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3D Simulation of diffusion induced stress in realistic $LiCoO_2$ electrode particles of lithium ion battery generated by nano-CT

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ABSTRACT

Diffusion induces stresses in the electrode during charge and discharge processes of lithium ion batteries, which can cause deformation and even fracture, further result in the fade of capacity and duration. The 3D model coupling diffusion and induced stress is applied to the reconstructed $LiCoO_2$ electrode particles determined by X-ray nano-computed tomography technology, of which the nonuniform electrochemical intercalation reaction takes place on the surface. A code is developed to simulate the fully coupled diffusion and induced stress in the $LiCoO_2$ electrode particles at different discharge rates. The simulations demonstrate the variable distribution such as concentration, reaction rate, hydrostatic stress, Von-Mises stress, and so on. The influence of the geometric characteristics of $LiCoO_2$ electrode particle and material properties on the variables is revealed. The investigation can help to improve lithium ion battery design and manufacture through understanding the relationship between electrode morphology and mechanical endurance.