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IMAGE-BASED 3D RECONSTRUCTION AND MODELLING OF HETEROGENEOUS BATTERY ELECTRODE MICROSTRUCTURE

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ABSTRACT

There is a constant need for the improvement in the performance of lithium-ion batteries (LIB) regarding charge/discharge time, capacity, and safety issues to satisfy the increasing requirements. The practical performance of lithium-ion battery materials is heavily dependent on their 3D microstructural characteristics. Their heterogeneous microstructural characteristics induce heterogeneity in mechanical and electrochemical performances of the battery materials. Physics-based 3D microstructure model resolving the microstructural characteristics of all phases in a porous electrode is critical for a better understanding of the correlation between battery microstructure and performance. The primary motivation of the 3D microscale model is to explore the influence of active material particle shape and size (morphology), particle placement and their inter-connectivity on the degradation predicted during battery operation. With the rapid development of tomographic technologies, the X-ray CT technique is widely used for the reconstruction of the 3D morphology of LIB electrodes. It also provides a non-destructive platform to explore the microstructure with sub-micron resolution. In this work, we employed a machine-learning algorithm to segment the active particles from the tomographic data obtained for an inhomogeneous porous microstructure of the LIB cathode electrode. Geometric characterization analysis of the segmented tomography data gives information such as the particle size distribution, porosity, tortuosity, and the connectivity of the particle system. We propose a methodology for stochastic reconstruction of electrode microstructure which is statistically equivalent to the empirical microstructure in terms of geometric characteristics. In the development of stochastic 3D model, spherical harmonics allow accurate representation of the non-spherical particle morphology. The developed stochastic microstructure model is validated with the experimental tomographic data through model-based computer simulation. Herein, stochastic reconstruction enables generating virtual microstructure designs beyond the limit of empirical datasets.