Multiscale modeling of dendrite formation in Lithium-ion batteries

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Lithium anode-based Lithium-ion batteries (LIBs) have received much attention as next-generation batteries due to their large energy density. However, commercialization of LIBs has been hindered due to dendrite formation, which significantly deteriorates battery life and performance. Inspired by this, we have developed a multiscale model to elucidate complex interactions between microscopic dendrite growth and macroscopic variables (i.e., current density, Li-ion concentration, and cell voltage). Specifically, a first-principled kinetic Monte Carlo model describing the dendrite growth at the anode surface has been integrated with a macroscopic electrochemical model. The proposed multiscale model was able to successfully explain the effect of current density and cell voltage on dendrite growth and has been validated with experimental data. Furthermore, the proposed multiscale model can be extended to simulate multiple charge-discharge cycles in future studies and would pave the way to devise effective dendrite mitigation strategies.