Karlsruher Institut für Technologie

Institute for Applied Materials
Electrochemical Technologies
Adenauerring 20 b
76131 Karlsruhe

Bachelor/Master thesis

Modelling the solid electrolyte interphase in lithium metal batteries using Kinetic Monte Carlo simulations

Research area

- ☒ Batteries
- ☐ Fuel Cells and Electrolyzers
- ☐ Electrocatalysis

Focus

- ☐ Experimental
- ☐ Electrical characterization
- ☐ Materials analysis
- ☒ Modelling
- ☒ Simulation
- ☒ Literature research

Studies

- ☒ Chemistry
- ☒ Chemical engineering
- ☒ Electrical engineering
- ☒ Mechanical engineering
- ☒ Material science

Starting date

Upon agreement

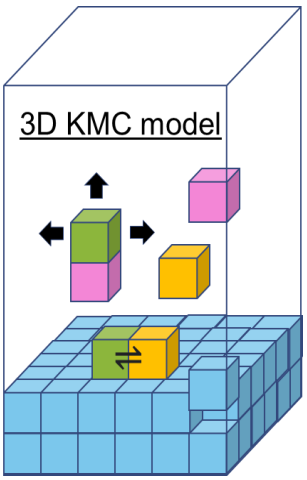
Contact person

Aravind Unni
Building 70.03
Room: 004
E-Mail: unni@kit.edu

http://www.iam.kit.edu/et/

Motivation

Lithium metal batteries (LMBs) represent the next generation in battery technology, offering significant advancements over current lithium-ion batteries. The primary challenge in realizing this technology lies in understanding and stabilizing **the Solid Electrolyte Interphase (SEI),** a critical boundary layer formed during battery operation. The SEI's composition and structure are influenced by various factors such as electrolyte composition, charging currents, and ambient temperature. Its complexity and variability over a battery's life make it difficult to fully comprehend. Here, at the IAM-ET we use the 3D Kinetic Monte Carlo (kMC) model to simulate the SEI formation. This allows for a detailed tracking of SEI growth and the associated reaction kinetics. Through the model we aim to gain fundamental insights into the SEI formation and provide these as input for SEI design, which can help design of lithium metal batteries.



Task definition

The task involves formulating plausible Solid Electrolyte Interphase (SEI) lattice structures and simulating their natural re-arrangement into a crystalline order, with a focus on utilizing the Kinetic Monte Carlo (KMC) model and diffusion processes. The key objective is to capture how nanostructures evolve under different diffusion scenarios and to develop a better overall understanding of the heterogeneity of the SEI.

Planned work packages:

- Literature Study on the KMC Model and Process Models
- Prepare plausible lattice configurations of the SEI
- Mapping Lattice Configurations to SEI in the Electrolyte + Anode KMC Model
- Study SEI structures for different diffusion models

Notes

Please enclose a **CV** and a current **overview of your grades** with your application. We offer you good supervision and the opportunity to work in an interdisciplinary team in a forward-looking field. **Independent work** and the motivation to familiarize yourself with new subject areas are required. **Programming experience in MATLAB** is desirable. For further information, please contact Mr. Aravind Unni.

Prof. Dr. -Ing. Ulrike Krewer