
MEDE+ HIGHLIGHTS 2023



CAIMEE

CENTER ON ARTIFICIAL INTELLIGENCE
FOR MATERIALS IN
EXTREME ENVIRONMENTS

WHAT IS MEDE+?

MATERIALS IN EXTREME DYNAMIC ENVIRONMENTS PLUS (MEDE+) IS A CONGRESSIONALLY DIRECTED SET OF PROJECTS FOCUSED ON DEVELOPING ADVANCED MATERIALS AND SCIENCE FOR MILITARY APPLICATIONS. MEDE+ CURRENTLY INCLUDES TWO COOPERATIVE AGREEMENTS: ARTIFICIAL INTELLIGENCE FOR MATERIALS DESIGN (AIMD) AND AI-DRIVEN INTEGRATED AND AUTOMATED MATERIALS DESIGN FOR EXTREME ENVIRONMENTS (AMDEE). RESEARCHERS AT THE CENTER ON ARTIFICIAL INTELLIGENCE FOR MATERIALS IN EXTREME ENVIRONMENTS (CAIMEE) AT JOHNS HOPKINS UNIVERSITY WORK IN CLOSE COLLABORATION WITH DEVCOM ARMY RESEARCH LABORATORY TO FURTHER RESEARCH WITHIN MEDE+ AND ACCELERATE THE MATERIALS DISCOVERY PROCESS.



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FROM THE CAIMEE DIRECTOR

At the Center on Artificial Intelligence for Materials in Extreme Environments (CAIMEE), we continue to innovate and discover, accelerating traditional timelines for materials discovery and bringing new ideas and approaches to materials science in extreme environments. The AIMD project is nearing completion while the AMDEE project is currently in its first year, and we have already made great strides towards our goal of accelerated materials discovery.

With 11 principal investigators in AMDEE, the overall team includes more than 45 people, including postdoctoral researchers, research and administrative staff, and graduate and undergraduate students. This booklet highlights the diverse activities of this multidisciplinary team, which includes expertise in materials science, robotics, experimental mechanics, computational modeling, and AI-driven design. The goals, challenges, and successes of each task in this project are provided, along with an outline of how these tasks fit into the greater AMDEE mission and strategy.

The Artificial Intelligence for Materials Design Laboratory (AIMD Lab) that serves as the focal point for much of the activity in AMDEE continues to grow and develop. The AIMD Lab (featured on page 12) currently has six stations in place, with the ability to expand its capabilities as future research needs arise. This high-throughput facility has the potential to revolutionize the way we discover new materials and to tailor the characteristics of materials for applications of interest to ARL.

We would like to thank our partners, without whom this project would not be possible. The support of our partners at the U.S. Army Research Laboratory and the Department of Defense has been crucial to our research activities. We have also been privileged to engage with outstanding students from our partners at the Maryland Institute College of Art (MICA) and Morgan State University (MSU). These students bring valuable new perspectives on the research we do.

An exciting future lies ahead for autonomous design of materials, and I am proud to say that the MEDE+ team is at the forefront of these developments for defense materials applications.

Onward and upward,
Lori Graham-Brady



LORI GRAHAM-BRADY

Director, CAIMEE
Professor, Department of
Civil and Systems Engineering
Johns Hopkins University

LEADERSHIP



JAAFAR EL-AWADY

Associate Director, CAIMEE
Interim Director, Hopkins Extreme
Materials Institute
Professor, Department of
Mechanical Engineering
Johns Hopkins University



BESS BIELUCZYK

Program Manager, CAIMEE

ABOUT MEDE+

The U.S. Army established the Materials in Extreme Dynamic Environments (MEDE) program in 2012 to design, develop, and test improved soldier protection materials. Johns Hopkins University led the MEDE Collaborative Research Alliance, which included 25 university and research centers across 13 states, the United Kingdom, Germany, and Switzerland. Researchers worked in close collaboration with DEVCOM Army Research Laboratory, and **the MEDE program accelerated the development of armor materials by an estimated 10 years.**

Based on the success of the MEDE program, congressionally directed funding was appropriated to establish MEDE+. MEDE+ invests in the future of advanced materials and is composed of two major projects: AI for Materials Design (AIMD) and AI-Driven Integrated and Automated Materials Design for Extreme Environments (AMDEE).

The **AIMD** project has resulted in a new, state-of-the-art laboratory which integrates multiple stations focused on high-throughput and machine learning (ML)-driven materials development. A centrally controlled robotic automation system links high-throughput characterization and dynamic testing, all driven by ML and computational modeling, and AI-guided decision-making. The AIMD Lab provides a proof of concept for high-throughput fabrication, characterization, and testing of materials in extreme environments. While the framework of this capability can be applied to a variety of materials design questions, the facility currently addresses the critical research question of which alloys exhibit optimal dynamic properties. As a result, AIMD will have a significant impact on U.S. Army material applications and on the broader materials research community.

AMDEE is a multi-year project that focuses on AI- and data-driven materials design. AMDEE is expanding the current hardware capabilities of the AIMD Lab to generate high quantities of valuable application-relevant data (e.g., by incorporating integrated thermal/mechanical laser shock, novel ultraviolet microscopy, and a broader range of materials such as RMPEAs and light alloys). The basic robotic automation developed in AIMD will be extended to reach more stations and demonstrate a new level of sophistication in applying materials and processing data. Most importantly, this project focuses on developing and implementing machine learning and AI tools, not only to evaluate materials, but to make actionable design decisions in the context of an automated system, as a large step towards an autonomous materials design capability.

CONNECTION TO ARMY GOALS

The MEDE+ projects provide foundational research for DEVCOM Army Research Laboratory's (ARL) **Sciences of Extreme Materials (SEM)** core competency. SEM focuses on the materials and related manufacturing methods for mechanical response and performance extremes, including novel manufacturing science for energetic materials and active, adaptive, and flexible/soft materials.

Within the SEM core competency, MEDE+ projects directly support the following focus areas:

- High strain rate materials response
- Mechanics of materials
- Materials and data science
- Structural and ballistic materials synthesis, processing, and characterization

MEDE+ researchers work in close collaboration with researchers at ARL, striving to discover materials that can survive and perform in extreme environments often encountered during military operations. These harsh military environments include those of high acceleration (e.g. projectile launch and flight), high temperature and rapid ablation (e.g. hypersonic flight), and high-velocity impacts (terminal ballistics).

The knowledge gained through MEDE+ projects will lead to improved protection materials for the Army, supporting two of its modernization priorities: **Next Generation Combat Vehicle** and **Soldier Lethality**.

MEDE+ also supports the Department of Defense's (DoD) **Advanced Materials** critical technology area, with a focus on autonomous materials development. This critical technology area explores novel materials and manufacturing techniques that can dramatically improve many of the DoD's capabilities. Materials developed as part of this effort may have higher strength, lighter weight, higher efficiency, or greater resistance to extreme temperatures. As a result, these materials will have the potential to better protect military service members and enhance their ability to accomplish their missions.

ORGANIZATION

PRINCIPAL INVESTIGATORS



LORI GRAHAM-BRADY



JAAFAR EL-AWADY



PAULETTE CLANCY



DAVID ELBERT



MARK FOSTER



TODD HUFNAGEL



AXEL KRIEGER



JOCHEN MUELLER



KT RAMESH



TAMER ZAKI



TIM WEIHS

STAFF

Bess Bieluczyk, *Program Manager*

Joseph Nkansah-Mahaney, *Associate Staff Engineer*

Sarah Preis, *Communications Specialist*

Phyllis Sevik, *Senior Grants & Contracts Analyst*

Matt Shaeffer, *Senior Staff Engineer*



SPOTLIGHT: RAYNA MEHTA

Rayna Mehta is a graduate student in the Department of Materials Science and Engineering at Johns Hopkins University. She has worked on AIMD and AMDEE and is advised by Prof. Tim Weihs.

