Karlsruher Institut für Technologie

Institute for Applied Materials
Electrochemical Technologies
Adenauerring 20 b
76131 Karlsruhe

Master thesis

Multiscale modeling of the anode-electrolyte interface in next generation lithium metal batteries

sResearch 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

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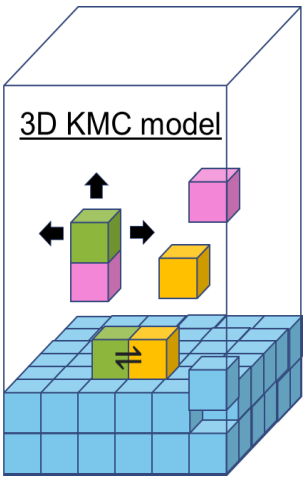
Motivation

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. To tackle this, at the IAM-ET we use a **multiscale simulation approach**, combining 3D Kinetic Monte Carlo (kMC) model with a continuum model. This allows for a detailed tracking of SEI growth and the associated reaction kinetics, particularly during the initial charging cycles. By better understanding the molecular processes behind SEI formation, the aim is to optimize the SEI, enhancing the longevity and safety of the cells, thereby bringing the promise of lithium metal batteries closer to fruition.



Task definition

In this work, a multiscale education model available at the Institute, which uses mesoscale models according to the kinetic Monte Carlo approach (kMC) with battery cell models based on partial differential equations, extended and applied to a new electrolyte chemistry. For this purpose, a new reaction network is to be implemented in the existing model. Simulation studies will then be carried out to investigate how SEI formation can be influenced by the electrolyte composition and applied charging currents.

Planned work packages:

- Literature research on the influence of macroscopic parameters on SEI formation
- Adaptation of the existing model and implementation of the new reaction network
- Simulation study on the effect of different macroscopic parameters on SEI formation
- Evaluation of the results and identification of optimal macroscopic parameters

Notes

Please enclose a **CV** and a current **overview of your grades** with your application. We offer you excellent 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