscopic data analysis, (2) identifying and mitigating search space bias through model disagreement, and (3) demonstrating how to use active learning to create optimally informative datasets for model training.

2:10 PM
Accelerated Discovery of Material Physics Using AI/ML Approaches: *Surya Kalidindi*[1]; [1]Georgia Institute of Technology

Accelerated refinement of multiscale material models (ranging from atomistic to the macroscale) demands the development and implementation of novel high throughput strategies in both experimentation and physics-based simulations, and their seamless integration using the emergent AI/ML (artificial intelligence/ machine learning) toolsets. This talk presents a novel information gain-driven Bayesian machine learning framework with the following salient features: (i) explicit consideration of the physics parameters as inputs (i.e., regressors) in the formulation of the material physics models needed to drive materials discovery, design and development workflows; (ii) Bayesian design of experiments strategies that maximize the expected information gain; (iii) versatile feature engineering for multiscale material internal structure using the formalism of n-point spatial correlations; (iv) amenable to a broad suite of surrogate model building approaches; and (vi) Markov chain Monte Carlo (MCMC)-based computation of posteriors for physics parameters using available experimental observations (usually disparate, incomplete, and uncertain).

2:30 PM
Tailoring Metastability Due to Rapid Solidification to Achieve High-strength Printable Al Alloys: *S. Mohadeseh Taheri-Mousavi*[1]; [1]Carnegie Mellon University

Printable aluminum alloys with high strength are a highly demanding class of alloys that are used, eg, in the body of airplanes and cars. However, there are few high-strength alloys that are printable. We exploited metastable phases due to the rapid solidification of powder bed fusion and transformed the length scale of our strengthening $L1_2$ phases from micro to nanoscale. The strength has an inverse relationship with this length scale. We combined integrated computational materials engineering and advanced machine learning methods and designed a composition for our target nanoscale $L1_2$ phases that have extremely low coarsening rates and all are initially precipitated as metastable phases. The hardness of the as-built samples is comparable to wrought Al7075. We also performed tensile tests and our alloy showed 410 MPa strength. The combined numerical and experimental techniques provide an efficient pathway for transformative future alloy design by various manufacturing techniques, especially additivemanufacturing.

2:50 PM
Advancing Multiscale Materials Characterization Through Machine Learning Integration: *Reeju Pokharel*[1]; [1]Los Alamos National Laboratory

We address the difficulty of characterizing mesoscale materials behavior across various spatial and temporal scales, emphasizing the need for faster data analysis capability to enable multiscale experiments at light sources. The present bottlenecks in the data inversion process hinder instantaneous feedback, thereby limiting our capability to pinpoint key areas of interest in real-time during experiments for guiding multiscale measurements. In this work, we demonstrate machine learning (ML) techniques to reconstruct crystal orientations from diffraction patterns, the refinement of ML algorithms for superior prediction accuracy, and the integration of physics-based principles to strengthen the robustness of these ML models. The overarching goal is to enable multiscale material characterization studies in beamline settings, ensuring immediate feedback and reducing the time required for data analysis and interpretation. Such integrated approach is anticipated to improve our understanding of mesoscale material dynamics.

3:10 PM Networking Break

4:00 PM Cancelled
Nanoindentation Study on the Hydrogen Effects in High- and Medium-entropy Alloys: Zhe Gao[1]; Yakai Zhao[2]; Upadrasta Ramamurty[3]; *Jae-il Jang*[1]; [1]Hanyang University; [2]Institute of Materials Research and Engineering; [3]Nanyang Technological University

4:20 PM
Approaching Plasticity Through Elastic-plastic Strain Gradients: Saurabh Kumar[1]; Bhargav Sudhakar[1]; Namit Pai[1]; *Indra Samajdar*[1]; [1]Indian Inst of Tech

This study involves microscopic digital image correlation, with high resolution microtexture measurements in scanning and transmission electron microscopes. The objective is to bring out the formation of new dislocation boundaries and lattice curvatures, during interrupted but controlled tensile deformation. In particular, direct observations are used to establish the role of elastic-plastic strain gradients on the plasticity of both cubic (bcc-iron) and hexagonal (titanium) polycrystalline metallic material. These observations range from slip transfer across grain boundaries, lattice curvatures in the grain interior and formation of non-crystallographic micro-bands. It was shown that the formation of such varied features includes both plastic and elastic strain gradients.

4:40 PM
Corrosion Fatigue Behaviour of Repititive Corrugation and Straightening Processed AA5083 Alloy: *Balasivanandha Prabu Shanmugavel*[1]; Sri Rathinamani Ramdoss[1]; Manikandan Murugan[1]; Pooja Kathiresan[1]; [1]Anna University

This work discusses the corrosion-fatigue behaviour of ultrafine-grained (UFG) AA5083 alloy. The UFG specimens were prepared by Repetitive Corrugation and Straightening (RCS) Process. The hardness and the tensile strength of the UFG alloy increased up to 27% and 24% respectively compared with the unprocessed alloy. Fatigue tests were conducted in a corrosive medium of 3.5% NaCl with a pH level of 6.3 in case of both unprocessed and RCS processed alloy, at a constant stress ratio of R= -1 and frequency = 20 Hz. Due to a more rapid formation of a passive layer on the UFG alloy, decreases the corrosion rate by 68%. In fact, a nearly 20% increase in fatigue life was observed in the RCS processed material compared with the unprocessed variant. In the unprocessed AA 5083 alloy, crack propagation at all stress levels is mediated by inter-granular corrosion.

5:00 PM
Eliminating Brittle Failure by Advanced Casting: *John Campbell*[1]; [1]University of Birmingham

Enhanced casting techniques are now demonstrated to raise properties simply by avoiding the formation of defects. The potential for increased properties by eliminating defects appears to exceed by far the capabilities of the usual metallurgical techniques of alloying and heat treatment. It is discovered that precipitates such as carbides in steels do not form on grain boundaries, they form on bifilm cracks (a high proportion of which are at grain boundaries). Closed bifilm cracks are prized open by the precipitation of inclusions, causing the metal to be sensitized to fracture by fatigue, creep, stress corrosion cracking and hydrogen embrittlement. The mysterious fracture feature, the fisheye, is an integral part of the fracture mechanism. Enhanced steels and Al alloys are currently being demonstrated (at reduced cost). For the first time we will be capable of manufacturing metals resistant to failure by fracture, possibly irrespective of mechanism. Metals we can trust.

Symposium on Digital & Robotic Forming 2024
Microstructure In Deformation Processing

Wednesday PM
June 19, 2024

Room: Center Street Room B&C
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

1:40 PM possible invited slot

2:10 PM
Modifying AM Microstructure and Process Defects by Post-process Forging: *Austin Ngo*[1]; Noah Kohlhorst[2]; Svitlana Fialkova[3]; Glenn Daehn[2]; Bradley Jared[4]; Jian Cao[5]; John Lewandowski[1]; [1]Case Western Reserve University; [2]The Ohio State University; [3]North Carolina Agricultural and Technical State University; [4]University of Tennessee, Knoxville; [5]Northwestern University

Additive Manufacturing (AM) processes have versatile capabilities but are susceptible to the formation of as-cast non-equilibrium microstructures, process-induced defects, and porosity, which have deleterious effects on the mechanical performance. Isothermal forging was investigated as a novel post-processing technique for refining microstructure, reducing process defect severity, and thereby improving mechanical properties. Specimens of Laser Powderbed Fusion (LPBF) AlSi10Mg were fabricated over a range of process parameters and tensile tested, in addition to examining the effects of isothermal forging at different temperatures and strain rates on the as-deposited materials. The microstructures, process defect populations, and tensile properties of both as-deposited and forged materials were quantified and analyzed by OM, EBSD, CT, and SEM. The effects of deposition conditions and forge post-processing on LPBF AlSi10Mg will be discussed in terms of microstructure, mechanical properties, and fractography.

2:30 PM
Refinement of Microstructure and Mechanical Properties of Robotic Wire Arc Additively Manufactured (WAAM) AISI 316LSi Using Forging.: *Vishnu Ramasamy*[1]; Brett Ley[1]; Noah Kohlhorst[2]; Glenn Daehn[2]; Jan Dzugan[3]; Zhigang Xu[4]; Bradley Jared[5]; Tony Schmitz[5]; Jian Cao[6]; Jennifer Carter[1]; John Lewandowski[1]; [1]Case Western Reserve University; [2]Ohio State University; [3]COMTES FHT a.s.; [4]North Carolina Agricultural and Technical State University; [5]University of Tennessee; [6]Northwestern University

The effects of forging on the microstructure and mechanical properties of AISI 316LSi produced via Wire Arc Additive Manufacturing (WAAM) were investigated in this work, using Cylindrical and novel Double Cone samples. Large-scale deposits (10" x 7" x 2.5") of AISI 316LSi were prepared in collaboration with Lincoln Electric Additive Solutions using their WAAM robot cell. The effects of changes in strain rate and forging temperature on the microstructure, ferrite content, and hardness properties of the deposits will be reported for two different orientations (Deposition direction – X axis and Building direction – Z axis), along with the changes in the anisotropy of tensile properties before and after forging.