1. What are your current activities within AMDEE?

I am working on the fabrication and processing task—this means making different samples and thermomechanically processing them before they are characterized through x-ray diffraction and spall testing. We fabricate our samples through sputter deposition, which involves building our material atomic layer by atomic layer. Creating materials this way gives us more control over the microstructure, which is integral to obtaining our desired properties. We then anneal and roll them, creating textures that mimic a material made through bulk processing. I also coordinate with the characterization tasks, making sure that the materials we are making meet the specs of what they need to properly analyze them (sample thickness, surface finish, etc.).

2. What do you hope to accomplish?

I hope to help create a series of samples that improve our understanding of RHEAs and their properties—most initial studies focus on equiatomic alloy compositions, and I think our method enables more discovery of the in-between composition space. Sample synthesis so far has been a frustrating and rewarding process—it requires lots of adjusting of parameters which is a slow-going process, but when it works its extremely satisfying.

3. What are your professional interests?

I'm very indecisive about this, but I'm on the fence between industry and national labs. I love being hands-on with my research and want to keep that up in my career after my PhD... but other than that I'm not sure yet.



One of the coolest moments of my career so far was presenting at Hopkins on the Hill earlier this year. Thanks to the AIMD/AMDEE program, I had the opportunity to visit the Russel Senate Office Building in D.C. and speak with congressional staffers, JHU alumni, and the general public about the research I was doing, my experiences in grad school, and why I like science.”



FACILITIES SPOTLIGHT: AIMD LAB

The Artificial Intelligence for Materials Design Laboratory (AIMD Lab) represents a collaborative effort among leaders in materials science, robotic automation, artificial intelligence, and data science. The facility features a closed-loop system that connects various stations for testing, processing, and characterization.



A **Conveyance system:** A U-shaped conveyance system carries material specimens from station to station. The inner and outer tracks move in opposite directions, allowing samples to move clockwise or counterclockwise throughout the system as needed.



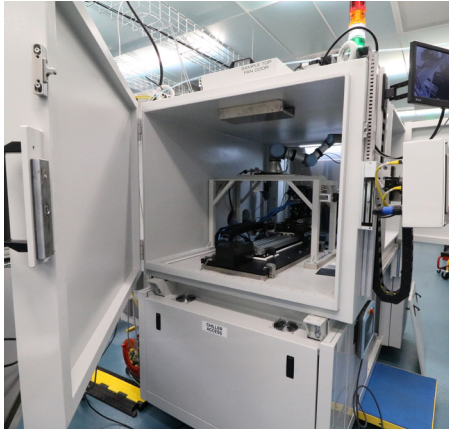
B **UR10e robots:** Each robot has a reach of 51.2 inches and is capable of carrying a 27.55 lb payload. Equipped with vacuum grippers, the robots move material specimens from the conveyance system to their proper positions for processing, testing, and characterization.



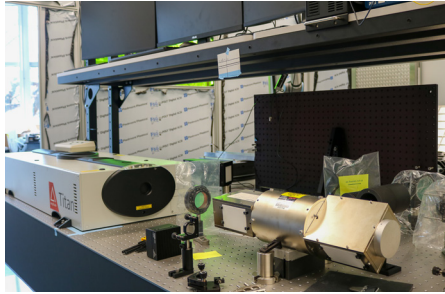
C **Station manning infeed/outfeed:** Samples (each mounted within a rectangular sample frame) begin and end their journey on these large trays, where a robotic arm adds them to or removes them from the conveyance system.



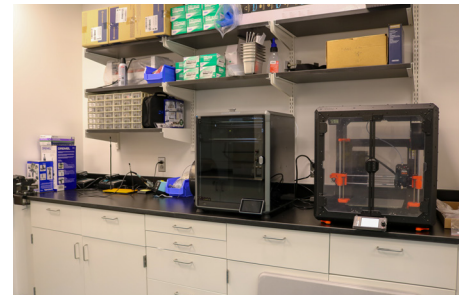
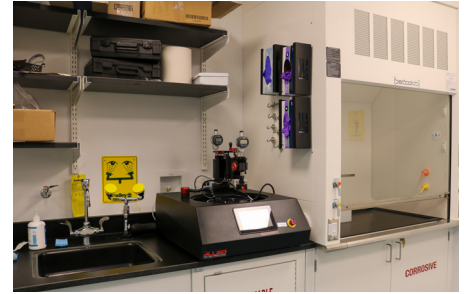
D **Laser engraver:** A nanosecond pulse laser engraves sample frames with QR codes, allowing samples to be tracked easily throughout the system. This computer-controlled laser has an average output of 20W and is powerful enough to engrave metals, ceramics, and plastics.



E **MAXIMA:** MAXIMA simultaneously performs high-transmission x-ray diffraction (XRD) and x-ray fluorescence spectroscopy (XRF) to characterize samples. A UR10e robot transfers samples from the conveyance system into MAXIMA through a small door in the side. A smaller UR3e robot handles samples within MAXIMA. Automation and rapid data collection helps reduce bottlenecks in characterization.



F **Laser shock:** A high-energy infrared laser launches disk-shaped impactors (flyers) at target materials. Another laser measures the deformation of the target materials in real time.



G **Wet lab:** AIMD's wet lab features a fume hood, polisher, 3D printers, and a soldering station.

RESEARCH ACTIVITIES WITHIN AMDEE

To achieve the goal of discovering novel RMPEAs using artificial intelligence, AMDEE's research activities strive to address five key AI needs. Each of AMDEE's research tasks aims to address one of these needs.

FIVE KEY AI NEEDS	ASSOCIATED TASKS
1. Significant quantity of coordinated materials data relevant to extreme environments;	<ul style="list-style-type: none">• Fabrication and Processing of Material Specimens and Novel Alloy Powders• Dynamic Testing of Material Specimens• High-throughput Specimen Characterization
2. Efficient prediction of the future ramifications of various decisions;	<ul style="list-style-type: none">• Physics-based & Machine Learning-driven Models
3. Reliable approaches to identify optimal decision(s);	<ul style="list-style-type: none">• AI-driven Decision Making for Optimal Materials Design• Bayesian Optimization for Connecting Materials Processing, Properties, and Performance
4. Actionable response to the decision(s);	<ul style="list-style-type: none">• Robotic Automation and On-the-fly Learning for Automation and Control
5. Event-driven integration of data to connect the design, decision, and control loops.	<ul style="list-style-type: none">• Data Management and the Event-driven Data Layer

KEY AI NEED 1

SIGNIFICANT QUANTITY OF COORDINATED MATERIALS
DATA RELEVANT TO EXTREME ENVIRONMENTS

FABRICATION AND PROCESSING OF MATERIAL SPECIMENS AND NOVEL ALLOY POWDERS

PROF. TIM WEIHS, CO-PI

RAYNA MEHTA, GRADUATE STUDENT

GOAL: TO FABRICATE, THERMOMECHANICALLY PROCESS, AND CHARACTERIZE DIFFERENT ALLOY SYSTEMS USING A COMBINATORIAL APPROACH.

