Improved Grain Growth Models through Multi-scale Modeling and Machine Learning

About DEVCOM ARL:

The DEVCOM Army Research Laboratory (ARL) is designed to significantly increase the involvement of creative and highly trained scientists and engineers from academia and industry in scientific and technical areas of interest and relevance to the Army. Scientists and engineers at ARL help shape and execute the Army's program for meeting the challenge of developing technologies that will support Army forces in meeting future operational needs by pursuing scientific research and technological developments in diverse research fields.

RESEARCH LOCATION: Aberdeen Proving Ground, MD

PROJECT DESCRIPTION:

This project seeks to improve the performance of Potts Monte Carlo grain growth models through the incorporation of atomistic simulation results. Two thrusts will be pursued to increase the realism these simulations, with both utilizing machine learning techniques to enable the scale bridging.

1. Advanced atomistic descriptors will be utilized to construct relations for predicting the energetic cost of removing/inserting atoms into a grain boundary within molecular dynamic simulations. These relations will then be implemented into a developed Monte Carlo grain boundary optimization scheme to construct better distributions of possible energy states for a given grain boundary orientation.

2. Macroscopic orientation descriptors will be utilized to construct relations for the prediction of grain boundary energy from a database of atomistic structures. These relations will then be implemented into a developed Potts Monte Carlo grain growth code and a comparative study performed on the resultant microstructure when an average energy, an orientation dependent energy, and an orientation dependent distribution of energies is utilized.

HPC resources will be utilized both developing the ML models (scikit-learn) and testing their implementation within parallelized software (LAMMPS, SPPARKS).

Atomistic Simulations: A developed workflow for a MC grain boundary structure optimization scheme utilizes trained ML models to predict the energetic cost of altering atoms at a grain boundary. This will enable the intern to construct models on an available database and quickly implement and test the performance of different descriptors, fitting metrics, and sampling strategies.

Grain Growth Models: SPPARKS grain growth code allows for a mapping of the energies of possible orientation to be performed at the outset. This will enable the intern to construct models on an available database and quickly implement into the code. A study can then be performed to understand the influence of these models on the resultant microstructure.

The Army Research Laboratory has an active intern program that includes tours of several individual laboratories at locations in Aberdeen Proving Ground and Adelphi, MD. Throughout the summer, there are planned functions/socials at the team, branch, and division level to interact. Furthermore, there are frequent program, team, and branch meetings to help introduce interns to the culture at ARL.

Throughout the summer, the intern will receive hands-on training on using the DSRC systems, running simulations, and analyzing simulation data. Linux workstations will be used to train the intern on accessing the DSRC resources and transferring data to/from the clusters. The intern will be provided extensive training on fitting machine learning models and running parallelized software (LAMMPS/SPPARKS). Additionally, the intern will be trained on using post-processing tools for studying the simulation results (Paraview/OVITO).

There are multiple opportunities to network with other interns, postdoctoral associates, and ARL S&Es. The mentor will facilitate individual meetings between the intern and specific staff members whose research portfolio or professional experience best align with the student's intended professional path. Additionally, the intern will have the opportunity to interact with human resources and learn more about careers in the government defense laboratories.

The proposed research plan is flexible enough to fit the experience of the interns, so specific expectations of technical activities will be adjusted accordingly. These range from constructing ML models and utilizing developed scripts to test their effects to much more involved research where they can attempt to improve the underlying workflows/code.

ANTICIPATED START DATE:

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

QUALIFICATIONS:

Graduate students with interest in materials modeling.

Preferred skills:

- Python or C/C++
- Basic/moderate understanding of parallel computing
- Understanding of microstructural evolution or grain boundary structure
- Knowledge on numerical methods or machine learning
- Experience with molecular dynamics or Potts Monte Carlo codes

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Master's
- Doctoral

DISCIPLINE NEEDED:

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