2:50 PM
Generating Digital Shadows of Workpiece Temperature During Thermomechanical Processes: *Albert Ostlind*[1]; Suzanne Tkach[2]; Rob Mayer[3]; Amy Clarke[1]; Kester Clarke[1]; [1]Colorado School of Mines; [2]Tkach Consulting; [3]Queen City Forging Company

Due to the sensitivity of mechanical properties as a function of temperature observed in many structural materials, predicting temperature distribution during thermomechanical processing is of great interest. However, in many cases there is no feasible way to directly observe or measure the internal temperature and surface contact measurements may also be impossible. This work utilizes non-contact surface measurements made by infrared cameras to generate initial conditions for finite element models of forging and heat treatment processes. Time synchronized measurements made under controlled conditions of tooling internal temperatures, and workpiece surface temperature by K-type thermocouples were used to validate the camera surface readings and the simulated internal predictions.Toward future integration of such a system into an Industry 4.0 manufacturing process, the data pathways and critical parameters needed to accurately pass information automatically between generic temperature sensors and finite element software were investigated.

3:10 PM Networking Break

4:00 PM
Deep Drawing and Spin Forming: A Comparison Study: *Melissa Thrun*[1]; Allie Glover[1]; Matthew Zappulla[1]; Kayla Molnar[1]; Paul Gibbs[1]; [1]Los Alamos National Laboratory

Incremental forming techniques rely on strain paths that may be radically different than traditional methods. Importantly, the final properties of the metal are rarely independent from the strain history associated with the processing method: understanding differences between representative strain histories is key to advancing incremental forming techniques. This work seeks to relate the geometry, microstructure, and properties of mild steel cylinders to the strain history resulting from two forming methods: spin forming and deep drawing. Experimental results indicate distinct microstructures arising from the two methods: spin forming produces microstructures with elongated, dislocated grains with edge-to-edge variation, while drawing produces dislocated grains with variation from center to edge. Corresponding changes in the local hardness and mechanical properties were measured. These data are expected to facilitate a discussion of material property variation which may be rationalized through consideration of the local strain gradients arising from each method.

4:20 PM
Adaption of Double-cone Forming Geometry to Reduce the Experimental Expenditures Necessary to Create Forming Process Maps: Brett Ley[1]; Vishnu Ramasamy[1]; Jackson Smith[1]; Caleb Campbell[2]; Brett Brady[2]; Noah Kohlhorst[3]; Brian Thurston[3]; Glenn Daehn[3]; Bradley Jared[2]; Zhigang Xu[4]; John Lewandowski[1]; *Jennifer Carter*[1]; [1]Case Western Reserve University; [2]University of Tennessee, Knoxville; [3]The Ohio State University; [4]North Carolina A&TSU

A process map is an explicit representation of the microstructural response of a material to imposed process parameters. Historically, creating these maps has required a large design of experiments (DOE) to characterize the flow performance and microstructure from uniaxial compression experiments conducted at six or more strain rates and temperatures to various incremental total strain accumulation. In 2000, Jackson et al. (DOI: 10.1179/026708300101507433) introduced the double-cone geometry. This novel geometry reduced the volume of material necessary for the DOE by imposing a linearly increasing effective strain over the radius. We adopt this approach to establish microstructurally-informed process models in 316 stainless steel in the presented work. We discuss modification of the geometry for material constraints of additively manufactured preforms and sheet/plate material; the quantification of microstructural metrics; and first attempts at computationally efficient models that would enable on-line modification of robotic incremental rolling and forming operations.

4:40 PM
Microstructural Evolution and Corrosion Resistance of 316 Stainless Steel by Double-sided Incremental Sheet Forming: *Nhung Nguyen*[1]; Putong Kang[1]; Fanglei Hu[1]; Zhigang Xu[2]; Svitlana Fialkova[2]; Jian Cao[1]; [1]Northwestern University; [2]North Carolina A&T University

The 316 stainless steel is a popular grade of stainless steel in engineering materials for its exceptional blend of mechanical properties and excellent corrosion resistance, making it suitable for various structural and fabrication purposes. We study the microstructural evolution and corrosion resistance of 316 stainless steel sheets deformed by Double-Sided Incremental Forming and rolling in saline solution, connecting to deformation-induced phase transformation from austenite to martensite and processing parameters. The 316 stainless steel sheets undergo incremental deformation at room temperature, which induces martensitic phase transformation on the surface. The different processing condition has promoted different deformed microstructures, including surface roughness and martensite phase volume. The other 316 stainless steel sheets undergo various thickness reductions at different strain rates and temperatures by rolling. The microstructural characterization by Electron Backscattered Diffraction is used to assess the impact of forming conditions on the microstructural evolution and investigate the weight loss during corrosion.

5:00 PM
Influence of Feedrate on Microstructure and Hardness of Conventionally Spin-formed 6061-O Plate: *Andrew Boddorff*[1]; Cecilia Mulvaney[1]; [1]NASA Langley Research Center

The influence of feedrate on the properties and microstructure of spin-formed aluminum alloy 6061 is explored utilizing microhardness mapping and microtextural analysis via electron backscatter diffraction (EBSD). The varying hardness profiles and microtexture are compared not only between samples spin-formed at various feedrates, but through the thickness of the samples to understand microstructural gradients that could lead to mechanical anisotropy and changes in formability. The resulting hardness data show a clear gradient from the outer mold line to the inner mold line that varies with feedrate and can relate to the imparted strain in the material. The microtextural mapping indicates a slight influence from feedrate, but shows trends through the thickness of the material that suggest varying locationally dependent stress states. The results show for the first time the influences of spin forming on hardness and texture that could be utilized to optimize spin forming processing parameters and mechanical performance.

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) Machine Learning - Microstructure

Thursday AM
June 20, 2024

Room: Hope Ballroom A
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

8:30 AM Invited
Reproducible Quantification of the Microstructure of Complex Quenched and Quenched and Tempered Steels Using Modern Methods of Machine Learning: *Björn Bachmann*[1]; Martin Müller[1]; Dominik Britz[2]; Marie Stiefel[1]; Frank Mücklich[1]; [1]Saarland University; [2]Materials Engineering Center Saarland

This study aims to address the limitations of conventional methods for assessing microstructures by using machine learning techniques. By using representative data and objective ground truth, ML models can achieve reproducible and automated microstructure evaluations. However, creating a definitive ground truth can be challenging in complex use cases. The study uses microstructures of highly complex Q/QT steels as a showcase, using patch-wise classification and a sliding window technique to segment entire microphotographs. The researchers used correlative microscopy, including micrographs from light optical microscopes (LOM) and scanning electron microscopes (SEM), and data from electron backscatter diffraction (EBSD) to train accurate machine learning models for classifying LOM or SEM images. Despite the complexity of the steels processed, the automated ML approaches achieved classification accuracies of 88.8% for LOM images and 93.7% for high-resolution SEM images, demonstrating close-to-superhuman performance compared to traditional subjective evaluations by experts.

9:00 AM
Enhancing Machine Learning Classification of Microstructures: A Workflow Study on Joining Image Data and Metadata in CNN: *Marie Stiefel*[1]; Martin Müller[1]; Frank Mücklich[1]; [1]Saarland University

In view of the paradigm shift towards data-driven research in materials science and engineering, handling large amounts of data becomes increasingly important. The applying FAIR data principles emphasize the importance of metadata describing datasets. We propose a novel data processing and machine learning pipeline to extract metadata from micrograph image files, then combine image data and their metadata for microstructure classification with a deep learning approach compared to a classic machine learning approach. The pipeline consists of a metadata extractor followed by transfer of both metadata and TIF image files into readable formats and an encoding step for the metadata. Image data is processed using a feature extractor such as ResNet50 or VGG16 as a backbone, followed by several dense layers, and then combined with processed metadata in a concatenating layer. In this use case, the impact of metadata strongly depends on the machine leaning approach and the model hyperparameters.

9:20 AM
Impact of Different Training Datasets on Machine Learning Based Grain Growth Model and Grain Growth Kinetics: *Vishal Yadav*[1]; Joseph Melville[2]; Amanda Krause[3]; Joel Harley[2]; Michael Tonks[1]; [1]Department of Materials Science & Engineering, University of Florida; [2]Department of Electrical and Computer Engineering, University of Florida; [3]Department of Materials Science & Engineering,Carnegie Mellon University

In this study, we investigate the influence of training datasets generated from Monte Carlo Potts (MCP) and Phase-field (PF) simulations on the PRIMME (Physics-Regularized Interpretable Machine Learning Microstructure Evolution) model for isotropic grain growth prediction. Despite nearly identical initial conditions, the PRIMME model trained with MCP simulation data captures most normal grain growth characteristics but fails to reproduce the von Neumann-Mullins' relationship and circular grain evolution. In contrast, the PRIMME model trained with PF simulation data successfully replicates all typical normal grain growth characteristics. Notably, both PRIMME models, whether trained with MCP or PF data, exhibit accelerated kinetics compared to the underlying training datasets, highlighting the significant impact of the simulation method on the model's learning behavior. This insight is invaluable for optimizing the PRIMME model's performance when training with experimental data.

