Professorship of Multiscale Modeling of Fluid Materials
TUM School of Engineering and Design
Technical University of Munich

Developing a Multi-Element Neural Network Potential for the Simulation of Aluminum Alloys

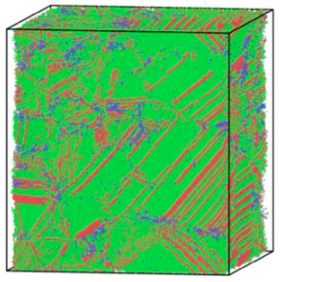
Motivation

Additive Manufacturing (AM) allows the production of parts with complex geometries that are unattainable with conventional manufacturing processes. Laser powder bed fusion (LPBF) is particularly relevant for constructing strong, lightweight metal parts. However, standard metals for lightweight applications, such as aluminum (Al), are only printable in a certain processing window and thus not well suited for these applications. Next to process design, material design is a key factor in overcoming this issue. Microalloying Al with other metals, such as titanium (Ti) and zirconium (Zr), can influence the microstructures developing during the solidification, making the alloy usable for LPBF.

Neural networks (NNs) have recently enabled high-accuracy molecular dynamics (MD) simulations of physically relevant system sizes. Training accurate NN potentials, however, requires large amounts of data, which are accessible for common systems such as pure Al yet are increasingly rare for alloys containing multiple elements. As these alloys are crucial for the application in AM, it is important to train an NN under the constraint of scarce data. Several approaches for this, such as transfer- or meta-learning have been proposed and can be advantageous for this task.

Goal

This Thesis aims to extend existing NN potentials for pure aluminum simulations and train new ones applicable to its alloys. Using this, the influence of adding different metals to aluminum in varying quantities on the resulting crystal structures and material properties after solidification should be evaluated.



Crystal structure (left) and grains (right) of stainless steel after directional solidification simulated in LAMMPS

Tasks

- Implement an approach for training multi-element NN potentials in our in-house research code ***chemtrain***
- Train a multi-element NN potential for aluminum alloys using multiple datasets
- Simulate solidification of different aluminum alloys in LAMMPS
- Evaluate the mechanical properties of the solidified alloys
- Understand the impact of additives on the crystalization process

Requirements

- Experience with machine learning, especially neural networks
- Strong proficiency in Python
- Experience with JAX is advantageous
- Highly motivated

Application

If you are interested in this project or have further questions, please write an email to ian.stoermer@tum.de including:

- A brief introduction of yourself (motivation, background, CV)
- Transcript of Records from your Bachelor and Master program.