Phase field model for stress evolution in an arbitrarily shaped elastoplastic electrode during two-phase lithiation

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Abstract

Stresses play an important role in lithium ion batteries, strongly coupled with the process of phase transformation during two-phase lithiation. It is a challenge to simulate the evolution of stresses in a three dimensional elastoplastic two-phase electrode. We develop a phase field model to simulate processes of galvanostatic and potentiostatic lithiation in an arbitrarily shaped particle, in which the distribution of stress is investigated based on the phase field microelasticity theory. It should be emphasized that we combine the electrode and the surrounding electrolyte together to form a regular simulation system, and thus the regular grid is used. We use a static order parameter to characterize the shape of the particle, where $\varphi=1$ represents the electrode while $\varphi=0$ represents the electrolyte, and the values between 0 and 1 denote the boundary of the particle. It is demonstrated that the smoothed boundary is adopted to determine the normal vector to the particle surface in order to introduce the galvanostatic and potentiostatic lithiation conditions. Chemical eigenstrain and plastic eigenstrain are introduced to describe the process of phase transformation and plastic deformation, respectively. Moreover, a virtual eigenstrain is employed to characterize the heterogeneous modulus of the simulation system. Our model has an advantage of simulating the evolution of stresses in arbitrarily shaped particles by adjusting the shape order parameter without changing the grid of the simulation box. Our simulations show that hoop tensile stress is prone to develop at the concave surface, which can initiate cracks during lithiation.

Keywords: phase field; lithium ion battery; stress; phase transformation; elasto-plasticity;