THE OHIO STATE UNIVERSITY
INSTITUTE FOR MATERIALS AND MANUFACTURING RESEARCH

Symposium on Computational Materials and Manufacturing
Student Poster Session

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Poster 1 - Mechanical Property Determination of Canine Femur through Multiscale Finite Element Simulations and Experimental Tests to Assess Fracture Risk

Presenter: Behzad Amirzade, Integrated Systems Engineering

Author(s): Behzad Amirzade, Tareq Zobaer, Janis Lapsley, Do-Gyoon Kim, Laura Selmic, Ali Nassiri

Advisor(s): Ali Nassiri

Abstract:

This study aims to develop a comprehensive computational modeling approach for characterizing the anisotropic mechanical behavior of trabecular and cortical bones in a canine femur using finite element analysis (FEA) of representative volume elements (RVEs) reconstructed from micro-Quantitative Computed Tomography (μQCT) data. A homogenization technique for cellular materials was applied to the RVEs to simulate the trabecular bone's large-scale mechanical response. The RVEs of bone were assumed to have a repetitive porous structure, characterized by an elastic orthotropic material model. To enhance the accuracy of the results, a Genetic Algorithm (GA) was employed to minimize the difference between the experimental force-displacement curve and the one generated by FEA simulations in ABAQUS, effectively balancing exploration and refinement to achieve a more accurate representation of the bone's mechanical response. The experimental data were derived from sapphire spherical tip nanoindentations performed on the same canine femur. This multiscale modeling approach enables more precise material property assignments in FEA, leading to improved fracture risk prediction and implant performance evaluation in clinical applications.

Poster 2 - CFD-based Molten Pool Model to Predict Hardness in Temper-bead Welding

Presenter: Aryan Aryan, Material Science and Engineering

Author(s): Aryan Aryan, Obinna Onwuama, Desmond Bourgeois, Wei Zhang

Advisor(s): Wei Zhang

Abstract:

Creep strength enhanced ferritic steels like Grade 91 are widely used in power plants, but they suffer degradation due to prolonged high-temperature exposure during service. Field welding repairs are used to restore the performance of degraded welds, often using a controlled temper-bead technique to temper the newly formed martensite during welding. However, knowledge of weld repairability is limited, and optimizing the microstructure and joint properties through experimental methods is costly and time-consuming. Many existing computational models, such as finite element models, solve only the heat conduction equation and neglect convective heat transfer due to molten metal flow. This omission can lead to over-prediction of peak temperatures in the weld pool and heat-affected zone, affecting tempering accuracy. To address this, a molten pool-based, multi-pass, multi-layer model has been developed using computational fluid dynamics and the Volume of Fluid method. This model eliminates the need for pre-determined bead profiles by calculating bead formation. The thermal cycles obtained from the molten pool model are used as inputs for microstructure models, such as Johnson-Mehl-Avrami-Kolmogorov and Grange-Baughman model, to predict tempering kinetics. These models are then applied to generate hardness maps for both single-pass and multi-pass welds, enabling a comparative study of the resultant hardness.

Poster 3 - Integrating Material's Behavior into JAX-Finite Element

Presenter: Rana Bakhtiyarzade, Material Science and Engineering

Author(s): Rana Bakhtiyarzade and Stephen R. Niezgoda

Advisor(s): Stephen Niezgoda

Abstract:

The research that will be presented focuses on integrating the recrystallization behavior of 316 stainless steel into the JAX-Finite Element Method (JAX-FEM) framework. By incorporating material behavior models directly into the finite element analysis, this work improves the predictive capability of FEM for materials processing simulations, particularly in forging and other metal-forming applications.

Poster 4 - Unveiling the Origins of Induced Magnetism in $LaCoO_3$

Presenter: Ali Barooni, Materials Science and Engineering

Author(s): Ali Barooni, Maryam Ghazisaeidi

Advisor(s): Maryam Ghazisaeidi

Abstract:

Lanthanum Cobaltite ($LaCoO_3$, LCO) is a perovskite oxide that has attracted considerable interest due to its complex and fascinating magnetic properties. In its bulk form, LCO behaves as a diamagnetic insulator at low temperatures, a phenomenon attributed to the low-spin state of Co^{3+} ions. However, in epitaxial films, LCO demonstrates ferromagnetic insulating properties, although the precise nature of this ferromagnetic state remains a topic of debate. In this project, we investigate the origins of this induced magnetism, focusing on the contributions of epitaxial strain and oxygen vacancies in facilitating spin-state transitions. Employing first-principles calculations, we examine how these factors affect the magnetic and electronic properties of $LaCoO_3$. Our results provide new insights into the mechanisms underlying spin-state transitions and the resultant ground-state magnetic configuration, thereby enhancing the understanding of LCO's potential for next-gen spintronic applications and other magnetic technologies.