Research Strategy:

Refractory multi-principal element alloys, or RMPEAs, are of interest for future use in high-temperature applications. We are interested in RMPEAs with a specific geometry; single-phase, body-centered cubic (BCC) materials have uniform properties throughout and have been shown to have high ductility at elevated temperatures. Our team is working to identify alloy systems of interest by utilizing CALPHAD modeling, an approach designed to predict or calculate thermodynamic and kinetic properties. We fabricate free-standing thick foils of varying chemical compositions through sputter deposition, a process by which alloys are sprayed onto a substrate in thin layers.

To create these foils, we first investigated how key parameters such as sputter rate, argon pressure, bilayer spacing, and others affect film stress, helping us find suitable deposition parameters. Through thermomechanical processing, we will introduce a bulk-like texture in our 50–200 μm thick foils. Our high-temperature furnace is capable of reaching 2200°C and has the ability to quench samples, cooling them rapidly to achieve specific properties. When used with a rolling mill, this furnace allows us to obtain a variety of phases, grain sizes, and

orientations. With machine learning and artificial intelligence methods, we will screen samples for desired material and mechanical properties, identifying ideal grain sizes, phases, hardness, and ductility.

Once we identify promising alloy compositions, we will synthesize 40–100 μm sized powders in bulk using an ultrasonic atomizer. These powders will be used as feedstock for a directed energy deposition (DED) process, producing samples in structures of further interest to the Army. These steps will help scale and accelerate the materials development process for applications in extreme environments. Aside from RMPEAs, other alloy systems of interest include aluminum alloys with eutectic strengthening and structural alloys with reversible phase transformations.

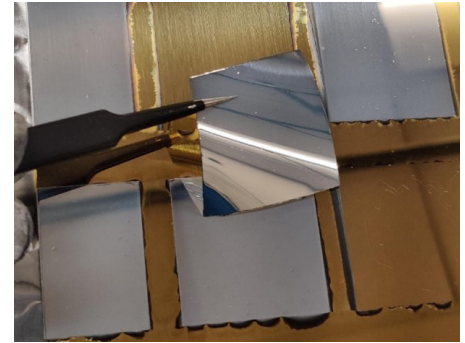


Figure 1: Free-standing 30 μm foil with varying Ti/Zr composition

DYNAMIC TESTING OF MATERIAL SPECIMENS

PROF. KT RAMESH, CO-PI

DR. PIYUSH WANCHOO, POSTDOCTORAL FELLOW

DR. AHMAD MIRZAEI, POSTDOCTORAL FELLOW

GOAL: TO DEVELOP THE ABILITY TO PERFORM TENS OF THOUSANDS OF DYNAMIC TESTS EACH WEEK USING HIGH-THROUGHPUT LASER SHOCK EXPERIMENTS.

Research Strategy:

High-throughput laser shock experiments will provide the critical dataset needed to build AI-driven models of material behavior under extreme conditions, and this in turn will help the Army discover new materials for critical applications. The goal is to provide a robust capacity to rapidly interrogate new materials as they are made, integrating our efforts with high-speed characterization and robotics to drive automated scientific discovery. The new materials themselves are created by the synthesis, processing, and fabrication group. Our basic approach is to use pulsed lasers, together with a high heating rate capability, to obtain dynamic material properties as a function of shock stress and temperature in a material of known microstructure. We study ductile metals as well as brittle and quasi-brittle materials using thick foil specimens. Using a high-power infrared laser that generates five pulses per second, we are able to launch miniature disk-shaped impactors into our target materials, and we then use another laser operating at low power to measure the real-time deformation of the target material. Such measurements allow us to determine the strength and impact resistance of the new material. All data from each experiment is collected and analyzed with an automated protocol. Significant safety concerns arise with such high-power lasers which must be addressed, but automation significantly reduces the risk to humans.

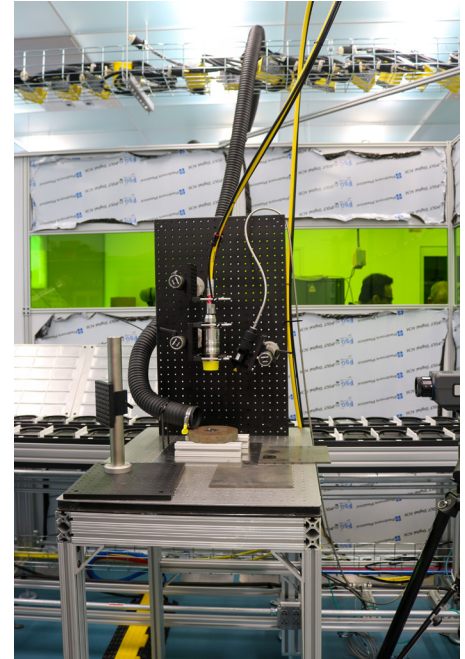


Figure 2: High-power lasers can present serious safety concerns, but automation and the use of safeguards like an enclosure and laser safety windows help reduce the risk of harm to humans.

HIGH-THROUGHPUT SPECIMEN CHARACTERIZATION

PROF. TODD HUFNAGEL, CO-PI

PROF. MARK FOSTER, CO-PI

PROF. KT RAMESH, CO-PI

GOAL: TO PROVIDE ACTIONABLE INFORMATION ABOUT MICROSTRUCTURE TO GUIDE AUTOMATED MATERIALS EXPLORATION CAMPAIGNS.

Research Strategy:

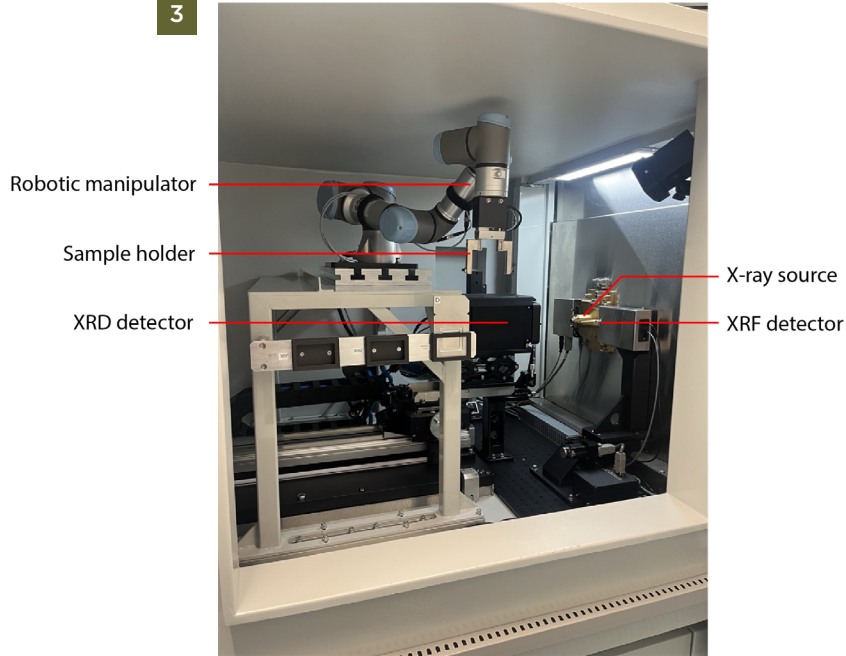
The emphasis is on obtaining, as rapidly as possible, sufficient information to allow decisions to be made about the next step(s) in automated materials exploration campaigns. Our research strategy emphasizes the development of novel, high-throughput techniques that avoid traditional bottlenecks in microstructural characterization, particularly the need for meticulous sample preparation.

