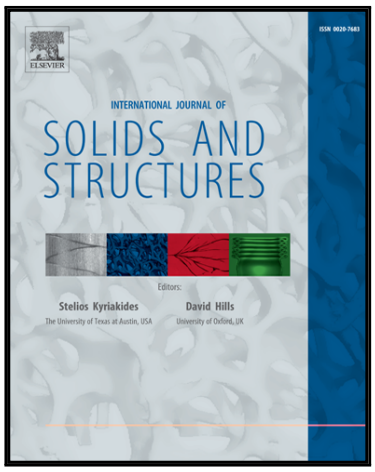

Phase field model for two-phase lithiation in an arbitrarily shaped elastoplastic electrode particle under galvanostatic and potentiostatic operations

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Phase field model for two-phase lithiation in an arbitrarily shaped elastoplastic electrode particle under galvanostatic and potentiostatic operations

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Abstract: A phase field model is developed to study the effect of charging methods on the stress evolution in an arbitrarily-shaped elastoplastic electrode particle. The model integrates Cahn-Hilliard equation with smoothed boundary method for two-phase lithiation under galvanostatic and potentiostatic operations and phase field microelasticity theory for inhomogeneous lithiation-mediated elasticity and plasticity. During two-phase lithiation, we show that the lithiation rate approximately remains constant under galvanostatic operation but slows down as lithiation proceeds under potentiostatic operation. While, the evolution of surface tangential stress during two-phase lithiation is similar under both galvanostatic and potentiostatic operations. Our results show that the surface tangential stress monotonously varies with the Li-rich phase volume, changing from compression to tension. The larger current density, as well as the larger chemical potential on the electrode particle surface, leads to the larger surface tangential compression in the early stage of lithiation but the larger surface tangential tension in the late stage. Our model is capable of probing the connection among the operating conditions, the complex particle geometry and the lithiation-induced stress.

Key words: phase field; smoothed boundary method; plasticity; lithium ion battery.

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