Modeling the phase transformations in tin-based anodes for sodium-ion batteries

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Abstract

Keywords: Sodium-ion batteries, Phase transformation, Cahn-Hilliard theory.
Sodium-ion batteries (NaBs) have risen as a viable alternative to lithium-ion batteries, driven by the widespread availability of sodium and their potential for sustainable, high-capacity energy storage. This work primarily concerns conversion type tin-based anodes for NaBs, which hold considerable potential. Tin forms binary alloys with sodium, thereby generating compounds with enhanced capacity. In contrast to carbon anodes, tin's alloying interaction with sodium induces phase transformations that can favor electrode degradation (1,2), mostly due to the expansion and subsequent fragmentation of electrode materials.

We aim at formulating a model that captures the mechanical and chemical properties of these phase transformations. To this end, we adopt a dual approach that combines viscoplasticity to account for mechanical stresses and strains, and the Cahn-Hilliard equation (3) to manage the chemical diffusion dynamics. The complexity of the coupled and uncoupled versions of the fourth-order Cahn-Hilliard equation necessitates the use of a split-method approach and a penalty term to simplify it into manageable second-order PDEs (4,5).

Numerically approximated phase diagrams and segregation metrics effectively demonstrate the dynamics of phase segregation over time, highlighting the model's alignment with experimental validations and its relevance to understanding the mechanisms of material behavior in sodium-ion batteries.

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