9:40 AM
Equivariant Neural Networks for Controlling Dynamic Spatial Light Modulators: *Sumukh Vasisht Shankar*[1]; Rui Wang[2]; Darrel D D'Souza[3]; Jonathan Singer[3]; Robin Walters[1]; [1]Northeastern University; [2]MIT; [3]Rutgers University

Spatial Light Modulators (SLMs) are devices that manipulate light via phase/intensity-altering pixels. A recent alternative design involves creating a phase mask by directing a thin film of fluid with thermocapillaryforces generated by a controlled temperature map. However, determining the required input temperature for a specific height profile proves challenging due to the intricate thin film equation governing temperature-height relations. To solve this, we employ deep neural networks, crafting equivariant models with scale and rotation symmetry. These models outperform non-equivariant counterparts in accuracy and computational efficiency, addressing the numerical challenges associated with the thin film equation. Beyond offering insights into the temperature-height relationship, this research holds implications for numerous applications, particularly in high-power laser systems. Its success demonstrates more efficient and effective ways to deploy the process of modulation of light in SLMs in a variety of applications.

10:00 AM Break

10:20 AM
Using Unsupervised Learning to Cluster Fatigue Life Based on Small Crack Characteristics: *Katelyn Jones*[1]; Paul Shade[2]; Patrick Golden[2]; Reji John[2]; Elizabeth Holm[3]; Anthony Rollett[1]; [1]Carnegie Mellon University; [2]Air Force Research Laboratory; [3]University of Michigan, Ann Arbor

This work collects scanning electron microscope (SEM) images of Ti-6Al-4V fatigue fracture surfaces and applies convolutional neural networks to build a dataset of fatigue fracture surface images and make a connection between them and fatigue life. Round bar specimens used in a previous study on fatigue life at various stress levels have been imaged in regular intervals with an SEM. The images capture the crack initiation site, short crack, and steady crack regions; multiple magnifications were utilized to determine which length scale allows the machine learning algorithms to infer physically meaningful information. The images are used to train CNNs from scratch and compared using unsupervised machine learning methods to determine if fracture surface alone can be linked to the fatigue lifetime. The images taken, the algorithms used, identified fatigue properties, and fracture characteristics will be presented.

10:40 AM
Persistent Homology for Microstructure Manifold Construction: *Simon Mason*[1]; Jeff Simmons[2]; Megna Shah[2]; Stephen Niezgoda[1]; [1]Ohio State University; [2]AFRL

Quantitative microstructure metrics are an integral component of understanding processing-structure-property relationships. Persistent homology can be used to summarize microstructural features at multiple length scales and fingerprint equivalent microstructures. By developing a method to construct a continuous manifold from microstructure descriptors that can be mapped back to processing conditions, a bi-directional relationship on how processing and microstructure impact each other can be learned. This microstructure manifold can be exploited to better understand regions of processing parameters where local changes have a small or large impact on resulting microstructure, as well as help define safe boundaries for potential processing conditions.

11:00 AM
Utilizing Machine Learning to Generate Representative Euler Angles for Large EBSD Datasets: *Janith Wanni*[1]; Dan Thoma[1]; [1]Universiy of Wisconsin Madison

Generating reduced-order synthetic grain structures that accurately represent the grain structures of a material is important for efficient crystal plasticity modeling. In this study, a novel machine-learning-based approach for generating representative Euler angle datasets that mimic the crystallographic texture of EBSD datasets is introduced. The method employs K-means clustering and density-based sampling in a closed-loop iteration to create representative Euler angle datasets. Proof-of-principle experiments were performed on a quench and tempered steel. Validation of the new approach was extended to twenty datasets, including BCC, FCC, HCP, orthorhombic, and monoclinic unit cells, thereby encompassing a broad range of materials and crystal structures. Pixel-wise comparisons of the pole figures indicate a match exceeding 94%, outperforming traditional methods, which achieve less than 80% accuracy. The new method is capable of achieving a 6-fold reduction in dataset size without compromising the crystallographic texture of the EBSD data.

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) Machine Learning Simulations

Thursday AM	**Room: Hope Ballroom B**
June 20, 2024	**Location: Hilton Cleveland Downtown**

Session Chair: To Be Announced

8:30 AM Invited
Machine Learning Approach to Phase Recognition and Prediction of Mechanical Properties: Bin Zhang[1]; Aiyshe Jin[1]; Akanksha Parmar[1]; *Yung Shin*[1]; [1]Purdue University

This presentation covers a deep learning scheme of phase recognition for steel materials. A convolutional neural network (CNN) classifier is established, such that the martensite phase, which has a substantial impact on the mechanical properties of steels, can be recognized from microstructure images and its volumetric fraction can also be estimated from multi-phase microconstituents. The testing results on an ultrahigh carbon steel dataset proved that the developed scheme has good phase recognition accuracy. The estimated martensite fraction can be used as an essential feature to predict the mechanical properties of materials in additive manufacturing. The procedures were applied to train a CNN model using H13 SEM collected from the literature and then the martensite fraction was extracted with this trained model. Subsequently, a multilayer ANN model was constructed and trained to predict the mechanical properties with 11 input elements, including the martensite fraction and the grain size area density bins.

9:00 AM
Inverse Design of High-temperature Al-alloys Using Hybrid CALPHAD-based ICME Techniques: *Benjamin Glaser*[1]; S. Mohadeseh Taheri-Mousavi[1]; [1]Carnegie Mellon University

High temperature strengthening Al-alloys are in high demand for automotive and aerospace industries due to their high strength, lightweight, machinability, and low cost. We discovered a pathway to strengthening by enabling significant length scale reduction of $L1_2$ particles by activating metastable phases due to rapid solidification and their transformation after aging. Precipitates formed in this way develop at a nanometer length scale, significantly enhancing strength. The performance of this record high-temperature strength printable Al alloy from the Al-Ni-Er-Zr-Y-Yb system was validated in experiments. To further enhance this, on data from CALPHAD-based ICME calculations, we applied various unsupervised machine learning techniques and Bayesian optimization to efficiently explore high dimensional compositional space and optimized the complex objective functions. We discovered that changing the composition enables a 6x increase in volume fraction of strengthening precipitates versus benchmark designs, while retaining the nanometer length scale achieved by activating the metastable phase.

9:20 AM

Real-time Predictions of Distortion and Residual Stress Resulting From Weld Sequences Using Machine-learning Algorithms: *James Sobotka*[1]; Matthew Robinson[1]; Jake Janssen[1]; [1]Southwest Research Institute

Physics-based simulation is a common tool in the fabricated components and structures community. Unfortunately, these simulations do not account for real world manufacturing variation, i.e., geometric ill-fit, that may dictate or drive a process change. Using advances in artificial intelligence and new machine learning frameworks, we now have an opportunity to train a real-time algorithm that can assess the input variation to a process and to update in real-time a process based on the geometry presented, even though it deviates from CAD. In this talk, we outline a framework to enable an intelligent robotic system to visualize a presented condition and leverage learning from physics-based simulations and ongoing production history to generate optimal process plans. These developments take advantage of both new approaches for machine learning based frameworks as well as the ability to execute at the rate of production, leading to improved operational efficiencies and better performing fabricated products.

9:40 AM

In-situ Melt Pool Morphology Estimation From Thermal Imaging via Vision Transformers: *Odinakachukwu Ogoke*[1]; Peter Pak[1]; Alexander Myers[1]; Guadalupe Quirarte[1]; Jack Beuth[1]; Jonathan Malen[1]; Amir Barati Farimani[1]; [1]Carnegie Mellon University

Insufficient overlap between the melt pools produced during Laser Powder Bed Fusion (L-PBF) can lead to lack-of-fusion defects and deteriorated mechanical response. In-situ monitoring of the below surface morphology of the melt pool requires specialized equipment that may not be readily accessible or scalable. Therefore, we introduce a machine learning framework to correlate in-situ thermal images observed via two-color thermal imaging to the two-dimensional profile of the melt pool cross-section. Specifically, we employ a temporal Vision Transformer to establish a correlation between single bead off-axis thermal image sequences to melt pool cross-section contours measured via optical microscopy. Our framework is able to model the curvature of the below surface melt pool, with improved performance in high energy density regimes compared to analytical melt pool models. The performance of this model is evaluated through dimensional and geometric comparisons to the corresponding experimental melt pool data.

10:00 AM Break

10:20 AM

Machine Learning-enhanced Prediction of Surface Smoothness for Inertial Confinement Fusion Target Polishing Using Limited Data: *Antonios Alexos*[1]; Junze Liu[1]; Akash Tiwari[2]; Kshitij Bhardwaj[3]; Sean Hayes[3]; Satish Bukkapatnam[3]; Pierre Baldi[1]; Suhas Bhandarkar[3]; [1]University of California, Irvine; [2]Texas A&M University; [3]Lawrence Livermore National Laboratory

In the Inertial Confinement Fusion (ICF) process, roughly a 2mm spherical shell made of high-density carbon is used as the target for laser beams, which heat it to the energy levels needed for a high fusion yield [1]. The surface quality of the shell (smooth, round, defect-free) has been identified as one of the drivers which can be controlled during the fabrication process [3]. To meet these specifications, the shells are meticulously polished, in multiple stages. The process is monitored by measuring shell surface roughness after each step, but this measurement is labor-intensive, time-consuming, and requires a human operator. To speed up this process, we propose to use Machine Learning to automatically predict surface roughness from the vibration data collected from an accelerometer connected to the polisher. Such models can generate surface roughness of the shells in real-time, allowing the operator to make changes to the polishing for optimal results.

