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Abstract

Development of high-performance phase transformation electrodes in lithium ion batteries requires comprehensive studies on stress-mediated lithiation involving migration of the phase interface. It brings out many counter-intuitive phenomena, especially in nanoscale electrodes, such as the slowing down migration of phase interface, the vanishing of miscibility gap under high charge rate, and the formation of surface crack during lithiation. However, it is still a challenge to simulate the evolution of stress in arbitrarily-shaped nanoscale electrodes, accompanied with phase transformation and concurrent plastic deformation. This article gives a brief review of our efforts devoted to address these issues by developing phase field model and simulation. We demonstrate that the miscibility gap of two-phase state is affected not only by stress but also by surface reaction rate and particle size. In addition, the migration of phase interface slows down due to stress. It reveals that the plastic deformation generates large radial expansion, which is responsible for the transition from surface hoop compression to surface hoop tension that may induce surface crack during