Geometric characteristics of 3D reconstructed anode electrodes of lithium ion batteries

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Abstract: The realistic 3D microstructure of lithium ion battery electrodes plays a key role in studying the effects of inhomogeneous microstructures on the performance of LIBs. However, the complexity of realistic microstructures implements significant computational cost on numerical simulation of large size samples. In this work, we used tomographic data obtained for a commercial lithium ion battery graphite electrode to evaluate the geometric characteristics of the reconstructed electrode microstructure. Based on the analysis of geometric properties, such as porosity, specific surface area, tortuosity, and pore size distribution, a representative volume element that retains the geometric characteristics of the electrode material was obtained for further numerical studies. In this work, X-ray micro-CT with 0.56 μm resolution was employed to capture the inhomogeneous porous microstructures of lithium ion battery anode electrodes. The Sigmoid transform function was employed to convert the initial raw tomographic images to binary images. Moreover, geometric characteristics of an anode electrode after 2400 1 C charge/discharge cycles were compared with those of a new anode electrode to investigate morphological change of the electrode. In general, the cycled electrode shows larger porosity, smaller tortuosity, and similar specific surface area compared to the new electrode.

Keywords: Lithium ion batteries; computed tomography; geometric characteristics; representative volume element