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Coupled electrochemical-mechanical modeling with strain gradient plasticity for lithium-ion battery electrodes. (English) Zbl 1472.74054

Eur. J. Mech., A, Solids 87, Article ID 104230, 8 p. (2021).

Summary: We first present a model coupling the electrochemical reaction with strain gradient plasticity for a spherical electrode, which aims to analyze the evolutions and distributions of electrochemical-reaction dislocations and diffusion-induced stress during lithiation process. Several critical features viewed by *in-situ* TEM are incorporated into this model, such as the two-phase boundary and high-density dislocations at the reaction front. It is shown that the microstructure evolution can impact the mechanical properties and electrochemical performances of electrode materials. The results obtained by a finite difference method indicate that, as lithiation proceeds, the circumferential stress on the surface of the lithiated shell changes from compression to tensile stress, which may cause fracture of the active materials. Especially, the electrochemical-reaction dislocation zone results in fairly large stresses at the front of the interface. Furthermore, the lithiation reaction displays a strong size effect, and the movement rate of reaction front reduces as the size of the particles decreases. This work provides a framework for large-capacity, multi-scale research on high-capacity lithium-ion battery electrodes.

MSC:

74E40 Chemical structure in solid mechanics
74C99 Plastic materials, materials of stress-rate and internal-variable type
74S20 Finite difference methods applied to problems in solid mechanics
78A55 Technical applications of optics and electromagnetic theory

Keywords:

spherical electrode; reaction dislocation; strain gradient plasticity; diffusion-induced stress; finite difference method

Software:

ReaxFF

Full Text: DOI

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