10:40 AM

Graph-based Machine Learning to Assess Particle Growth Kinetics From Image Sequences: *Sameera Nalin Venkat*[1]; Thomas Ciardi[1]; Preston DeLeo[1]; Mingjian Lu[1]; Frank Ernst[1]; Yinghui Wu[1]; Roger French[1]; Laura Bruckman[1]; [1]Case Western Reserve University

We present a graph neural network framework to assess particle growth kinetics in different materials systems. We define a metric for similarity, quantitatively accounting for particle eccentricity, radial growth rate, and final size between particles. Using a graph neural network architecture, we predict the similarity between particles across various materials systems at different stages of growth. We design our training dataset by choosing particle pairs that obey established growth kinetics models and using domain expertise. Based on pairwise particle similarity analysis, we infer the overall behavior of materials systems using various machine learning algorithms. We implement this framework for fluoroelastomer films undergoing crystallization due to thermal aging. We track the pairwise similarity for crystallite pairs at different times and correlate them to growth kinetics models. As a result, we can quantify particle behavior in a pairwise fashion, leading to improved statistics.

11:00 AM

Uncertainty Quantification in Machine-learning Models for Predicting β-phase Volume Fraction From Synchrotron X-ray Diffraction Patterns: *Ayorinde Olatunde*[1]; Weiqi Yue[1]; Pawan Tripathi[1]; Roger French[1]; Anirban Mondal[2]; [1]Materials Data Science for Stockpile Stewardship: Center of Excellence, Case Western Reserve University; [2]Department of Mathematics, Applied Mathematics and Statistics, Case Western Reserve University

While many machine learning methods focus on deterministic and accurate prediction, we aim to quantify the uncertainties in these predictions. In particular, we focus on predicting the -phase volume fraction, with its uncertainties, in a Ti–6Al–4V alloy during heat treatment from image sequences of 2D diffraction patterns recorded at a synchrotron beamline. In the first approach, we used Gaussian Process (GP) to model the relationship between optimal principal components of the 2D diffraction pattern and the -phase volume fraction. A GP represents a distribution over a functional relationship by specifying a multivariate normal (Gaussian) distribution over all possible function values, from which, given a set of data points, we can make predictions on an unobserved data point and then carry out uncertainty analysis using predictive probability distribution. We quantitatively compared the GP results with an alternate procedure that used Convolution Neural Network and quantified its uncertainty by Monte Carlo ensemble.

11:20 AM

Closing the Loop in Direct-chill Casting of Aluminium Alloys, a Deep Learning Approach: *Loic Fracheboud*[1]; Julien Valloton[1]; [1]GAP Engineering SA

In Direct-Chill casting, the process is driven by a set of instructions (a recipe). The machine then measures the variables and adjusts them to match the recipe, but it can only adjust the process variables that it can measure and compare to the given setpoints. This is where our solution can bring novelty to the industry. We propose to use a Deep Learning model to predict the process variables that are not measured by the machine, and to extract more information than the sum of the measured variables. The goal is to tie the experience of failed and successful, or even exceptional, castings to the process variables used to produce them. By learning what makes a successful and great quality ingot, the model can then be used to avoid the pitfalls of the process and to help adjust the process variables to produce the best quality ingot possible.

Accelerating Discovery for Mechanical Behavior of Materials 2024 Design III

**Thursday AM
June 20, 2024**

**Room: Center Street Room D
Location: Hilton Cleveland Downtown**

Session Chair: To Be Announced

8:30 AM Invited
Higher-order Continuum Models Based Upon Granular Micromechanics Predict Metamaterials With Granular Motif: Theory and Experiments: *Anil Misra*[1]; [1]Florida International University

Granular materials are examples of materials systems that exhibit a range of behavior that have defied descriptions based upon either classical continuum or discrete models. Micro-macro analysis of such materials using granular micromechanics approach (GMA) shows that higher-order continuum models predict interesting non-standard emergent behaviours at the macro-scale. Using this analysis we have designed and fabricated (meta)materials with prescribed grain-pair interactions. The microscale deformation under extension and compression of these (meta)materials were analysed using digital image correlation (DIC). In this presentation, we will describe the theoretical development founded upon micro-macro kinematical identification and principle of virtual work leading to higher-order continuum model that connect the macroscale behavior to the microscale mechanisms. Metamaterials of granular motif and unusual emergent behavior are conceived using the derived theoretical model. We then experimentally evaluate the designed metamaterial, particularly in relation to the grain motions and the emergent non-standard macro-scale response.

9:00 AM
Tungsten Carbide-modified Nimonic 80A Alloy: *Martina Koukolikova*[1]; Pavel Podany[1]; Sylwia Rzepa[1]; David Hradil[1]; Michal Brazda[1]; [1]COMTES FHT a.s.

Nimonic 80A is a highly regarded nickel-based superalloy known for its exceptional high-temperature properties. In applications like forming tools, the demand for improved wear resistance is critical to prolong the material's lifespan while maintaining mechanical integrity and microstructural stability. The research focuses on incorporating tungsten carbide (WC) particles into Nimonic 80A. The powder-based directed energy deposition (DED) method added WC particles at varying concentrations (5%, 10%, 15%, and 20%) to comprehensively understand their impact. The microstructure of the modified material remains stable within specified concentration ranges, opening possibilities for applications in forming tools. This study provides valuable insights into the microstructural optimization of Nimonic 80A with WC reinforcement and highlights its potential for high-temperature and wear-resistant applications. The findings contribute to the development of advanced materials with tailored mechanical properties for demanding engineering applications in high-stress environments.

9:20 AM
Adapting FAIR Practices in Materials Science: Digital Representation of Material-specific Characterization Methods: *Bernd Bayerlein*[1]; Markus Schilling[1]; Jörg Waitelonis[2]; Philipp von Hartrott[3]; Thomas Hanke[3]; Henk Birkholz[4]; June Lau[5]; Birgit Skrotzki[1]; [1]Bundesanstalt für Materialforschung und -prüfung; [2]Leibniz-Institut für Informationsinfrastruktur; [3]Fraunhofer-Institut für Werkstoffmechanik (IWM); [4]LeLeibniz-Institut für Werkstofforientierte Technologien; [5]National Institute of Standards and Technology

Age-hardenable aluminum alloys undergo precise heat treatments to yield nanometer-sized precipitates that increase their strength and durability by hindering the dislocation mobility. Tensile tests provide mechanical properties, while microstructure evaluation relies on transmission electron microscopy (TEM), specifically the use of dark-field TEM images for precise dimensional analysis of the precipitates. However, this manual process is time consuming, skill dependent, and prone to errors and reproducibility issues. Our primary goal is to digitally represent these processes while adhering to FAIR principles. Ontologies play a critical role in facilitating semantic annotation of (meta)data and form the basis for advanced data management. Publishing raw data, digital workflows, and ontologies ensures reproducibility.This work introduces innovative solutions to traditional bottlenecks and offers new perspectives on digitalization challenges in materials science. We support advanced data management by leveraging knowledge graphs and foster collaborative and open data ecosystems that potentially revolutionize materials research and discovery.

9:40 AM
A Crystal Plasticity Study on the Effects of Strength Anisotropy on the Deformation Response of BCC Polycrystal: *Ezra Mengiste*[1]; Dominic Piedmont[2]; Mark Messner[3]; Meimei Li[3]; James Stubbins[2]; Jun-Sang Park[3]; Xuan Zhang[3]; Matthew Kasemer[1]; [1]University of Alabama; [2]University of Illinois Urbana-Champaign; [3]Argonne National Laboratory

Metallic alloys subjected to irradiated environments have been observed to possess increased yield strength and reduced ductility compared to unirradiated samples. It is important to understand the micromechanical source of these effects for the reliability of components utilized in irradiated environments. Assuming that a major contributor to this behavior is slip system strength anisotropy, we perform a study using a full-field crystal plasticity model to simulate the deformation response of idealized polycrystalline samples with strength anisotropy parameterized. We execute a suite of simulations and explore the effects of increasingly severe strength anisotropy on the reorientation trajectories and fragmentation of grains within a BCCpolycrystal. We will scrutinize individual grains and their mechanical states as a function of their local grain neighborhood, as well as the effects of the activation of secondary slip families, and results will be analyzed through the lens of insights from high energy X-ray diffraction experiments.

10:00 AM Break

10:20 AM
Microstructural Investigation of Wire Arc Additively Manufactured 316LSi in the As-deposited Condition and After Forging: *Brett Ley*[1]; Vishnu Ramasamy[1]; Noah Kohlhorst[2]; Glenn Daehn[2]; Bradley Jared[3]; Zhigang Xu[4]; Kornel Ehmann[5]; Jennifer Carter[1]; John Lewandowski[1]; [1]Case Western Reserve University; [2]The Ohio State University; [3]University of Tennessee; [4]North Carolina Agricultural and Technical State University; [5]Northwestern University

Wire Arc Additive Manufacturing (WAAM) is a near net shape solution for printing large-scale metal components. A thick wall deposit of 316LSi stainless was printed using WAAM where the heat input and interpass temperature were controlled. Several tension and fatigue crack growth (FCG) samples were machined along the x and y directions and tested. The as-deposited macrostructure, microstructure, and fracture surfaces were examined using a combination of optical metallography, scanning electron microscopy, and optical profilometry. Grain structure along the entire build direction for the deposit was characterized using optical metallography. The effect of sample orientation on the WAAM structure and mechanical performance will be summarized including Young's modulus anisotropy and orientation dependent fatigue crack growth properties. Additional characterization of the structure was performed on as-deposited material that was machined into a double cone geometry and forged.