One thrust in this task has been the development of an instrument and associated data analysis techniques to permit fully automated high-throughput transmission high-energy x-ray diffraction (XRD) characterization of microstructure (see figures 3 and 4). High-energy XRD provides microstructural information including the identities and amounts of specific crystalline phases present in the sampled region, along with their lattice parameters, grain size, and crystallographic texture. The small spot size of the x-ray beam (approximately 0.2 mm)

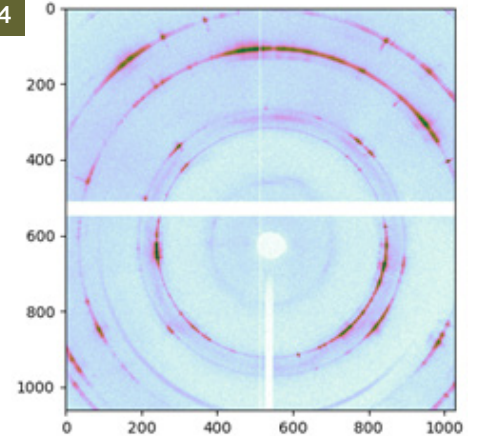
permits mapping of microstructural variations over a large area. The advantages of high-energy XRD are that there is no need for extensive sample preparation, and that the x-rays are sufficiently penetrating that the true bulk microstructure is sampled (as opposed to electron-based techniques that can only analyze the sample surface). Simultaneously with XRD, the instrument can perform x-ray fluorescence spectroscopy (XRF) which provides quantitative, point-by-point measurements of the chemical composition.

This task is also pursuing the development of novel techniques for coherent ultraviolet (UV) microscopy of sample surfaces, which have the potential to provide higher spatial resolution than traditional optical microscopy techniques, while not requiring the sample to be held in vacuum (as in electron microscopy).

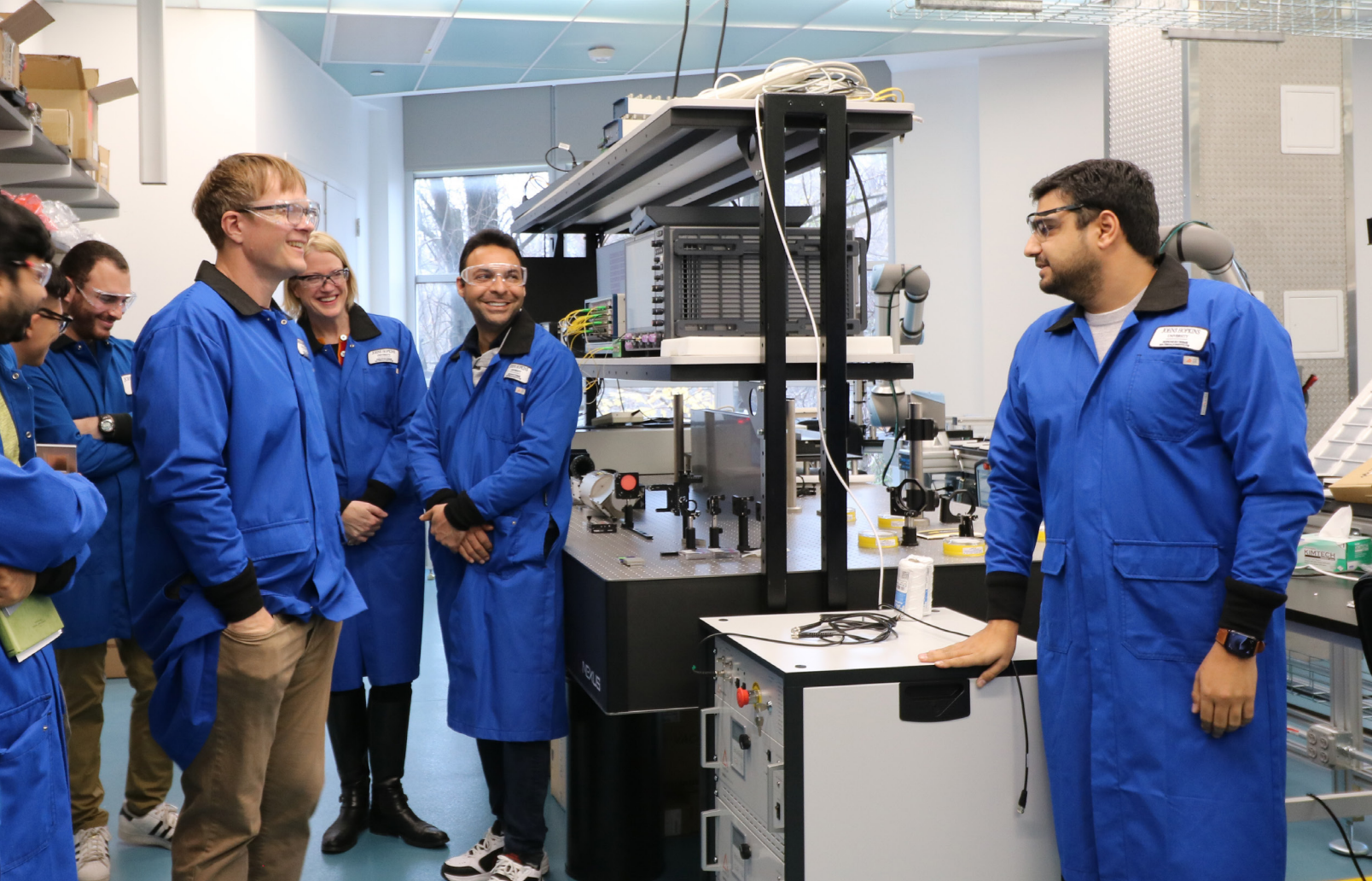
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4



Figures 3 and 4: (3) Instrument for high-throughput XRD and XRF. (4) Sample XRD data from a 200 μm thick specimen of aluminum alloy.



KEY AI NEED 2

EFFICIENT PREDICTION OF THE FUTURE
RAMIFICATIONS OF VARIOUS DECISIONS

PHYSICS-BASED & MACHINE LEARNING-DRIVEN MODELS

PROF. JAAFAR EL-AWADY, CO-PI

PROF. LORI GRAHAM-BRADY, CO-PI

PROF. TAMER ZAKI, CO-PI

GOAL: TO INTEGRATE MACHINE LEARNING AND PHYSICS-BASED MODELING WITH EXPERIMENTAL RESEARCH IN ORDER TO ACHIEVE A HOLISTIC UNDERSTANDING OF RMPEAS AND ELUCIDATE THE RELATIONSHIP BETWEEN MICROSTRUCTURE AND MECHANICAL PROPERTIES LIKE STRENGTH, DUCTILITY, AND SPALL RESISTANCE.

Research Strategy: Physics-based Models

Models of spall under shock loading in alloys are highly computationally intensive, requiring accurate representation of plastic deformations at the sub-grain scale, damage due to void initiation and growth at grain boundaries, and the equation of state. To support rapid materials design, the AMDEE program needs accelerated models that can approximate behavior such as spall strength in real time—a much faster rate than the physics-based models can achieve. After developing the physics-based finite element model (FEM) that represents all these phenomena, this team has used an ensemble of FEM results to train a three-dimensional U-net capable of predicting the evolving velocity profile in a microstructure under shock loading. This U-net model generates accurate evaluations, in orders of magnitude less time than the corollary FEM models. This figure shows the predicted velocity profile at the final step of the model, using both FEM and U-net models. Although the U-net model is trained only on microstructures with 20 grains, it is capable of capturing accurately the velocity profile in a microstructure with 70 grains. In other words, the U-net model is capable of predicting behavior in as-yet unseen microstructures, potentially serving a critical role in designing materials with improved spall strength and other key dynamic properties.

