Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Mechanics & Materials Laboratory
Prof. Dr. Dennis M. Kochmann
www.mm.ethz.ch

Master Thesis

(Spring / Autumn 2024):

Data-driven atomistic mass diffusion in crystalline solids over long time scales

Description: Studying the long-term diffusion of solutes in metals is crucial for a variety of present and futuristic engineering applications. This includes the design of safe and compact solid-state hydrogen reservoirs for automobile applications, designing corrosion-resistant materials for nuclear applications, and much more. The time scales involved in such mass diffusion processes for potential applications range from seconds to minutes. However, most state-of-the-art atomistic techniques can simulate an ensemble of atoms as large as some micrometers and for a real-time of some microseconds at best. Hence, the computational modeling of atomistic mass diffusion presents many challenges, which is why the design of these devices has relied on experiments. This project deals with an emerging class of atomistic simulation techniques based on statistical mechanics [1], which aims to track the relevant statistics of the ensemble rather than tracking all atomic positions and momenta. In such a statistical framework with multiple atomic species, every atomic site ceases to be a pure species and is instead identified by probabilities of finding different types of species at that site.

In order to introduce mass transport in such a setting, one needs to update the concentrations of different species at the atomic sites based on a phenomenological model, or by an atomistically informed master equation for the site probabilites. We are more interested in the latter approach, which involves computing the energy barriers and minimum energy pathways needed for atoms of different types to hop from one site to another. As this computation needs to be done for every possible atomic hop in the ensemble, the concentration update becomes computationally expensive. In this project, we plan to bypass this by employing graph neural networks (GNNs) to learn the hopping energy barriers as a function of local atomic environments and using a pre-trained GNN to update the site probabilities, which would enable us to reach higher time scales relevant for potential applications.

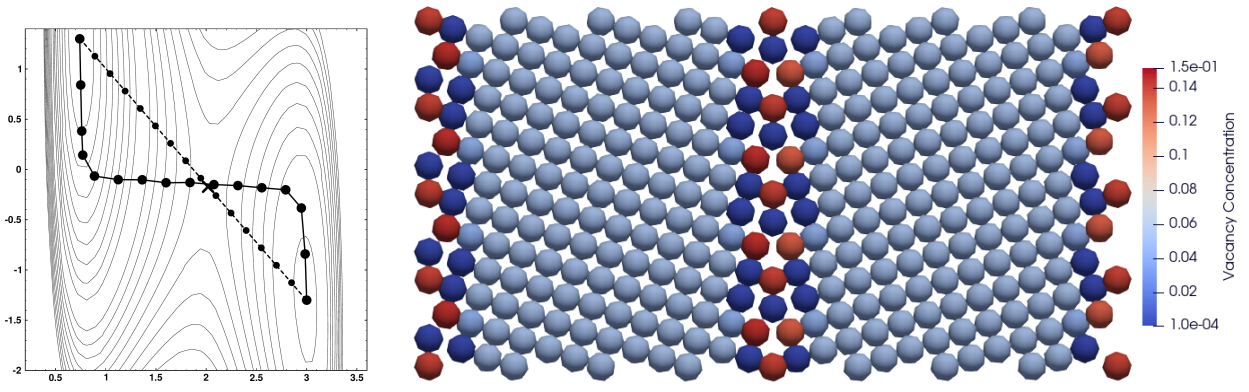

Figure 1: Minimum energy pathway for a vacancy hop (left) and vacancy clustering at a $\Sigma 5$ grain-boundary in FCC copper (right)

Tasks:

- Literature review of stat-mech-based atomistic techniques and familiarization with our in-house C++ code
- Familiarization with a state-of-the-art GNN architecture for atomistic applications (NEQUIP)
- Adapt the NEQUIP framework to enable learning of energy barriers
- Filter and preprocess the training data to optimize the learning process
- Train GNN models and access their reliability over a wide range of test data

Pre-requisites:

- Good coding skills, especially comfortable with Python. Knowing C++ is an added advantage.
- Strong background in machine learning, ideally with GNN's.

For more information, please contact:

Shashank Saxena
Mechanics & Materials Lab
Department of Mechanical and Process Engineering
Leonhardstrasse 21, LEE N223
email: ssaxena@ethz.ch

References

[1] Gupta, P., Ortiz, M., Kochmann, D.M., 2021. Nonequilibrium thermomechanics of gaussian phase packet crystals: Application to the quasistatic quasicontinuum method. Journal of the Mechanics and Physics of Solids , 104495URL: https://www.sciencedirect.com/science/article/pii/S0022509621001630, doi:https://doi.org/10.1016/j.jmps.2021.104495.