

PROCEEDINGS

A Peridynamic Model for Lithium Dendrite Growth in Solid Electrolyte

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ABSTRACT

The uncontrolled lithium dendrites penetrate into solid electrolyte is the major obstacle of the practical deployment of all-solid-state batteries (ASSBs) [1,2]. In this study, we present a Peridynamic (PD) model for lithium dendrite growth in solid electrolyte by coupling the Poisson-Nernst-Planck (PNP) system, continuum surface reaction (CSR) and the mechanical effects. The PD formulation decouples nonlocal PNP and CSR equations via operator splitting method, enabling natural accommodation of evolving dendrite interfaces without interface tracking or mesh reconstruction. Benchmark simulations demonstrate high accuracy and convergence for ion transport and lithium deposition processes. Applications to lithium electrodeposition reveal the model's capability to capture dendrite morphology evolution, showing a transition from reaction-limited dense growth to diffusion-limited tip propagation with increasing Damköhler number. Further simulation of the penetration of lithium dendrites into solid electrolytes is conducted. Results demonstrate that the growth of lithium dendrites in nanoscale pores significantly amplifies the internal hydrostatic pressure, leading to tensile stress buildup in the electrolyte grain boundary (GB) and ultimately causing intergranular and transgranular fracture. These findings indicate that the proposed PD model can be effectively used in the designing of the dendrite-resistant solid electrolytes.

KEYWORDS

Peridynamics; lithium dendrites; lithium metal anodes; fracture; surface reaction

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