Phase-field modeling of Li deposits growth in Li-ion batteries

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Abstract:

Formation of Li deposits on the anode surface during cell charging of Li-ion batteries leads to a decrease in reversible capacity and potential short-circuiting as deposits grow towards to the cathode. In this presentation, we will discuss a nonlinear phase-field model for predicting the electrode-electrolyte interface motion and electrode microstructure evolution during the electrochemical deposition. It is able to simulate and predict the lithium deposit formation and growth on anode surface during charging operations. The main thermodynamic driving forces for the electrode-electrolyte interface evolution are local variations of overpotential and chemical potential. It explicitly describes ion diffusion in the electrolyte, Li^+ deposition on the electrode surface and an electrochemical reaction at the electrode-electrolyte interface. The lithium electrodeposition rate follows the classical Butler-Volmer kinetic with exponential dependence on the overpotential and cation concentration at the electrode surface. The local variations of overpotential and ion concentration cause the instability of electrode surface which eventually produce a fiber-like lithium deposit growth. The morphologies of lithium deposits and their evolutions under different charging current densities and reaction rates will be discussed.