Poster 5 - Prediction of the creep strength of single crystalline superalloys via a microstructure-informed deep neural network

Presenter: Andreas Bezold, Materials Science and Engineering

Author(s): A. Bezold, T. Albert, M. Göken, S. Neumeier

Advisor(s): Michael Mills

Abstract:

This study aims to develop a robust, generalized model for accurately predicting the creep life of single-crystalline superalloys by incorporating microstructural images as input parameters into a deep neural network. A comprehensive database of over 1,000 creep experiments on Ni-, NiCo-, and Co-based superalloys, along with their corresponding microstructural images, was compiled. To address the inherent biases towards a limited set of alloy compositions and the narrow composition space typical of traditional superalloy research, a strategic approach was taken to divide training and testing data. While the initial predictive performance was limited, it improved significantly through the use of a ResNet-based AutoEncoder-like neural network to extract meaningful representations of the alloys' microstructures. After hyperparameter optimization, the model outperformed baseline approaches, demonstrating that incorporating microstructural data enhances predictive accuracy. The model's high generalizability was further validated and potential pathways for practical implementation in multi-criteria alloy design algorithms are discussed.

Poster 6 - Displacive to Order-Disorder Crossover in the Structural Phase Transition of Niobium (IV) Oxide

Presenter: Paul Cuillier, Materials Science and Engineering

Author(s): Paul Cuillier, Wenqian Xu, Vicky Doan-Nguyen, Wolfgang Windl

Advisor(s): Wolfgang Windl

Abstract:

Niobium (IV) oxide exhibits a temperature-dependent band gap and an insulator-to-metal transition, which yield nonlinear electronic behavior desirable for applications like neuromorphic computing. From an average structure perspective, this has been connected to a second-order displacive transition with a critical temperature concomitant with the insulator-to-metal transition. Efforts to understand and engineer this behavior have led to ongoing debates about whether Peierls structural instabilities or Mott electron-electron correlations are the primary driving force. To address gaps in the structural description of bulk NbO_2, we apply in-situ X-ray pair distribution function analysis and machine learning molecular dynamics simulations to show that the structural phase transition is not purely displacive. Rather, it crosses over from displacive to order-disorder character near the insulator-to-metal transition, providing an alternative explanation for the complex electronic behavior. The high temperature metallic phase largely retains the local structure of the insulating phase, but long-range order is frustrated by dynamic 2-dimensional fluctuations. Furthermore, the agreement at high temperature between experiment and machine learning molecular dynamics, which does not consider changes in electronic temperature, suggests a Mott transition is not needed to describe the structural phase transition. This supports the notion that NbO_2 undergoes a Peierls-assisted Mott transition.

Poster 7 - Simulation of Spray Processes to Train a Machine Learning Algorithm for Autonomous Path Generation

Presenter: Erik Furterer, Integrated Systems Engineering

Author(s): Erik Furterer, Josh Groves

Advisor(s): Michael Groeber

Abstract:

Robotic spray-processes are used in many industries, including automotive and aerospace. Path planning for these spray process, particularly spray painting, is challenging when attempting to account for how the process interacts with complex geometries. One can use computer simulation to help train machine learning methods, such as a convolutional neural networks, to use images to learn a path planning policy. In this work, we feature engineer input channels for these images to provide the network with key geometric and process information during the spray process. This poster will show the development of these features, the architecture of the learning system, and the results and transferability of the policy learned.

Poster 8 - Prediction of Metal Deformation with Graph Neural Networks to Enable Forging Policy Learning

Presenter: Joshua Groves, Integrated Systems Engineering

Author(s): Joshua Groves, Sam St. John (UT), Thomas Banko, Rana Bakhtiyarzade, Chris Stanulet

Advisor(s): Michael Groeber

Abstract:

We utilize finite-element analysis as a method for generating synthetic data to train a graph neural network (GNN) on the deformation of metal in a forging process. Early training of the GNN shows it successfully learns to model the physics of metal deformation. The GNN can then be used as a surrogate model to train a reinforcement learning agent to learn a policy for automating the forging process with a robotic arm and hydraulic press.

