Finite element study of Li diffusion and stress in $LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ cathode using microstructures reconstructed by synchrotron X-ray tomography

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$LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ is a good substitute for $LiCoO_2$ because of its good thermal stability and high energy density. In this study, the diffusion and stress in $LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ cathode with realistic three-dimensional (3D) microstructures have been studied systematically. Synchrotron X-ray tomography was used to obtain the 3D reconstructions of porous $LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ microstructures. Li concentration distributions under various C-rates were investigated. The obtained charge/discharge curves under various C-rates were compared with the results from Newman's model. The stress generation in the cathode was computed coupled with the diffusion. The hydrostatic stress, shear stress and von Mises stress in the particles were analyzed. The results show that the von Mises stress in particle boundaries is higher than the stress inside the particle due to the Li concentration gradient during discharge, which is consistent with the literature. Additionally, the von Mises stress near the particle contact region is much higher than other areas.