Deep Learning and Human-Machine Teaming for Efficient and Targeted Fabrication of Liquid Metal/MXene Composites

About AFRL:

Air Force Research Laboratory (AFRL) is a scientific research organization operated by the United States Air Force Materiel Command. AFRL is dedicated to leading the discovery, development, and integration of aerospace warfighting technologies, planning, and executing the Air Force science and technology program, and providing warfighting capabilities to United States air, space, and cyberspace forces.

The Air Force Research Laboratory Materials and Manufacturing Directorate uses a combination of novel and high-impact experiments, in-house high-fidelity HPC simulation software, and machine learning to characterize and predict the performance of current and emerging materials.

RESEARCH LOCATION: Wright-Patterson AFB, OH

PROJECT DESCRIPTION:

The morphology of liquid inclusions in composite materials has a profound impact on their performance. This project aims to leverage computational statistical mechanics, high-end computing, and machine learning to uncover processing to liquid morphology relationships.

This project intends to investigate the intricate relationships between processing parameters and resulting morphologies in liquid metal/MXene (LM/MX) included composites, building upon previous efforts by the team, and through the HIP program. HEC will be leveraged as we employ computationally intensive dimensionality reduction techniques, such as UMAP and Variational Autoencoders, to uncover hidden correlations within high dimensional processing parameter space. This includes, but is not limited to, factors like temperature, mixing times, mixing speeds, volume fractions, and chemical compositions. Integrating materials science expertise through human-machine teaming, meaningful insights will be extracted from these correlations. Data will include a mix of low-fidelity simulation data (Ising-like lattice gas models for agglomeration), high-fidelity models (agglomeration of sticky particles in LAMMPs), and experimental data.

The aim of the project is to enhance understanding of morphology control of LM/MX composites and to also foster synergistic relationships between materials scientists and deep learning methodologies for efficient and targeted fabrication of these composites.

To achieve the goals of the project, the intern will:

Week 1: The intern will spend the first week getting acclimated to AFRL, getting access to computational resources, and will have the opportunity to review the research goals, the fundamentals of Monte Carlo, liquid inclusions, and machine learning.

Weeks 1-3: Because both the processing parameters and morphological features live in high dimensional space, powerful dimensional reduction techniques will be used to probe processing-morphology relationships. The intern will research with materials science experts to uncover important and hidden relationships in the reduced dimensional space.

Weeks 4-5: The intern will train a variational auto-encoder and explore the latent variable space to discover any further, missing, or hidden correlations between processing parameters and morphology.

Weeks 6-8: From the learned correlations, the intern will collaborate with the team to further employ deep learning models and/or design rules to target efficient fabrication of LM/MXene composites.

Weeks 9-10: The intern will complete participation on projects, participate in the annual AFRL poster session, final HIP presentation, and create documentation to ensure facile intellectual transfer and continuation of the research.

The intern will learn debugging, automated workflows, data management, data analysis, data visualization, and applied ML--all of which are broadly applicable to STEM fields. Monte Carlo methods are ubiquitous in modeling systems with randomness (e.g., weather forecasting, ground water, biology, financial markets, etc.). Beyond technical research, the intern learns about AFRL, network, attend talks and seminars (e.g., "MIrACLE Forum" on machine learning), and enhance communication skills.

ANTICIPATED START DATE:

June 2025 – Exact start dates will be determined at the time of selection and in coordination with the selected candidate.

QUALIFICATIONS:

Preferred qualifications include:

- Degree obtained or sought in Data Science, Chemical Engineering, Physics, Chemistry, Computer Science, Mechanical Engineering
- Advanced undergraduate or graduate student
- Some knowledge of programming such as MATLAB, Python, C++, and/or Julia is preferred
- Knowledge of machine learning is a plus

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Bachelor’s
- Master’s
- Doctoral

DISCIPLINE NEEDED:

- Computer, Information, and Data Sciences
- Engineering
- Chemistry and Materials Sciences
- Physics
- Science and Engineering related