10:40 AM
A Strong Fracture-resistant High-entropy Alloy With Nano-bridged Honeycomb Microstructure: A Critical Role of 3D Printing in Promoting Strength Without Compromising Toughness: *Punit Kumar*[1]; Sheng Huang[2]; David Cook[1]; Kai Chen[3]; Upadrasta Ramamurty[4]; Xipeng Tan[5]; Robert Ritchie[6]; [1]Lawrence Berkeley National Laboratory; [2]Massachusetts Institute of Technology; [3]Xi'an Jiaotong University; [4]Nanyang Technological University, Singapore; [5]National University of Singapore; [6]University of California Berkeley

Strengthening materials via conventional "top-down" processes involves restricting dislocation movement by precipitation or grain-refinement, which invariably restricts the movement of dislocations away from, or towards, the crack tip, thereby severely compromising their fracture resistance. A high-entropy alloy Al0.5CrCoFeNi was produced by the laser powder bed fusion process, a "bottom-up" additive manufacturing process similar to how nature builds structures, with the microstructure resembling a nano-bridged honeycomb structure consisting of a fcc matrix and an interwoven hexagonal net of an ordered bcc B2 phase. While the B2 phase, combined with high-dislocation density and solid-solution strengthening, provides strength to the material, the nano-bridges of dislocations connecting the fcc cells, i.e., channels between the B2 phase on the cell boundaries, provide highways for dislocation movement away from the crack tip. Consequently, the nature-inspired microstructure imparts the material with an unprecedented combination of strength and toughness, details of which will be discussed during the presentation.

11:00 AM
Designing Materials With Engineered Interfaces by Exploiting Underlying Structure-property Linkages: *Ankit Gupta*[1]; Garritt Tucker[1]; [1]Baylor University

Crystalline interfaces (grain boundaries (GBs)) are vital to understanding the deformation behavior of materials. As such, it becomes important to study different GB mechanisms (sliding, migration, dislocation emission) and how the interplay between these mechanisms dictates the overall interfacial strength. In this study, we leverage continuum-based metrics to identify and delineate individual GB mechanisms by mapping changes in local atomic environments during deformation. Insights into kinematic signatures of GB mechanisms and their linkages with GB structures are discussed. We further calculate contributions of GB mechanisms to the overall deformation based upon amount of microstructural strain accommodation. It is shown that the strength of interfaces is closely linked with the underlying mechanistic competition. Finally, strategies to rationally tailor the interfacial properties by altering the governing mechanistic landscape, are presented. This study will inform avenues to engineer interfaces in functional materials geared towards superior properties, like, improved nanocrystalline stability or radiation tolerance.

11:20 AM
Effects of Process Parameters on Mechanical Behavior of Wire Arc Additively Manufactured (WAAM) AISI 316LSi.: *Vishnu Ramasamy*[1]; Brett Ley[1]; John Lewandowski[1]; [1]Case Western Reserve University

The effects of changes in process parameters on the microstructure and mechanical properties of AISI 316LSi produced via Wire Arc Additive Manufacturing (WAAM) will be reported. Large-scale deposits (10" x 7" x 2.5") of AISI 316LSi were prepared in collaboration with Lincoln Electric Additive Solutions using their WAAM robot cell. The effects of changes in process parameters (Heat Input and Interpass Temperature) on the microstructure, ferrite content, mechanical properties (Tension, Impact, and Fatigue Crack Growth) and preliminary corrosion properties of the deposits will be reported for all three orientations (X [Deposition direction], Y and Z [Building direction]), along with measurements of surface roughness on the as-deposited conditions.

11:40 AM
Investigating the Nucleation and Growth of Deformation Twinning in HfNbTaTi Refractory High Entropy via a Machine Learned Interatomic Potential: *Wenqing Wang*[1]; Madelyn Payne[1]; Pedro Borges[1]; David Cook[1]; Punit Kumar[1]; Mark Asta[1]; Robert Ritchie[1]; [1]Lawrence Berkeley National Lab

Refractory high-entropy alloys (RHEA) are characterized by high strength and compressive ductility at elevated temperatures. However, their practical application is hindered by brittle failure modes when subjected to tension at ambient temperatures. The plastic deformation behavior of RHEAs is closely tied to the energetics of deformation twinning, a well-known plasticity mechanism in refractory elements at low temperatures (below room temperature). In the HfNbTaTi alloy, abundant twinning is observed across a broad temperature range from 77 K to 1073 K, potentially playing a pivotal role in its mechanical properties. Recognizing its significance and the current knowledge gap regarding deformation twinning in HfNbTaTi RHEA, we explore the nucleation and growth of deformation twinning using a machine-learned atomic cluster expansion (ACE) potential. Our findings reveal a layer-by-layer growth pattern of deformation twins initiating from a 2-layer twin embryo, characterized by a near-isosceles equilibrium twin boundary structure.

Accelerating Discovery for Mechanical Behavior of Materials 2024 In-situ and In-process of Extreme Environments

Thursday AM **June 20, 2024**
Room: Center Street Room A
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

8:30 AM Invited
In-situ XRD Fragmentation Experiments to Accurately Measure Film Fracture Stresses: *Megan Cordill*[1]; [1]Erich Schmid Institute of Materials Science

Fragmentation testing has been used for decades to assess thin film fracture and delamination through uniaxial tensile straining. Hooke's law is generally used to determine a film fracture stress from the crack onset strain observed in micrographs or measured as an electrical resistance increase. While this method is in theory suitable in the elastic regime, it neglects important film characteristics, such as residual stress, microstructure, or film architecture. Thus, there is a need to improve fracture analysis using fragmentation to avoid significant errors in measuring fracture stress or apparent fracture toughness of thin films. In-situ X-ray diffraction fragmentation experiments can measure the film fracture stress even for individual layers being part of multilayer. Which characteristics influence the apparent fracture behavior will be demonstrated on Mo thin films on polyimide.

9:00 AM

Solute Hydrogen Leads to Residual Stress Changes in Surface Engineered High Strength Steels: *David Bahr*[1]; Jia-Huei Tien[1]; Megan Reger[1]; David Johnson[1]; [1]Purdue University

Processing of many engineering components containing tempered martensitic steels often involves surface engineering steps such as shot peening, laser shock peening, or induction heat treating. These processes create compressive stresses and high dislocation densities in the near surface region of parts. Shot peened quench and tempered steel with a hardness over 45 Rockwell C in the Almen strip geometry was measured for bow, electrochemically hydrogen charged, and then the residual stresses and hardness were measured using x-ray diffraction and nanoindentation respectively. For moderate intensities H charging led to a larger bow but lower surface stress. The hardness increases with solute hydrogen. X-ray diffraction verified that severe plastic deformation and compressive residual stresses caused dislocation recovery, leading to a more gradual but deeper residual stress profile on the part, in line with a hydrogen enhanced plasticity process where charged specimens with high compressive stresses were able to undergo dislocation rearrangement.

9:20 AM

Review About In-Situ Studies at Very High-temperatures of Superalloys Using Neutrons and Complementary Methods: *Ralph Gilles*[1]; Frank Kümmel[1]; Massimo Fritton[1]; Cecilia Solis[2]; Alexander Mutschke[1]; Andreas Kirchmayer[3]; Steffen Neumeier[3]; Masood Haghighat[4]; Bodo Gehrmann[4]; [1]TU Munich; [2]Helmholtz-Zentrum Hereon GmbH; [3]Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU); [4]VDM Metals International GmbH

The development of gas turbine materials requires high-temperature strength, ductility, corrosion resistance and high creep resistance. Ni-base superalloys are the most common material for these tasks because size and volume fraction of hardening precipitates can be tuned up to very high temperatures. Using the example VDM®Alloy 780 (developed as a further improvement of the 718 alloy series) it is shown how neutron methods (neutron diffraction, small-angle neutron scattering) and complementary methods (scanning electron microscopy and atom probe tomography) support the microstructure characterization and the behavior at high-temperature processes. A sophisticated testing machine was built to perform unique experiments. [1] R. Gilles, Journal of Surface Investigations: X-Ray, Synchrotron and Neutron Techniques, (2020), 14, Suppl. 1, S69. [2] F. Kümmel et al., Metals (2021),11,719. [3] C. Solis et al., Journal of Alloys and Compounds (2022),928,167203.[4] F. Kümmel et al., Metals (2022),12,1067.

9:40 AM

Mechanical Properties of Oxide Dispersion Strengthened Inconel 625 Alloys Produced by Selective Laser Melting: *Kadir Demirci*[1]; Eda Aydogan[2]; Ilhan Bukulmez[1]; Selen Nimet Gurbuz Guner[1]; Erhan Aksu[1]; [1]Turkish Energy, Nuclear and Mineral Research Agency; [2]Middle East Technical University

Nickel-based superalloys have widespread application areas which often require harsh environments (e.g., high temperature, large radiation flux, corrosive media) and intricate shapes. To this end, a new grade of oxide dispersion strengthened (ODS) Inconel 625 (IN625) was developed using additive manufacturing (AM). The powders were mixed using various ball milling parameters. The designed alloy was produced by Selective Laser Melting (SLM) with optimized process parameters. Proper heat treatment routes were determined for optimal amount and distribution of nano-oxides and strengthening " phases. To understand the effect of additive manufacturing and existence of nano-oxides, both wrought and additively manufactured IN625 were subjected to the same heat treatment routes. Comprehensive microstructural analyses as well as mechanical tests at RT and 700 ˚C were conducted comparatively. It has been demonstrated that the AM produced ODS IN625 shows better mechanical properties.