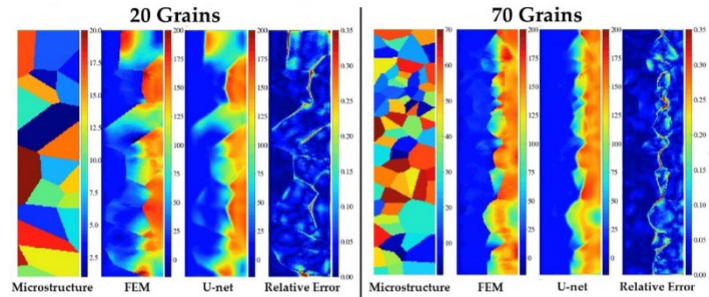


Figure 5: Velocity maps predicted from finite element models (FEM) with crystal plasticity and damage, vs those predicted from U-net. U-net is trained only on microstructures with 20 grains, but it can accurately predict behavior of microstructures with 70 grains, with orders of magnitude less computational time as compared to the FEM model.

Data-driven Representations and Machine Learning

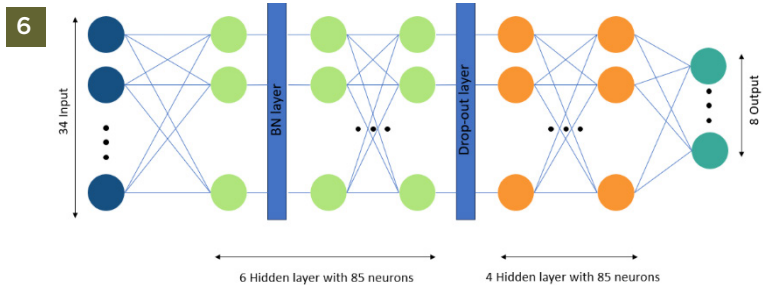
Machine learning framework: We are developing a coupled artificial neural network framework to guide RMPEA design. The first multi-layer perceptron (MLP) network predicts phase composition based on 34 chemical descriptors. RMPEAs classified as single-phase body-centered cubic (BCC) microstructures will be passed to a second MLP network, which predicts their mechanical performance. By actively exploring the design space, this framework will identify BCC RMPEA candidates with optimal predicted properties. The architecture comprises two sequenced MLP networks, continuously trained on both simulated and experimental data for enhanced accuracy. This integrated data-driven approach will rapidly steer RMPEA design towards alloys with exceptional strength and ductility. Further details on the MLP framework are provided in Figures 6 and 7.

Training database: The coupled MLP networks are trained on extensive datasets from both computational and experimental sources. The first network uses a database of thousands of RMPEAs with predicted phases from Thermo-Calc software. The second network trains a database of BCC RMPEA mechanical properties generated by a new experimentally validated theoretical model developed by our group. As more experimental data becomes available from AIMD, it will be incorporated to enhance the fidelity and practical applicability of both datasets. This focus on integrated computational and empirical validation will produce MLP networks with exceptional accuracy for guiding RMPEA design.

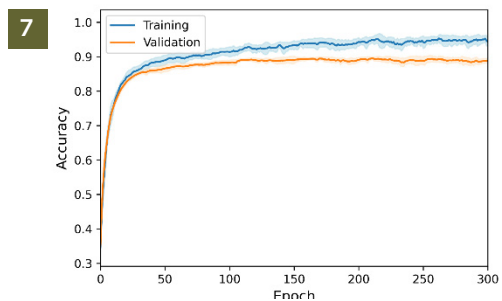
Key findings: The developed MLP framework demonstrates exceptional performance and new capabilities:

- Achieves over 90% prediction accuracy for RMPEAs containing Ti, Fe, Al, V, Ni, Nb and Zr, trained solely on computational data. The learning curve in Figure 7 illustrates rapid convergence.
- Predicts up to 8 potential phases simultaneously, namely: FCC, BCC, HCP, ordered BCC, Laves, Sigma, Heusler and Other. This enhanced the resolution of the predictions which exceeds previous works that only focused on a much smaller subset of phases.
- Incorporate Shapley values and feature distribution analysis to provide correlation between the chemical feature importance with respect to the development of different phases to enable the accurate prediction of a completely new alloy compositions outside the original training data.

By combining high accuracy, multi-phase prediction, and interpretation for new alloys, this MLP approach significantly advances high-throughput RMPEA design and discovery. Ongoing work includes integrating experimental data to further improve practical applicability.



Figures 6 and 7: (6) Architecture of the designed MLP network (7) Learning curve of the first MLP network





KEY AI NEED 3

RELIABLE APPROACHES TO
IDENTIFY OPTIMAL DECISION(S)

AI-DRIVEN DECISION-MAKING FOR OPTIMAL MATERIALS DESIGN

PROF. TAMER ZAKI, CO-PI

GOAL: TO DEVELOP ACCURATE AND PREDICTIVE AI MODELS THAT GUIDE DECISION-MAKING FOR THE DESIGN OF NEW MATERIALS.

Material performance on a larger scale depends on a material's composition, microstructural properties, processing details, and many other design and process decisions. The objective of this task is to regard these decisions as an optimization problem in order to objectively select these tunable parameters in a manner that optimally achieves the desired outcome. Mathematically, this process is a nonlinear optimization where we aim to maximize an objective function (e.g. spall strength of a material sample) or minimizing a cost function (e.g. probability of failure). Since the outcome invariably depends on a large number of design, or control, parameters, the optimization is performed in high dimensions. In addition, due to the nonlinear nature of the problem, the search for the optimal configuration must traverse a non-convex, tortuous decision terrain. The figure below is a simplified schematic of a cost function $J(c)$, where c are the control parameters to optimize. While the figure shows a

two-dimensional optimization $c=[c_1, c_2]^T$ for visualization purposes, in reality we are interested in higher dimensions. In the current stage of the project, we assume that the cost of performing experiments or simulations is not prohibitive, and therefore we can sample the space of parameters c using efficient approaches. We then proceed to learn the surface $J(c)$ from data, using a machine-learned model that we subsequently use as a surrogate to optimize our design decisions. Our optimization algorithm effectively navigates non-convex surfaces in search for the optimal. For our first demonstration, we will optimize the grain orientations for a microstructure with a fixed grain boundary and grain size distribution, with the objective of maximizing the spall strength. We will then expand the design space to include a larger number of design variables such as number of grains, grain size distribution etc.

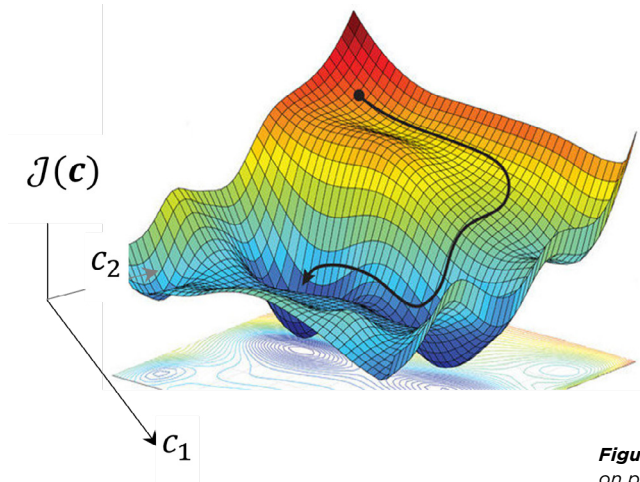


Figure 8: Schematic of decision landscapes, J , which depend on parameters \mathbf{c} . The landscape is inferred from data, and encapsulated in a surrogate machine-learning based model. The ML-model is subsequently used as a surrogate to experiments to inform and, more importantly, efficiently optimize decision-making.