Poster 9 - Mapping Indentation to Stress Strain of Shape Memory Alloys through Computation and Bayesian Inference

Presenter: Daniel Hong, Materials Science and Engineering

Author(s): Daniel Hong, Peter Anderson

Advisor(s): Peter Anderson

Abstract:

Shape memory alloy (SMAs) research is challenged with exploring a broad design space integrating composition, synthesis, and training to design materials with desired properties. Nanoindentation provides a method to characterize microstructures at various length scales. However, indentation presents additional challenges in complex stress and deformation states. This work presents on an effort to apply Bayesian Inference to draw relationships between indentation data and stress strain properties trained on finite element simulations of indentation into SMAs.

Poster 10 - Multiscale Modelling framework for Solid State Batteries

Presenter: Kartik Kashyap, Mechanical and Aerospace Engineering

Author(s): Kartik Kashyap

Advisor(s): Soheil Soghrati

Abstract:

The study replicates solid-state battery (SSB) manufacturing, a detailed framework involves several key steps. Start by synthesizing solid electrolytes and electrode materials using techniques like sol-gel or vapor deposition, followed by mixing them to form a composite. Thin-film layering or cold-pressing can be used to fabricate the SSB cell, ensuring uniform contact between the electrolyte and electrodes.

For the computational analysis, the microstructure of the battery is modeled using a combination of electrochemical and mechanical simulations. At the microscale, this involves capturing ionic transport, stress distribution, and the degradation of materials. Advanced simulation tools like COMSOL or custom meshing libraries can simulate these interactions within the microstructure, revealing crucial factors affecting battery life and performance.

The homogenization procedure bridges the gap between micro and macro levels by averaging microstructural behavior, like ionic flux and stress-strain responses, and applying them to the larger cell-scale model. This upscaled model helps predict overall battery behavior, including energy density, mechanical integrity, and thermal management, providing insights for optimization at the pack level.

Poster 11 - Physics Based Modeling of Space Weather Effects on Widegap Semiconductor Materials

Presenter: Vanessa Kramer, Materials Science and Engineering

Author(s): Vanessa Kramer

Advisor(s): Wolfgang Windl

Abstract:

Wide band gap (WBG) semiconductors, such as such as gallium nitride (GaN) and beta-gallium oxide (β-Ga2O3), are used frequently in spacecraft electronic systems because of their high thermal stability and efficiency. However, these materials face challenges low Earth orbit (LEO), where exposure to high-energy ions which can lead to significant degradation. Exposure to these conditions can lead to various defects in the semiconductors such as Frenkel pairs and extended defect plumes, which adversely affect the performance and longevity of spacecraft systems. Currently, there is a lack of physical based modeling systems that address the complex damage mechanisms associated with radiation in conjunction with varying thermal and electrical environments. The goal of this project is to develop post-irradiation damage evolution models for GaN and β-Ga2O3 used in spacecraft electronics and to determine the end of life criteria for the devices in low Earth orbit.

Poster 12 - Assessing Microstructure Descriptors for Processing-Structure Manifold Construction

Presenter: Simon Mason, Materials Science and Engineering

Author(s): Simon Mason, Megna Shah, Jeff Simmons, Dennis Dimiduk, Stephen Niezgoda

Advisor(s): Stephen Niezgoda

Abstract:

Quantitative representations of microstructure are fundamental to exploring processing-structure-property relationships for accelerated materials design. This work outlines the criteria by which different microstructure descriptors can be assessed with respect to their ability to describe material domains in navigable, lower-dimensional embeddings. The stochastic representation of microstructure allows for a continuous mapping between processing and structure, enabling the construction of a microstructure manifold for exploitation/exploration analysis.

Poster 13 - Integrated Crystal Plasticity and Cellular Automata Modeling for Dynamic Recrystallization Prediction in 304LN Stainless Steel

Presenter: Jinheung Park, Integrated Systems Engineering

Author(s): Jinheung Park, Reza Rezaei, Myoung-Gyu Lee, Taejoon Park, Farhang Pourboghrat

Advisor(s): Taejoon Park, Farhang Pourboghrat

Abstract:

Dynamic discontinuous recrystallization (DDRX) typically occurs in metals with low to medium stacking fault energy during thermo-mechanical processing. This process involves the formation of strain-free nuclei, which grow into refined grains by consuming the surrounding deformed material. In this work, we present a computational model to simulate the DDRX behavior of AISI 304LN stainless steel under hot compression. The model integrates the crystal plasticity finite element method (CPFEM) with a probabilistic cellular automata (CA) approach to predict the microstructure evolution and mechanical properties. CPFEM captures the heterogeneous plastic deformation at the grain level, while the CA model simulates the microstructure evolution due to DDRX. The recrystallization process is controlled by stored energy, represented by dislocation density, within a dislocation density-based crystal plasticity framework. The developed model successfully predicts experimental results across various temperatures and strain rates.

