Surface growth models for solid-state batteries

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Abstract

Traditional liquid electrolyte-based lithium-ion batteries are close to reaching their limits on energy density, while higher specific capacity is required from modern energy storage units (1). Solid-state batteries, combining a solid-state electrolyte with a lithium anode have emerged as a promising alternative, offering higher energy density (up to 50% on the cell level) and improved safety. However, during charge and discharge cycles uneven current density often causes dendrites to develop in the form of needle-like protrusions of lithium that propagate through the solid electrolyte by fracturing it. Suppression of their growth presents a critical challenge to developing solid-state battery technology as dendrites lead to mechanical degradation of the solid electrolyte, short-circuiting, and subsequent cell failure (2).
Lithium plating and stripping (deposition and ablation) during charge and discharge cycles are inherently surface growth phenomena that couple the stress state in the electrode, interface kinetics between the electrode and the electrolyte (commonly described by Butler-Volmer kinetics (3)), and ion transport in the bulk of the solid electrolyte with a dependence on the morphology of the interface. Current modeling of dendrite growth in solid-state batteries eludes the surface growth associated with lithium deposition.

As a first step towards formulating a fully coupled sharp-interface model of lithium plating or dendrite growth, we formulate a surface growth theory using a Lagrangian framework inspired by the work of Yavari and Sozio (4). To account for accretion of the body, an arbitrary time-dependent reference configuration is constructed that embeds an inelastic-strain field determined at the instant of deposition. We utilize the multiplicative decomposition of the deformation gradient to obtain the elastic strain tensor, related stress tensor in the growing body by a standard constitutive relation. As new material is accreted to the body, its stress components along the directions tangent to the growing surface remain undetermined by general principles, thus forming an additional constitutive quantity, referred to as the deposition protocol (5). We show that the choice of the deposition protocol as well as the history of deformation play a crucial role in the arising stress field and the inelastic-strain field. In contrast to existing formalisms of surface growth, the proposed theory does not rely on concepts of differential geometry, making it more accessible to the general mechanics community. It is also more amenable to numerical calculations using standard tools of nonlinear elasticity.

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