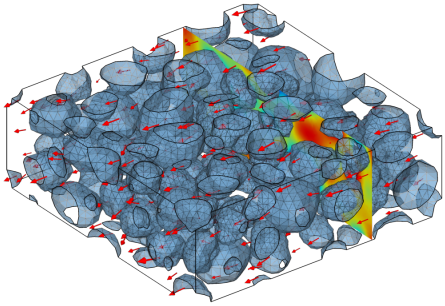
Lithium-Ion Batteries

Mathematical Modeling and Simulation

Background

Electrochemical storage technologies are a key component of the energy and mobility transition worldwide. Lithium-ion batteries (LIB) are of significant importance in this context, particularly due to technological advancements in recent decades. The enormous economic significance also creates a great demand for mathematical models for LIBs, which address a variety of different questions. Mathematical models based on non-equilibrium thermodynamics can already provide precise predictions for cell voltage as a function of state of charge and (dis)charge current, make statements about the distribution of lithium in porous electrodes, and predict hysteresis effects.



Section of a porous battery electrode with numerical solutions of a battery model (WIAS 3D grid).

Our Services

We are developing new mathematical models for all components of lithium-ion batteries as well as their current advancements. This includes models for various anode and cathode materials, liquid and solid electrolytes, porous electrodes, and electrode-electrolyte interfaces where electrochemical reactions occur. Furthermore, we are developing models for various aging effects, validating our models against experimental data, and developing numerical methods for porous electrodes. The models describe electrochemical processes and transport phenomena using partial differential equations, which are solved using numerical methods on our computers and clusters.

Key Features

- Derivation of homogenized models for porous electrodes (Newman-type models P1+1D, P3+1D, P3+N1D)
- Cahn-Hilliard-type models for multi-particle electrodes with phase separation (N-particles, M-phases) to describe graphite, $LiFePO_4$, and other active materials
- Models coupling diffusion and mechanical stresses within electrodes as well as in solid electrolytes
- Realistic 3D models for porous electrodes, including mesh generation, that fully resolve the electrolyte phase, conductive additives, and intercalation particles
- Determination of porous media parameters (diffusion corrector, tortuosity, specific surface area) based on homogenization theory
- Thermodynamically consistent transport models for ions in electrolytes, considering solvation effects, incompressibility, steric effects, and hydrostatic pressure
- Thermodynamically consistent reaction models for the intercalation reaction $Li^+ + e^- \rightleftharpoons Li$ and other side reactions (SEI, metallic lithium deposition, etc.), taking into account solvation shell effects, as well as the derivation of Butler-Volmer-like reaction rates

Fields of Application

- Scientific institutions in the fields of materials development, control engineering, and electrochemistry
- Material and cell manufacturers of lithium-ion batteries
- Automotive industry

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