10:00 AM Break

10:20 AM

Origins of Exceptionally High Strength Deformation Nanostructures/Crystallites and Their Universal Behavior: *Darcy Hughes*[1]; [1]Sandia National Labs (ret.)

Pressing and sliding nominally flat surfaces together creates gradients in structural size and strength with depth from the surface. Subsurface strengths reach 40% of theoretical maximum strength (E/10) via this method: micro ridges on a steel tool, high loads, and 77K in Cu plus ~ 1.5% Fe from the steel. Samples at different temperatures and loads were statistically examined via microscopy. Deformation structures follow the principal of grain subdivision identified under different deformation modes. Measured structure/strength parameters include the spacing, D_{av}^{GNB}, of deformation induced geometrically necessary boundaries that act like grain boundaries, and the incidental dislocation density in between, //961$_{av}^{ID}$. Dislocation mechanisms were demonstrated to dominate subsurface deformation at all size scales. Universal scaling of deformation structures in fcc and bcc alloys, unified by stress and physical constants, persists across 2 to 4 orders of magnitude for stress: 30MPa-4.4GPa, strain, structural size: D_{av}^{GNB}=10//956m-2.8nm, and dislocation density: //961$_{av}^{ID}$ =10>^{13}-10>^{17} m^{-2}.

10:40 AM Cancelled

Monitoring of Sintering With and Without Shrinkage via the Impulse Excitation Technique (IET): *Willi Pabst*[1]; Eva Gregorova[1]; [1]University of Chemistry and Technology, Prague (UCT Prague)

11:00 AM

Uncovering Superelastic Energy Dissipation in Monazite Ceramics via Elevated Temperature Nanoindentation: *Henry Afful*[1]; Corinne Packard[1]; [1]Colorado School of Mines

Energy damping based on phase transformation or point defect mechanisms has an extremely limited operating temperature range. For elevated temperature mechanical damping, an alternative superelastic mechanism with a wide operating temperature range is desired. Certain refractory rare earth orthophosphate ceramics exhibit energy recovery under nanoindentation hardness testing, and a reversible deformation twinning mechanism has been proposed as the origin of this recovery. Here, we investigate this recovery mechanism in two monoclinic rare earth orthophosphates (monazites) using spherical nanoindentation as a sensitive probe of deformation behavior. Cyclic loading across a range of peak loads and temperatures reveals the presence and persistence of superelastic energy damping across monazite compositions. The observed monazite behavior is similar to the elastic twinning phenomenon observed in calcite. In contrast to calcite, the damping is largely insensitive to temperatures up to at least 400C due to the refractory nature of the rare earth orthophosphates.

11:20 AM

Fracture of Refractory High Entropy Alloys in Extreme Temperature Environments: *David Cook*[1]; Punit Kumar[2]; Calvin Belcher[3]; Madelyn Payne[4]; Pedro Borges[4]; Wenqing Wang[1]; Flynn Walsh[4]; Mingwei Zhang[2]; Mark Asta[4]; Andrew Minor[4]; Enrique Lavernia[3]; Diran Apelian[3]; Robert Ritchie[4]; [1]University Of California, Berkeley; [2]Lawrence Berkeley National Labs; [3]University of California, Irvine; [4]University of California, Berkeley

Body-centered cubic (bcc) refractory high-entropy alloys (RHEAs) inhabit the two extremes of the strength-toughness trade-off across extreme temperature environments. While the group V-VI alloys, represented by the model NbMoTaW system, have high compressive strengths at high temperatures, they suffer from extremely poor tensile ductility and fracture toughness. On the other hand, the group IV-V alloys can exhibit significant tensile ductility, and high ambient temperature fracture toughness, but lose strength and ductility at higher temperatures. In this talk, a novel RHEA that beats the strength-toughness trade-off across extreme temperature regimes is discussed. This material exhibits high temperature strength, and high fracture toughness characterized by rising R-curve behavior, even in the cryogenic regime. These remarkable properties can be attributed to deformation mechanisms that cause strain softening, which runs counter to long-held notions that fracture toughness of metals is derived from mechanisms that prolong uniform ductility and delay plastic instability through strain hardening.

11:40 AM

Delineating the Alloying Elements on the Formation of Fe-Zn Intermetallics During the Liquid-metal Embrittlement of Advanced High-strength Steel: *Seungchang Han*[1]; Sang-Ho Uhm[2]; Du-Youl Choi[2]; Tijmen Vermeij[3]; Krzysztof Wieczerzak[3]; Xavier Maeder[3]; Dario Sanchez[4]; Daniel Grolimund[4]; Tea-Sung Jun[1]; [1]Incheon National University; [2]POSCO; [3]Empa; [4]Paul Scherrer Institut

Grain boundaries play a significant role in the behavior of polycrystalline materials and are often affected by intergranular degradation phenomena through liquid metal embrittlement (LME). Resistance spot welding is associated with rapid microscopic processes and drastic temperature changes, typically occurring in subsecond processing steps. The coexistence of solid substrate and liquid Zn phase further complicates direct observations at the microstructural scale. To gain more insights into the inhibition of LME and the associated nanoscopic microstructural changes in the Fe–Zn system, it is crucial to investigate these phenomena at a smaller scale. This study explores the LME behavior of two advanced high-strength steels with different chemical compositions. We reveal the presence of intermetallic phases at Zn-infiltrated grain boundaries, indicating high local stresses. Through cross-correlation-based high angular resolution electron backscatter diffraction (HR-EBSD), we confirm that boron addition can mitigate crack-initiating local stress heterogeneities arising from the intermetallic phase formation.

2nd World Congress on Artificial Intelligence in Materials & Manufacturing (AIM 2024) Poster Session

Tuesday PM
June 18, 2024

Room: Hope Ballroom E
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

An Advanced Machine Learning Approach for Identification of Grain Boundaries in Atomistic Simulation Data: Saksham Singh[1]; Akash Gupta[2]; Sumit Maurya[2]; *Surya Ardham*[3]; [1]Indian Institute of Technology Jodhpur; [2]Tata Consultancy Services; [3]TCS research

Atomistic simulations are considered a useful tool to study the defects in material. However, the analysis of results is always a tedious and time-consuming process. We present a deep learning-based approach for automated analysis of atomistic simulation data. The identification of grain boundaries (GBs) in molecular dynamics (MD) simulations of aluminum is chosen as test case. The atomic configurations representing GB are translated into a 3-dimensional array. The length and size of each element in the array are carefully optimized to create a dense representation of each atom's neighborhood while minimizing the memory and computational demands. Two variants of 3-D Convolutional Neural Networks (CNN) are trained on this dataset. The final model shows a test accuracy of more than 95% by using only the atomic coordinates as input feature. The model is further validated on an MD trajectory featuring two GBs in an aluminum supercell, showcasing its automated analysis capability.

Comparison of Prediction Performance Between Conventional and Transfer Learning for Magnetic Properties of Bulk Metallic Glasses: *Chunghee Nam*[1]; [1]Hannam University

This Study Demonstrated the Improved Prediction Performance of Magnetic Properties of Metallic Glasses with Transfer Learning to Overcome the Limitations of Scarce Data

Data-efficient Self-supervised Property Prediction for Materials Using Graph Networks: *Alex New*[1]; Michael Pekala[1]; Elizabeth Pogue[1]; Nam Le[1]; Janna Domenico[1]; Eddie Gienger[1]; Christopher Ratto[1]; Andrew Lennon[1]; Christine Piatko[1]; Christopher Stiles[1]; [1]Johns Hopkins Applied Physics Laboratory

Properties of interest for materials, such as band gap and elasticity, are related to each other: they are determined by the same underlying physics. However, materials in existing databases do not contain calculations of all properties of interest. Furthermore, subsets for which properties are calculated are often partially-intersecting and limited in size. To enable accurate and data-efficient prediction of multiple material properties, we propose a self-supervised learning (SSL) strategy, based on data augmentation strategies like perturbation and masking, as well as analyses of the spectral properties of loss function Hessians. This enables us to train property-agnostic graph networks on the large volume of materials with limited or no property calculations. Once trained, these models are finetuned on property-specific prediction tasks. We evaluate our SSL approaches on different matbench prediction tasks while varying the amount of data provided for finetuning and consider how these findings can inform further data-efficient property models.

Development for an Intelligent System for Controlling the Peripheral Temperature of the Blast Furnace: *Sumaila Omeiza Jimoh*[1]; [1]Mechanical Engineering Department, Federal University of Technology

Product policy is pivotal to the controlling the peripheral temperature of the blast furnace operations. It affect, production time and sale price and user acceptability. Hence, researchers and practitioners need to be intentional about the quality of products that are produced by PTB systems. In this work, therefore, aims to develop an intelligent system that will generate real- time product quality information for APTB technology. Based processes, with emphasis on the decision and develop an intelligent APTB decision-making support system with the goal of optimizing operations from a product evaluation perspective. The APTB systems information will enhance the pursuit of innovative works in product quality development and management. It will support stakeholder's decision- making during the design and development of tactical and strategic policy for product management.Keywords: Blast Furnace, Peripheral zone, Heat temperature, Policy, Quality, Artificial intelligence.

