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Analytical Model on Stress-Regulated Lithiation Kinetics and Fracture of Si-C Yolk-Shell Anodes for Lithium-Ion Batteries

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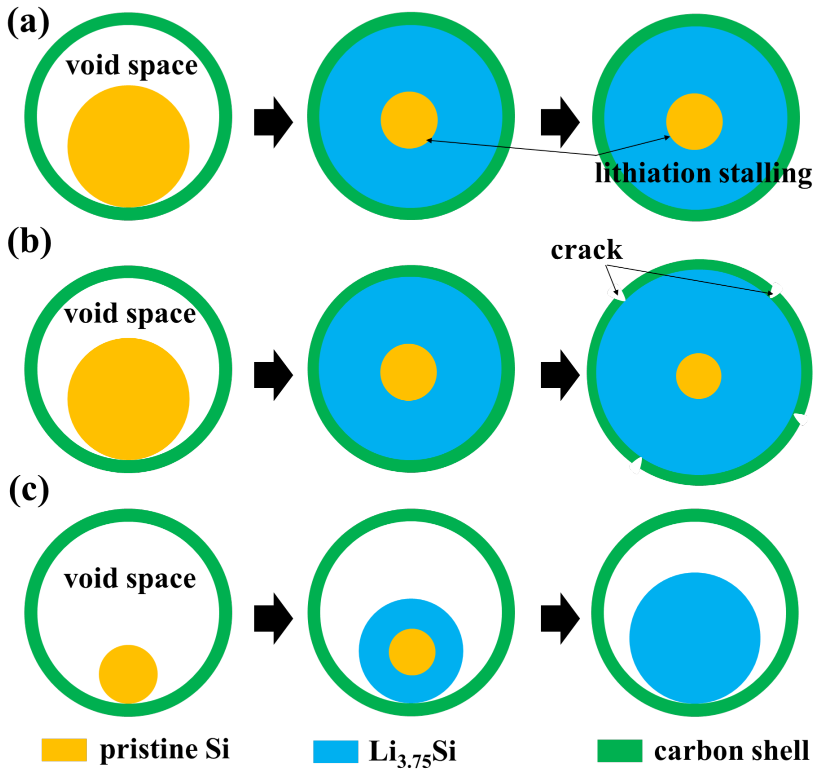

Caption: *(a) For a Si-C yolk-shell anode with insufficient void space, the expansion of Si particle first fully occupies the void space and then pushes the carbon shell to expand outwards. The contact between the carbon shell and the particle induces tensile hoop stresses in the carbon shell and compressive stresses in the particle. The compressive stresses in the particle may readily generate a large enough mechanical energy barrier to stall the lithiation reaction, ceasing propagation of the reaction front (interface between prinstine Si and $Li_{3.75}Si$). (b) For a Si-C yolk-shell anode with insufficient void space, after the lithiated Si particle fully occupies the void space, the tensile stresses generated in the carbon shell may rupture the carbon layer before the lithiation reaction stops. (c) For a Si-C yolk-shell anode with excessive void space, the particle expands inside the carbon layer without fully occupying the void space, so that the reaction stalling and rupture of carbon protective layer are avoided. However, excessive void spaces unacceptably increase the total volume of the battery pack, which is not be a good target design for Si-C yolk-shell anode.*

Scientific Achievement

We investigate how the void spaces in Si-C yolk-shell anodes impact the mechanical integrity and electrochemical behaviors of the anodes and seek for optimal void spaces. We calculate the stress fields resulting from lithiation reaction and mechanical contact between lithiated particle and outer carbon shell. Conditions to avoid catastrophic fracture of carbon shell in terms of the void space, the thickness of the shell, and the state of charge are also identified.

Significance

The research findings in this work capture experimental observations reported in the literature and shed light on optimal design of commercial Si-C yolk-shell anodes.

Citation

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