Poster 14 - The Origin of Photoplasticity in ZnS

Presenter: Sevim Polat Genlik, Materials Science and Engineering

Author(s): Sevim Polat Genlik, Roberto C. Myers, Maryam Ghazisaeidi

Advisor(s): Maryam Ghazisaeidi

Abstract:

ZnS is a brittle material but shows extraordinary plasticity during mechanical tests performed in complete darkness. This phenomenon is known as the photoplastic effect, whose underlying mechanisms have long been unclear. We study the impact of light, via photoexcited charge carriers, on the dislocation core structure and mobility using first-principles calculations. We calculate the core structure and the charge-dependent Peierls barriers of the glide set of Shockley partial dislocations in ZnS. Our findings reveal that locally charged dislocations capture excess carriers in the system, leading to core reconstructions that alter the Peierls barrier, resulting in higher barriers and lower mobility for these dislocations. This altered and asymmetric mobility, depending on dislocation character (edge or mixed) and local stoichiometry (Zn or S rich), is responsible for the brittle behavior of ZnS under light exposure and will be reversed in complete darkness

Poster 15 - Ab-Initio Simulation of Field Evaporation

Presenter: Jiayuwen Qi, Materials Science and Engineering

Author(s): Jiayuwen Qi, Emmanuelle A. Marquis and Wolfgang Windl

Advisor(s): Wolfgang Windl

Abstract:

This work involves the development and application of a novel approach—TAPSim-MD—to simulate the field evaporation process in atom probe tomography (APT). By integrating the electrostatics solver from TAPSim with the classical molecular dynamics (MD) code LAMMPS, we include field evaporation as part of an in-field MD simulation. This approach enables a full-dynamics description of the field evaporation process in an "ab initio" manner, without assuming any ad hoc evaporation fields or criteria as used in previous methods. By employing this full-dynamics simulation, we are able to obtain natural atom trajectories and investigate artifacts in APT data resulting from dynamic atomic effects, such as enhanced zone lines in field evaporation maps. Furthermore, by investigating field evaporation in the TiAl intermetallic compound, our simulation highlights the significant role of interatomic interactions and bond-breaking processes, which determine atomic behavior under the field and can significantly impact the evaporation results.

Poster 16 - Multiscale CA and CPFE Modeling for Predicting Mechanical Behavior of Low Carbon Steel Alloys

Presenter: Reza Rezaei, Integrated System Engineering

Author(s): Dr. Amir Asgharzadeh, Reza Rezaei, Dr. Jinheung Park , Dr. Taejoon Park, and Prof. Farhang Pourboghrat

Advisor(s): Farhang Pourboghrat, Taejoon Park

Abstract:

A multiscale modeling framework is developed to predict microstructure evolution and resulting mechanical behavior of steel alloys. Microstructure evolution during the annealing process is predicted based on Cellular Automata (CA) modeling, while the mechanical behavior is predicted by conducting Crystal Plasticity Finite Element (CPFE) simulations. To evaluate the effect of precipitates on the mechanical behavior, CPFE simulations are conducted with representative volume elements (RVEs) with varying the sizes and volume fractions of the precipitates. An integrated CPFE model is developed to efficiently predict the effect of precipitates under various loading conditions using a homogenization technique. For the validation, microstructure evolution and stress-strain behavior during the uniaxial tension tests are compared between the simulations and experiments.

Poster 17 - Phase Field Method for Ductile Fracture

Presenter: Ananya VK, Mechanical and Aerospace Engineering

Author(s): Ananya VK, Steve Niezgoda

Advisor(s): Stephen Niezgoda

Abstract:

Crack initiation and propagation are critical factors in the design of mechanical components. Phase field modeling is an effective method for predicting crack propagation, eliminating the need for predefined branching or propagation criteria. This study presents the implementation of a ductile phase field fracture model, developed by Kuhn et al., into an Abaqus user-defined material (UMAT). Unlike brittle fracture models, the ductile model shows damage initiation at the boundary without complete failure at similar strain levels. Future work will focus on extending the model to incorporate crystal plasticity.

Poster 18 - Automated Forging with DEFORM3D

Presenter: Tara Wagoner, Material Science and Engineering

Author(s): Sam St. John, Josh Groves, Rana Bakhtiyarzade, Thomas Banko, Tara Wagoner, Michael Groeber, Stephen Niezgoda

Advisor(s): Stephen Niezgoda

Abstract:

DEFORM3D is a metal forming software. DEFORM3D takes a material in a given shape and forms it in a method such as forging, extrusion, rolling, drilling, etc. to determine aspects such as stress distribution, strain, temperature change, material flow, and deformation.