Fluoroelastomers Genome: Analysis of Fluoroelastomers Growth Behavior Based on Spatio-temporal Scene Graphs: *Mingjian Lu*[1]; Sameera Venkat[1]; Thomas Ciardi[1]; Pawan Tripathi[1]; Roger French[1]; Yinghui Wu[1]; [1]Case Western Reserve University

In this research, we utilize Spatio-temporal Scene Graphs to examine the growth of fluoroelastomers through Atomic Force Microscopy (AFM) videos. This method allows a detailed analysis of the temporal and spatial evolution of crystallites. Our approach identifies distinct growth phases and the factors influencing them, offering insights into crystallite formation and expansion. By dissecting the growth process, we pinpoint parameters affecting growth rate and uniformity. The Spatio-temporal Scene Graphs facilitate an in-depth examination, linking observed patterns to material properties. This study enhances our understanding of fluoroelastomer growth and showcases the potential of Spatio-temporal Scene Graphs in material science research. It opens new avenues for investigating material behavior, illustrating the methodology's effectiveness in situ analysis of complex material dynamics. This work not only furthers knowledge in material science but also demonstrates the versatility of Spatio-temporal Scene Graphs for various material science applications.

Generative Closed-loop Discovery of Materials With Multi-property Targets: Christopher Stiles[1]; Elizabeth Pogue[1]; *Alex New*[1]; Brandon Wilfong[2]; Gregory Bassen[2]; Izze Hedrick[2]; Eddie Gienger[1]; Christine Piatko[1]; Janna Domenico[1]; Kyle McElroy[1]; Timothy Montalbano[1]; Michael Pekala[1]; Michael Pekala[1]; Nam Le[1]; Christopher Ratto[1]; Andrew Lennon[1]; Tyrel McQueen[2]; [1]Johns Hopkins Applied Physics Laboratory; [2]Johns Hopkins University

Machine learning (ML) holds immense potential for accelerating the materials discovery process; however, approaches based on screening existing databases limits what these techniques might ultimately achieve. Instead of being bound to lists of known materials, generative methods offer the potential to explore a broader space of possibilities. To date, the ML processes of generating novel out-of-distribution candidates and property prediction have been pursued independently. In this work we present the first successful application of these technologies together in a single coherent workflow which incorporates ML processes together with assessments of thermodynamic stability, experimental synthesis, and characterization. We demonstrate this workflow in the context of superconductor discovery - we identified promising candidate materials, and used these predictions to extrapolate to unreported ternary compounds in the Heusler family. This success demonstrates ML can be used to push beyond the limits of datasets biased by known phase spaces and experimentalist priors.

POSTERS

Learning a Reliable Compression of In-situ, High-speed Camera Data for Additive Manufacturing: *Tian Yu Yen*[1]; Anthony Garland[1]; Daniel Moser[1]; Cody Lough[2]; Ben Brown[2]; Jon Zettwoch[2]; [1]Sandia National Laboratories; [2]KCNSC

New experimental setups in additive manufacturing (AM) now allow for in-situ monitoring of the AM process via high-speed cameras centered at the point of interest. However, the volume of data generated from the high-speed camera even for a single layer of a build can be too large to store and analyze in a reasonable time frame. We propose utilizing a variant of autoencoders to learn a reliable compression algorithm from previous video data and show that the compressed representation encodes key quantities of interest relevant to the build quality, as well as the image reconstruction error. We discuss the limitations and benefits of our approach to in-situ monitoring of the AM process.

Machine Learning to Identify Composition and Heat Treatment Schedule of Low-alloyed TRIP-aided Steel Sheets With the Strength-ductility Trade-off: *Chang-Seok Oh*[1]; Jiwon Park[1]; [1]Korea Institute of Materials Science

The Transformation-Induced Plasticity phenomenon in advanced high-strength steels, involving the conversion of retained austenite to martensite during deformation, has been harnessed to delay plastic instability, leading to an excellent balance between strength and ductility. Nevertheless, the challenge of identifying the optimal combination of multi-component alloying chemistry and processing routes to achieve the desired tensile strength and ductility persists. In this study, we developed machine learning models to predict room temperature tensile properties of low-alloyed TRIP-aided steels. This predictive framework involved data augmentation by incorporating missing information and utilizing the CALPHAD approach, followed by validation against literature values. Furthermore, we elucidated the features that influence mechanical properties and microstructure through model interpretability analyses. To further optimize the strength-ductility trade-off, we applied a multi-objective optimization strategy, intending to expand the Pareto-front systematically. Finally, we derived composition-process combinations that yield tensile-strength balance of about 35,000 MPa%, a range consistent with experimentally reported values.

Physics Inspired Modelling of the Milling Process Using a Combined Deep Learning and Symbolic Regression Approach for an Efficient Production of Battery Materials: *Ahmed Eisa*[1]; [1]Technical University of Braunschweig

With soaring energy prices, efficiency optimization of power intensive processes in the production of battery materials has become of paramount importance. The trial and error method as well as simulation techniques are typically used for process optimization, but both have major disadvantages. A more efficient data oriented approach was needed. In this work an automated mechanistic process-modelling framework for process optimization was developed. The framework combines physics informed neural networks with symbolic regression adapted optimization algorithms, to determine existing physical relationships between process parameters. As a proof of concept, the framework was applied to model the milling process based on the Netzsch-LabStar laboratory mill. The data was generated through experiments and validated CFD-DEM simulations for non-experimentally measurable parameters. Based on the generated data, the framework estimated the process model in the form of a transparent equation.

An Insight Into Predictive Modelling of NiTi Shape Memory Alloys: *Sina Hossein Zadeh*[1]; Amir Behbahanian[2]; John Broucek[2]; Mingzhou Fan[2]; Guillermo Vazquez[2]; Mohammad Noroozi[3]; William Trehern[2]; Xiaoning Qian[2]; Ibrahim Karaman[2]; Raymundo Arroyave[2]; [1]Texas A&M; [2]Texas A&M University; [3]University of South Florida

Nickel-titanium (NiTi) shape memory alloys have become increasingly pivotal across various industries, primarily recognized for their exceptional mechanical properties and corrosion resistance amalgamation. These unique properties of NiTi alloys have extended their usage, opening a diverse range of applications that have shifted the paradigm in material science and engineering. This comprehensive study demonstrates how the generation, restriction, and employment of compositional and processing features aid in the advanced development of predictive models. These multifaceted models, devised with meticulous precision, have surpassed expectations and proven to be highly effective, with an average accuracy rate of 95%. This significant rate underpins the successfully predicted transformation properties; it opens the avenue for a revolutionary procedure in controlling alloy transformation properties based on the model predictions. This innovative methodology, merging materials science thinking and data-driven studies, helps shape our future toward an even more material-efficient society.

CRowdsourced Materials Data Engine for Unpublished X-ray Diffraction: *Abhishek Daundkar*[1]; Mengying Wang[1]; Hanchao Ma[1]; Yiyang Bian[1]; Alp Sehirlioglu[1]; Yinghui Wu[1]; [1]Case Western Reserve University

We propose CRUX, a CRowdsourced Materials Data Engine for Unpublished X-ray diffraction (XRD) data, addressing key challenges in data-driven materials science. Modern multidisciplinary materials research integrates various data resources, often underutilized. CRUX establishes a materials knowledge graph, built upon specialized ontology, capturing processing metadata. This graph houses abstract knowledge from XRD datasets, evolves by recommending new datasets, and facilitates user queries, supporting "Why" and "What-if" analyses for XRD. Our goal is to collect critical data without burdening contributors, allowing the expansion of experimental/modeling datasets and fostering open collaboration. CRUX empowers the exchange of unpublished XRD data, unlocking research opportunities, like predicting materials compositions from multi-phase data. It also inspires innovative machine learning pipelines for data-driven materials science, regardless of the analysis model's current state. In collaboration with industry partners and developers, CRUX fosters a sustainable, open platform to advance materials research and accelerate scientific discoveries.

Extreme Value Statistics Analysis of Process Defects in Additive Manufacturing Materials: *Ayorinde Olatunde*[1]; Kristen Hernandez[1]; Austin Ngo[2]; Arafath Nihar[1]; Thomas Ciardi[1]; Rachel Yamamoto[1]; Pawan Tripathi[1]; Anirban Mondal[3]; Roger French[1]; John Lewandowski[2]; [1]Materials Data Science for Stockpile Stewardship: Center of Excellence, Case Western Reserve University; [2]Department of Materials Science and Engineering, Case Western Reserve University; [3]Department of Mathematics, Applied Mathematics and Statistics, Case Western Reserve University

Fatigue and fracture studies focused on process defects that occur in Additive Manufacturing (AM) materials have shown that defect populations possess features which are better measured with extreme value statistics (EVS). In AM alloys, defect occurrences increase with material volume. This situation facilitates the need to model process defects in the path of fatigue crack growth with suitable statistical tools, such as EVS, which is more cost-effective when compared to destructive experiments. The application of EVS on defect space features helps determine the difference in defects present on fracture surfaces. As the fatigue quality of any material depends on its extreme value flaws, we use the Block Maxima and Peak over Threshold methodologies to study the distribution of the features of the defects in AM Ti-6Al-4V and make recommendations for the distributions of best fit based on different scenarios with different ranges of complexity of different defect types.

