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Revealing Multiscale Interaction in Batteries by Direct Coupling of KMC and Continuum Models

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The formation of solid films on electrochemically active surfaces in porous electrodes of batteries is often critical regarding the systems performance and degradation. A deep understanding of those problems is crucial for an optimal control of the growth process by current and temperature profiles. Since film thickness often is on nanoscale and structural properties are determined by heterogeneous reactions on atomistic scale, we propose the application of direct coupled kinetic Monte Carlo (kMC) and continuum models to reveal the multiscale interactions.

We have developed a multiscale modeling methodology for simulation of surface film growth in lithium-ion batteries [1]. Heterogeneity is introduced in a full order continuum battery model of the P2D type, by applying kMC simulations for heterogeneous film growth processes. The model is applied to solvent decomposition problems on graphite electrodes. Results illustrate the multiscale nature of this surface film growth problem. Thermodynamic and kinetic model parameters were identified at a set of electrochmical measurements. The simulated electrode potentials are shown to be in very good agreement with experimental data. Simulation results indicate that film thickness and structure can be influenced by externally applied current, which can lead to significant spacial deviations of film properties due to uneven distribution of electric potentials and concentrations.

This methodology provides the most advanced simulations of the frequently stated multi-scale nature [2] of film growth in lithium-ion batteries. As such, it enables a more detailed study of those highly complex but important problems in the development of batteries.

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