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A coupled phase field framework for mechanical and electrochemical dendrite propagation in lithium metal solid-state battery cells

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Extended Abstract

Abstract

Li-metal dendrites often initiate at imperfections [1] in the solid electrolyte/Li-metal electrode interface. During charging, Li metal deposits in these imperfections, generating stress concentrations that could form filaments in the solid electrolyte, which may propagate through it. This process can significantly degrade the solid electrolyte and impair battery performance, posing a risk of internal short circuits. To address this challenge, this work presents a phase-field model coupling electrochemical [2] and mechanical effects [3], capable of predicting dendrites growth in battery cells. This coupled approach captures the interaction between dendrites growth and the electrochemical, mechanical, and damage responses of the solid electrolyte. The model is implemented using the open-source finite element software FreeFEM++ [4]. To better understand each physical process, the problem is decoupled into an electrochemical part (Figure 1), a partially coupled electrochemical–mechanical part, and a fully coupled electrochemical–mechanical–damage part. This work aims to test and refine current thermodynamic formulations, focusing on the influence of mechanical confinement on lithium dendrites growth in all-solid-state batteries.

Keywords:

Multi-physics modelling phase field fracture mechanics Electrochemistry