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A Chemo-Mechanical model of delithiation in high-capacity anode materials

YANG, HUI, huy121@psu.edu, Zhang, Sulin, Pennsylvania State University, United States

ABSTRACT

We present a chemo-mechanical model to investigate the delithiation-induced phase transformation, morphological evolution, stress generation, void nucleation, and growth in high-capacity anode materials such as silicon (Si) and germanium (Ge). The model couples lithium (Li) diffusion with large elasto-plastic deformation by solving a set of coupled phase field and mechanical equilibrium equations using the finite element method, which leads to the coevolution of the Li concentration, stress distribution, and morphology of the anode materials during the delithiation process. The model conveniently simulates the phase boundaries, in addition to void nucleation and growth. Our simulations using this model identify a set of key chemo-mechanical parameters controlling the damage evolution and accumulation in the electrodes. As such, the model offers a generic framework for the study of the degradation mechanisms in the high-capacity electrode materials during electrochemical cycling.