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Chemo-Mechanical Peridynamic Simulation of Dynamic Fracture-Pattern Formation in Lithium-Ion Batteries

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ABSTRACT

Mechanical failure due to lithium-ion diffusion is one of the main obstacles to fulfill the potential of the electrode materials. Various fracture patterns in different electrode structures are observed in practice, which may have a profound impact on the performance and the service life of electrodes during operation. However, the mechanisms are largely unclear and still lack systematic understanding. Here we propose a coupled chemo-mechanical model based on peridynamics [1] and use it to study the dynamic fracture-pattern formation in electrode materials and solid electrolytes during lithiation/delithiation cycles. We found in hollow core-shell nanowires that geometric parameters such as the size of the nanowire and the thickness of the coating significantly influence the fracture patterns, leading to straight cracks, random crack networks and orthogonal cracks [2]. We also studied fracture-pattern differentiation in film-substrate structures [3], single crystalline electrodes [4], solid electrolyte/electrode interfaces, etc. We reveal the mechanisms by investigating the interplay between mechanical stress and lithium-ion insertion/extraction. The results provide insights into the phenomena of dynamic fracture in complex chemo-mechanical environments and the numerical tool is thus useful in guiding the future design of lithium-ion batteries.

KEYWORDS

Peridynamics; chemo-mechanical simulation; lithium-ion batteries; dynamic fracture

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