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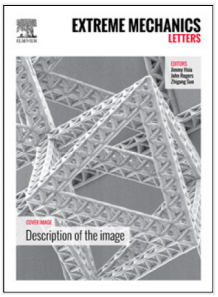

Phase transformations with stress generations in electrochemical reactions of electrodes: Multiscale-based mechanics for combined-phase reactions

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Phase transformations with stress generations in electrochemical reactions of electrodes: Multiscale-based mechanics for combined-phase reactions

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Phase transformations in most electrodes used for electrochemical energy storages follow the conserved dynamics of combined one- and two-phase reactions, which leads to complicated charge-discharge processes with various voltage plateaus; this could affect an electrochemical performance as a generic phenomenon in electrochemical system. In order to fully describe the combined-phase reactions from the atomic scale to the mesoscale, we propose a multiscale-based phase transformation model that also considers electrochemical states and mechanical deformations. This model predicts the miscibility gap, spinodal region, voltage profile, phase transformation, and stress generations of the combined-phase electrodes in the electrochemical reactions. We apply this multiscale model to high-rate cathode material Li_xFePO_4 to fundamentally understand the experimental phase transformation behaviors [Yamada et al., Nat. Mater. **5**, 357 (2006)]. This model is applicable to various electrodes for phase behaviors too complex to be detected experimentally due to combined-phase reactions.