BAYESIAN OPTIMIZATION FOR CONNECTING MATERIALS PROCESSING, PROPERTIES, AND PERFORMANCE

PROF. PAULETTE CLANCY, CO-PI

GOAL: TO ACCELERATE THE DISCOVERY OF MATERIALS WITH SUPERIOR PROPERTIES

Accomplishment: We used a Bayesian optimization code pipeline that we created (PAL 2.0)¹ to perform “feature engineering” to find the properties most correlated with the target of the optimization, and then use the optimization code to select better alternative materials. Unlike most deep learning approaches, we can work with small data sets (as few as 12 points), perfect for research labs with few and expensive data. We have completed a spectacular “stress test” of PAL using a 70,000-strong MOF database² to find the best MOF material for methane storage. We found the optimal solution in just 4 tries, beating the performance of a recent paper by Deshwal et al.; see Figure 9.³

This year, we started new collaborations with Prof. Tim Weihs (Mat. Sci.) and Eddie Gienger (APL) to predict better performing metal alloys. With the Weihs group, we helped identify the presence of a ternary alloy phase as a key metric and suggested improved Mg-alloys. We found an unexpected result that both corrosion rate and hardness depend on the ternary phase, $\text{Ca}_2\text{Mg}_6\text{Zn}_3$, explaining the slow decrease in these targets as the solution treatment time increases beyond 10 minutes; see Figure 10. These encouraging results, produced in just a short time, have prompted a second study, on Al-alloy fragmentation, to begin. A publication is in preparation.⁴

With Gienger, we have completed two design improvement cycles so far to suggest better high-entropy alloys, with improved strength for spacecraft actuators. A design cycle involves PAL predictions of compositions to try, followed by experimental synthesis and testing, with the results fed back to PAL for further optimization. We have added constraints for manufacturability and the cost of the elements. This work will be presented in November at a TMS conference.

References

- 1 M. Sharma Priyadarshini, O.V. Romiluyi, Yiran Wang, K. Miskin, P. Clancy. A new approach to incorporate physical domain knowledge for Bayesian optimization searches in high-dimensional chemical materials system, *Materials Horizons*, revision submitted 11/6 (2023)
- 2 R. Mercado, R.-S. Fu, A. V. Yakutovich, L. Talirz, M. Haranczyk and B. Smit, *Chem. of Matls.*, 2018, **30**, 5069–5086.
- 3 A. Deshwal, C. M. Simon and J. R. Doppa, *Molecular Systems Design & Engineering*, 2021, **6**, 1066–1086.
- 4 S. Raguraman, M. Sharma Priyadarshini, T. Nguyen, R. McGovern, A. Kim, A. Griebel, P. Clancy, T. Weihs, Machine Learning-guided rapid structure-property correlations in a lean magnesium alloy for biomedical implants, in prep. Nov. (2023)

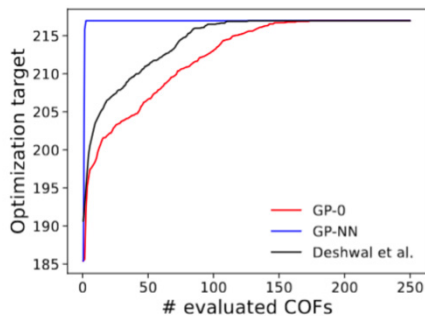


Figure 9: Progress of a Bayesian optimization approach to find the MOF candidate with the best methane storage capability. The fewer the number of evaluated COFs, the faster the optimization. Recent results by Deshwal et al. [3] are shown in black. A naive BayesOpt approach in red and PAL 2.0's very fast optimization is shown in blue.

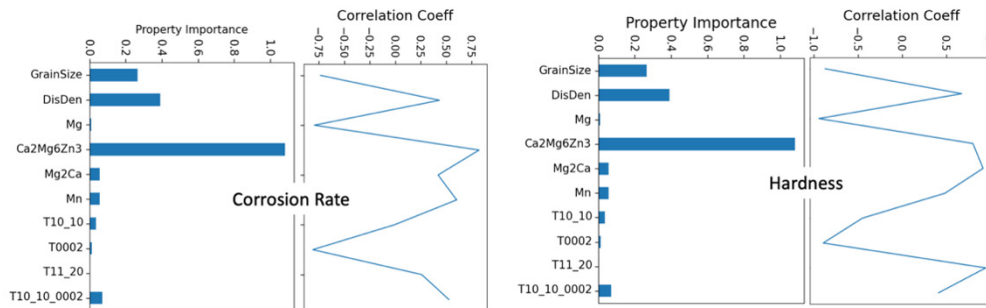


Figure 10: XGBoost analysis of the importance of posited physical properties and their corresponding correlation coefficient (labeled + or - to denote positive or negative correlations)

KEY AI NEED 4

ACTIONABLE RESPONSE TO THE DECISION(S)

ROBOTIC AUTOMATION AND ON-THE-FLY LEARNING FOR AUTOMATION AND CONTROL

PROF. AXEL KRIEGER, CO-PI

PROF. KT RAMESH, CO-PI

GOAL: TO CREATE A SYSTEM OF ROBOTS THAT CAN HANDLE SAMPLES IN A PRECISE, REPEATABLE FASHION TO FACILITATE HIGH-THROUGHPUT MATERIALS DISCOVERY WHILE COLLABORATING SAFELY WITH HUMAN RESEARCHERS.

Research Strategy:

We developed a robotic system to accelerate AI-directed material discovery by facilitating high-throughput testing and characterization. The system features a conveyor setup and six collaborative UR10e robots from Universal Robots to handle and manipulate the samples. The robots utilize vacuum grippers for precise sample handling, allowing them to move samples effectively between the conveyor and different subsystems.

A key aspect of this design is its precise and repeatable sample positioning at different stations. Its modular design allows for adaptability in handling different materials and sample sizes.

The communication between the central programmable logic controller (Siemens PLC) and each subsystem is established using OPC Unified Architecture (OPC UA). Additionally, the system's performance has been evaluated and simulated through simulations in Gazebo and SIMUMATIK.

Safe collaboration between the robotic system and researchers is paramount. Each collaborative robot is equipped with a force sensor that will automatically stop when it collides with a person or an object.

This fall, we installed the robotic automation system in our new facility and started integration with the different substations.



Figure 11: UR10e robots are installed at each station in the AIMD Lab. The robots are fitted with vacuum grippers to facilitate specimen handling.