Accelerating Discovery for Mechanical Behavior of Materials 2024 Poster Session

Tuesday PM
June 18, 2024

Room: Hope Ballroom E
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

Coating-free Method to Form Superhydrophobic and Superoleophilic Surface on 7075 Aluminum Alloy Surface: *Faez Qahtani*[1]; [1]Najran University

We report a coating-free method of fabricating a superhydrophobic and superoleophilic surface on aluminum 7075 alloys. High repetition rate picosecond pulsed laser is used for the generation of characteristic nanoscale surface roughness and direct writing of microscale patterns on the sample surface. Laser machining transitions the surfaces from nominally liquid-philic to nearly superhydrophilic and superoleophilic. Heat-treating the superhydrophilic and superoleophilic surface in the ethanol-vapor-rich environment reduces the surface energy and transforms the surface to superhydrophobic and superoleophilic. The fabricated surface showed no degradation in its superhydrophobicity and superoleophilicity during extended exposure to the ambient environment. The unique combination of the superhydrophobicity and superoleophilicity enables facile separation of oil and water mixtures as well as renders the surface icephobic. Repeated rinsing with DI water did not affect superoleophilicity. The water contact angle on the treated surface reduces after repeated rinsing, but reheating the surface in the alcohol-vapor-rich environment restores the superhydrophobicity.

PMD Core Ontology: Building Bridges at the Mid-level – A Community Effort for Achieving Semantic Interoperability in Materials Science: *Bernd Bayerlein*[1]; Markus Schilling[1]; Henk Birkholz[2]; Matthias Jung[3]; Jörg Waitelonis[4]; Lutz Mädler[5]; Harald Sack[4]; [1]Bundesanstalt für Materialforschung und -prüfung; [2]Leibniz-Institut für Werkstofforientierte Technologien; [3]Fraunhofer-Institut für Werkstoffmechanik (IWM); [4]Leibniz-Institut für Informationsinfrastruktur; [5]Universität Bremen

Knowledge representation in the materials science and engineering (MSE) domain is a vast and multi-faceted challenge: Overlap, ambiguity, and inconsistency in terminology are common. Invariant and variant knowledge are difficult to align cross-domain. Generic top-level semantic terminology often is too abstract, while MSE domain terminology often is too specific. This poster presents an approach to create and maintain a comprehensive and intuitive MSE-centric terminology by developing a mid-level ontology–the PMD core ontology (PMDco)–via MSE community-based curation procedures.The PMDco is designed in direct support of the FAIR principles to address immediate needs of the global experts community and their requirements. The illustrated findings show how the PMDco bridges semantic gaps between high-level, MSE-specific, and other science domain semantics, how the PMDco lowers development and integration thresholds, and how to fuel it from real-world data sources ranging from manually conducted experiments, simulations as well as continuously automated industrial applications.

Predicting Charpy Toughness From Fractographic Images: *Nathan Bianco*[1]; Kaitlynn Fitzgerald[1]; Dale Cillessen[1]; Nathan Brown[1]; Jay Carroll[1]; Kimberly Bassett[1]; Brad Boyce[1]; [1]Sandia National Laboratories

Evaluating the fracture toughness of failed in-service parts without physical material testing can accelerate failure analysis. In this study, additively manufactured Charpy bar samples were produced over a wide range of process conditions. The Charpy V-Notch toughness was measured on over 400 samples alongside corresponding optical images of the fracture surface. A series of convolution neural network models were trained to determine a correlation between these fracture toughness values and the corresponding fractographic images. In addition to analyzing the native images at 1800 x 1800 pixels, the images were downsampled to various levels to evaluate the tradeoff between image fidelity, predictivity, and computational efficiency. The models successfully predicted the fracture toughness for a diverse range of fractographic images while also identifying interpretable physical characteristics associated with changes in toughness, such as: porosity, shear lips, and fracture surface edges. This work illustrates a machine learning approach to facilitate failure analysis.

Temperature Dependence of Young's Modulus and Damping of Natural Basalt Rock and Melt Cast Basalt Products Determined via the Impulse Excitation Technique (IET): *Eva Gregorova*[1]; Willi Pabst[1]; [1]University of Chemistry and Technology, Prague (UCT Prague)

Symposium on Digital & Robotic Forming 2024 Poster Session

Tuesday PM
June 18, 2024

Room: Hope Ballroom E
Location: Hilton Cleveland Downtown

Session Chair: To Be Announced

Control System Development for a Lab-scale Forging Manipulator for Deformation Model Validation Experiments: *Lennard Poliakov*[1]; Evan Penczek[1]; Albert Ostlind[1]; Natalie Compton[1]; Mason Weems[1]; Kester Clarke[2]; [1]Colorado School of Mines; [2]Los Alamos National Laboratory

A linear-rotational actuator manipulator has been developed to support lab-scale forging experiments to evaluate cogging operations with an open-die press. The robotic actuator is designed to hold a metal bar, enables rotation and translation relative to the press and affords the ability to be used in conjunction with and induction heater. This experimental capability allows for the study of path-dependent deformation sequences that can inform deformation models. Due to the significant reactionary forces during the forging operations, some deviation between intended and actual deformation path have been observed. Python has been used to collect sensor data to determine appropriate thresholds and control parameters to optimize electronic motor control and facilitate accurate deformation paths during forging. Feedback on the rotational and linear position of the bar would allow implementation of a PID controller to reduce error.

POSTERS

Development of a Low-cost Open-source Wire Arc Additive Manufacturing (WAAM) Machine: *Vishnu Ramasamy*[1]; Bathlomew Ebika[1]; Robert Gao[1]; Kenneth Loparo[1]; Bradley Jared[2]; Tony Schmitz[2]; Michael Groeber[3]; Sun Yi[4]; Kornel Ehmann[5]; John Lewandowski[1]; [1]Case Western Reserve University; [2]University of Tennessee; [3]Ohio State University; [4]North Carolina Agricultural and Technical State University; [5]Northwestern University

The Wire Arc Additive Manufacturing (WAAM) process has gained considerable attention in academic and industrial research due to its advantages, including large-scale capabilities, minimal wastage, cost-effectiveness, and range of available materials. To address the current high capital investment and steep learning curve associated with existing WAAM machines, this study focuses on the development of a low-cost, open-source WAAM machine to enhance accessibility and encourage broader research engagement. The machine's open-source nature promotes flexibility, facilitating the easy implementation and testing of advanced hardware and software techniques. This initial work investigates the utilization of a Metal Inert Gas (MIG) based WAAM process on a 3-axis linear gantry system for the printing and characterization of ER70S-6 Low Carbon Steel. Additionally, the study explores the integration and application of advanced thermal and metrology systems within the machine to support further research endeavors.

Predictive Modeling of Material Deformation Using English Wheel Under Varying Loading Conditions: *Ahmad Mitoubsi*[1]; Sam St John[1]; Vispi Karkaria[2]; Derick Suarez[2]; Jie Chen[2]; Fan Chen[2]; Wei Chen[2]; Kornel Ehmann[2]; Jian Cao[2]; Nicholas Dewberry[3]; Chandra Jaiswal[4]; Kevin Benton Benton[4]; Issa AlHmoud[4]; Balakrishna Gokaraju[4]; Anahita Khojandi[1]; [1]University of Tennessee; [2]Northwestern University; [3]North Carolina Agricultural and Technical State University ; [4]North Carolina Agricultural and Technical State University

The English wheel, a traditional metalworking tool, is used to shape intricate curves and contours in metal sheets. This has applications spanning vital industries like automotive and aerospace. Finite Element Method (FEM) simulations have traditionally been used to calculate end-state geometry. This approach is often time-consuming and resource-intensive. To revolutionize manufacturing simulation, we focus on developing surrogate models for digital twin technology. This innovation leverages the potential of Graph Neural Networks (GNNs) for modeling complex relationships among metal sheet regions, enhancing multi-point displacement prediction and diverse structure simulations. The viability of this approach has been assessed through a preliminary neural network proof of concept. The research intends to provide more efficient and resource-conscious simulations that will benefit precision manufacturing and metal shaping industries. Our longer-term vision of this research includes an additional phase to incorporate the GNN into Virtual Reality (VR) simulations to provide enhanced modeling and visualization.

Late Breaking News

Time: TBD **Room: TBD**
Date: TBD **Location: Hilton Cleveland Downtown**

Session Chair: To Be Announced

Invited
Generative Methods to Discover Materials With Enhanced Mechanical Properties: *Markus Buehler*[1]; [1]Massachusetts Institute of Technology

In this talk we review how modeling, experiment and synthesis are integrated to understand, design and leverage novel smart material manufacturing for advanced mechanical properties through the use of physics-based generative AI. This allows us to mimic and improve upon natural processes by which materials evolve, and how they meet changing functional needs. Applied specifically to protein materials, this integrated materiomic approach is revolutionizing the way we design and use materials, and has the potential to impact many industries, as we harness data-driven modeling and manufacturing across domains and applications. The talk will cover several case studies covering distinct scales, from silk, to collagen, to biomineralized materials, as well as applications to food and agriculture. A specific focus will be on the use of multi-agent transformer-based attention models as foundational theories, ultimately applied to solve multi-modal material modeling, design and analysis problems.

Additional Late Breaking News can be viewed via the online session sheets and will be available in the final technical program.

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