I am working with DEFORM to create an API to autonomously run many cogging simulations.

I will be rotating an object and hitting it with a combination of varying angles, forces, and temperatures, in a series of steps to create the desired shape for what we want to forge.

My team plans to use this data to train a graph neural network and see if we can use that as a faster form of DEFORM3D. Ultimately, we want the GNN to perform automated forging within a reasonable time frame. Currently, DEFORM3D is too slow to run for automated forging. The simulations take at least 15 minutes to run. What we want is a software connected to a camera and robot to provide feedback on different parameters needed to create the desired object.

Poster 19 - Computational Discovery of B2 Phases in the Refractory High Entropy Alloys

Presenter: Junxin Wang, Materials Sciences and Engineering

Author(s): Junxin Wang, Maryam Ghazisaeidi

Advisor(s): Maryam Ghazisaeidi

Abstract:

The Multi-Cell Monte Carlo method for phase prediction for multicomponent alloys has demonstrated great potential in simulating coexisting phases in many-component crystalline systems. To find potential B2 structures in high entropy alloys, this method is applied to composition space, spanning through the refractory element range in the periodic table. First, we explore the refractory elements with BCC ground state structures (MoNbTaWV) and then the ones with HCP ground state structures (TiZrHfOsReRu). Ordered structures are found in both systems and their thermal stability are analyzed. We further look into the combination of all the refractory elements (both HCP and BCC elements) and try to identify the most possible groups to form a B2 structure.

Poster 20 - Dendrite Growth in Na/Na3Sb in Na3SbS4 Solid State Electrolyte Battery

Presenter: Chengyin Wu, Materials Science and Engineering

Author(s): Chengyin Wu, Yanzhou Ji

Advisor(s): Yanzhou Ji

Abstract:

Solid-state batteries play an indispensable role in modern electronic devices, from cellphones and automobiles to energy storage systems. The performance and lifespan of these devices are highly dependent on the condition of the installed battery. During the charge-discharge cycles, batteries undergo microstructural changes, such as dendritic growth at the anode and solid electrolyte interface, which can lead to a reduction in energy storage capacity or even device failure.

To address this challenge, we employed phase-field modeling and physics-based COMSOL simulations to analyze dendrite growth from a Na-Na_3Sb polycrystal anode to a Na_3SbS_4 solid electrolyte. By incorporating charge-discharge cyclic loading, we modeled the system as realistically as possible to gain a deeper understanding of how dendrites evolve during service.

Poster 21 - High and Moderate Temperature Deformation Modeling of High Entropy Alloys

Presenter: Charles Xu, Materials Science and Engineering

Author(s): C. Xu, Y. Wang, B. Viswanathan, S. Niezgoda

Advisor(s): Stephen Niezgoda

Abstract:

Al, Mo, Nb, Ta, Ti, Zr High-entropy alloys can form a superalloy-like microstructure with a B2 matrix and coherent bcc precipitates. Many members of this family have good high temperature strength but poor ductility below 600 °C due to coarse intermetallic grain boundary particles, but some composition show excellent mechanical properties. In this talk we explore the high- and moderate temperature deformation behavior of these alloys through crystal plasticity simulations with dislocation utilizing a dislocation based constitutive laws. Specifically, we explore the composite B2/bcc microstructure response and homogenization to calibrate effective single crystal grain scale constitutive response. These effective properties are then integrated into polycrystalline models to explore the effects of texture and grain boundary precipitates on the resulting response of the polycrystalline aggregate. Calibration data is obtained from a combination of TEM/SEM characterization, micro phase-field simulation, nanoindentation and small-scale mechanical testing.

Poster 22 - Goniopolar Materials for Semiconductor-Based Thermoelectrics in High-Efficiency Generators

Presenter: Bowen Yu, Material Science and Engineering

Author(s): Bowen Yu, Ziling Deng, Yaxian Wang, Joshua Goldberger and Wolfgang Windl

Advisor(s): Wolfgang Windl

Abstract:

Goniopolar materials exhibit unique charge carrier properties, where both electrons and holes coexist and transport orthogonally within a single crystal. This feature makes them highly desirable for thermoelectric applications, as they have the potential to significantly reduce energy losses and improve device efficiency using transverse device design. In this poster, we will show the electronic structure of goniopolar semiconductors, with a focus on materials like Re_4Si_7, using first-principles methods, including density functional theory (DFT) and BoltzTraP2 for transport properties.