KEY AI NEED 5

EVENT-DRIVEN INTEGRATION OF DATA TO CONNECT
THE DESIGN, DECISION, AND CONTROL LOOPS

DATA MANAGEMENT AND THE EVENT-DRIVEN DATA LAYER

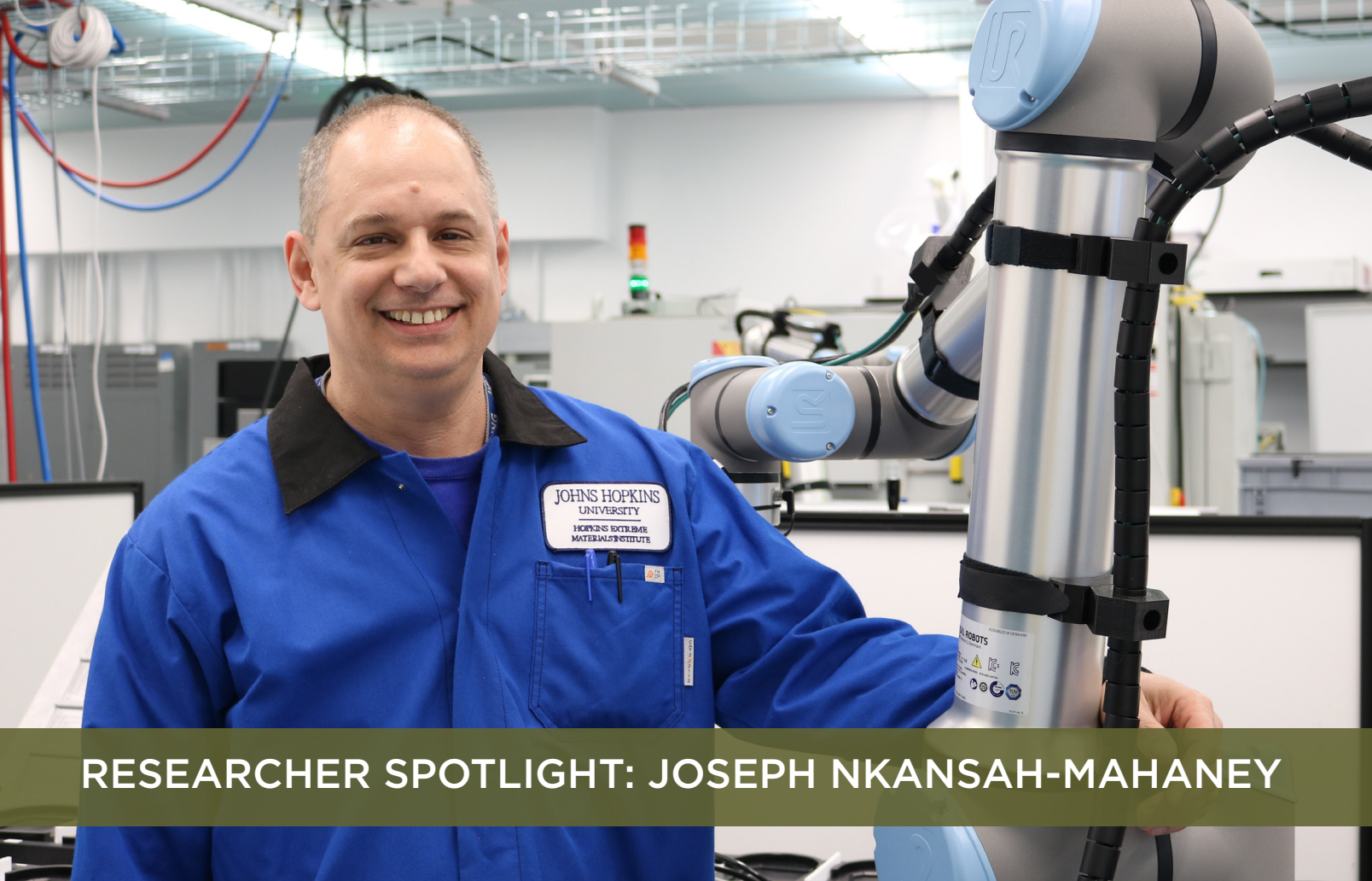
DR. DAVID ELBERT, CO-PI

GOAL: TO CONNECT AMDEE TASKS WITH EVENT-DRIVEN DATA STREAMING TO CREATE ORCHESTRATED WORKFLOW AUTOMATION

The AMDEE vision centers on integrating automation and decision-making to move the current state-of-the-art towards autonomous materials design. Making this a reality requires seamless integration of data from three components: 1) processing and characterization science, 2) AI/ML decision-making models, and 3) automated control system deployments for the varied, complex tasks. Our group is implementing a streaming data layer to seamlessly link events across these three main components and serve as a backbone for the development of event-driven methods, which will allow research tasks to react automatically to changes in state of other parts of the AMDEE system.

To realize this goal, we have developed an initial concept of AMDEE workflows factored into data creation, data analysis and visualization, and data curation. Work-to-date has included building object storage and streaming server clusters to support streaming movement and management of data. We have advanced our knowledge graph approach to data modeling to include streaming data from automated sample handling in the laser shock facility. Current efforts include over 30,000 linked data nodes that can be stored in file representations or a queryable graph database. We are currently working to automate decision deployment for the See-Move-Shoot algorithms being developed by the robotic automation group.

In addition to scientific data, AMDEE researchers (directed by Eric Walker) have developed a rich data layer for sample movement and analysis control. This summer, our group will focus on building streaming from the Facility Control and Data Layer. This control data provides a seamless source of information to link sample characterization parameters with scientific data, as well as a powerful point of contact to return ML decisions in the form of control scripts to guide next steps on the automated line. Once we have automated capture and curation of control data, we will create automated tools to inject new control directives safely and in coordination with the workflows entered manually on the line. This level of orchestrated interaction is believed to be unique in the materials research space and will accelerate advancement towards autonomous research.



RESEARCHER SPOTLIGHT: JOSEPH NKANSAH-MAHANEY

Joseph Nkansah-Mahaney is an associate staff engineer at the Hopkins Extreme Materials Institute at Johns Hopkins University. His primary focus is the AIMD Laboratory.

1. What is your role within AMDEE?

I am a staff engineer. I work as part of a team to tackle the technical challenges of the development of a complex autonomous, AI-driven materials research platform. Within the context of AIMD/AMDEE, I help coordinate and integrate the PIs, their teams, vendors, and the many disparate tools and parts that allows bringing the systems together chasing the vision of AI driven autonomous materials discovery. As a staff engineer working on the AIMD platform, I have a responsibility to learn and share knowledge in subjects extending from to the practical, such as connecting wires to pass DC signals, to the more abstract such as an understanding how AI works within the AIMD materials discovery process.

2. What is it like to work on AMDEE?

No two days are the same. I work in a place where I know I am on the cutting edge of discoveries which could have a positive impact on millions of people. I also get to work with extremely talented, focused, and dedicated scientists every day, all of whom are driven, like me, to help the AIMD Lab reach its full potential.

3. What are your professional interests?

I have acquired many while on life's unpredictable path. On my professional journey, I've found a consistent interest in bringing the scientific results from curious lab experiments to a scaled reality outside of the laboratory such that a measurable, societal impact can be made. In the past, I have often joked with colleagues that if they invented warp drive, I would build it. I love science—but I REALLY love when science makes a difference.



I love science—
but I REALLY love
when science
makes a difference.”

OTHER MEDE+ FACILITIES: THE WEIHS LAB

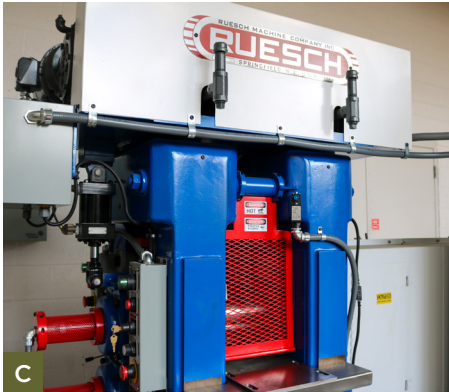
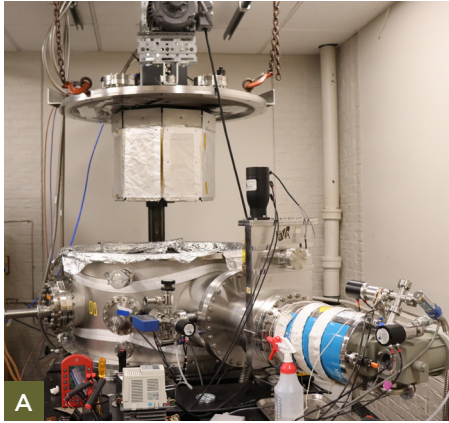
The **Weih's Lab**, led by Tim Weih, features a suite of equipment used for fabricating and processing samples. Researchers use thermomechanical processing methods to create samples with very specific characteristics.

EQUIPMENT	CAPABILITIES	USE FOR AMDEE
A. Sputter chamber—PVD Uses DC magnetron guns to deposit layers of atoms on a substrate.	<ul style="list-style-type: none"> • 30" diameter chamber provides the space to create hundreds of samples in a single deposition • Horizontal configuration allows for the creation of thicker samples, which can be removed from substrate for characterization • Gradients allow researchers to create many samples with large ranges of compositions efficiently 	Allows researchers to: <ul style="list-style-type: none"> • Finely control the microstructure of sample materials and create alloys with very specific compositions • Determine how composition affects material properties
B. High-temperature furnace with quenching capability	<ul style="list-style-type: none"> • Reaches temperatures up to 2200°C • Has built-in quenching capability to cool samples rapidly 	Allows researchers to: <ul style="list-style-type: none"> • Homogenize samples • Access more phases than a standard lab furnace • Anneal (heat treat) samples
C. Rolling mill	<ul style="list-style-type: none"> • Two rollers compress samples • Capable of both cold and hot rolling (up to 300°C) 	Allows researchers to change the textures of their samples, creating materials with oriented grains, increased dislocations, and greater strength



Most standard lab furnaces can only reach 1200°C, which could be enough to homogenize a material, but not really let us access every phase predicted. Our high-temperature furnace reaches 2200°C, which is particularly helpful when we are looking for single-phase BCC microstructures.”

Rayna Mehta, graduate student



SIGNIFICANT MEETINGS

HOPKINS ON THE HILL

Hopkins on the Hill is a biennial event which showcases the range, value, and impact of federally funded research and programming at Johns Hopkins University. MEDE+ was one of 14 major projects selected to represent Johns Hopkins at this event in 2023. The event, which was held in the historic Kennedy Caucus Room of the Russell Senate Office Building, was attended by the Maryland Congressional delegation, JHU alumni, and university leadership.

CONGRESSIONAL STAFFER VISITS

Legislative staffers from the offices of U.S. Senators Ben Cardin and Chris Van Hollen visited MEDE+ facilities at Johns Hopkins University on August 31, 2023. The visit included tours of the AIMD Laboratory and the labs of Todd Hufnagel and Tim Weihs.



RELATED ACADEMIC PROGRAMS

The Hopkins Extreme Materials Institute is committed to academic and professional development. In support of these values, CAIMEE facilitates several academic programs to broaden the impact of the AMDEE program.

EXTREME SCIENCE INTERNSHIP (ESI)

The ESI program, which is run in coordination with Morgan State University, is led by Prof. Birol Ozturk and offers paid internships year-round to MSU students. ESI interns participate in internal internships at Morgan State, allowing them to develop their research skills before participating in external internships at participating locations. Started during the MEDE program, ESI continues to model excellence in collaboration and student development.

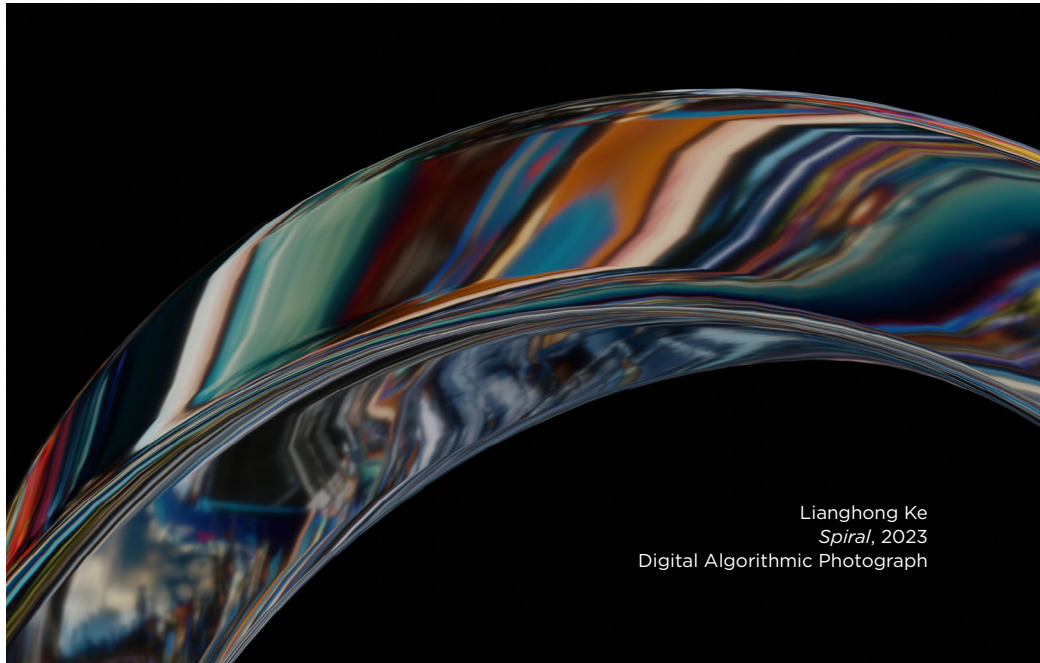
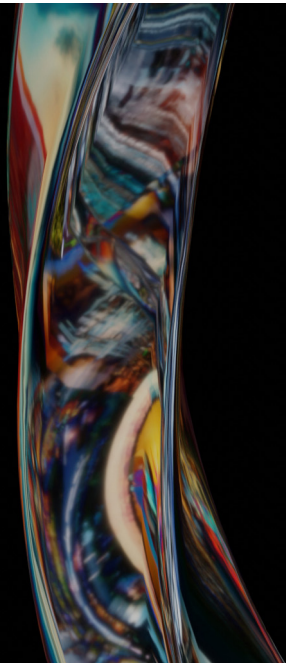
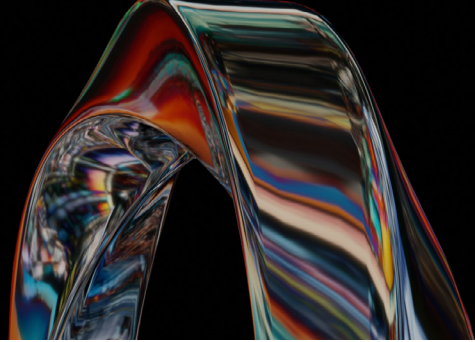


*In 2023, AMDEE supported ESI intern **Tomas Sujeta**. Sujeta's work involved quantum sensing experiments to detect magnetic fields with nitrogen vacancy defects in diamond.*

HEMI/MICA EXTREME ARTS INTERNSHIP

The HEMI/MICA Extreme Arts Program brings artists and scientists together to explore unique perspectives on extreme materials and events. HEMI/MICA Extreme Arts Internships bring students from the Maryland Institute College of Art to Johns Hopkins University, where they work with HEMI faculty hosts and MICA mentors to discover new scientific concepts and opportunities for creative expression.

In 2023, AMDEE supported Extreme Arts intern Lianghong Ke. Ke, a photographer, worked with HEMI Fellow Paulette Clancy and was inspired by artificial intelligence and the pursuit of technological advancements like superconductors. Ke's work, shown on page 44, conjures a warped, abstract reflection of what the world might look like as humanity continues its ceaseless march towards infinite knowledge and power.



Lianghong Ke
Spiral, 2023
Digital Algorithmic Photograph



HEMI.JHU.EDU/CAIMEE

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