3D Microstructure Reconstruction Based Numerical Investigation on the Energy Storage in Electric Double Layer of Super Lithium Ion Capacitor

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Super lithium ion capacitor (SLIC) is a hybrid energy storage system containing functionalities derived from lithium ion batteries and electric double-layer capacitors [1]. The energy storage in the electric double layer plays an important role and depends on the microstructure of the electrodes and the interfacial morphology at the electrolyte/electrodes interfaces [2]. However, it is hard to understand their influences on the energy storage performance of SLIC by using traditional testing methods.

In this respect, a numerical model based on the real structure of electrodes by 3D microstructure reconstruction technique [3] is developed in this study. At first, electrode samples from SLIC are scanned to obtain a series of two dimensional images by using x-ray micro/nano CT or dual-beam focused ion beam-scanning electron microscopy (FIB-SEM). Then, these images are used to reconstruct the 3D morphology of the SLIC electrodes by the commercial software MIMICS. The 3D reconstructed volumes obtained from MIMICS are converted into the computational domain in COMSOL. With following the porous electrode theory [4] and the electric double layer theory [5], a mathematical model of SLIC can be established, and thus the Model will be validated by a comparison of measurements and simulated results.

Using this 3D microstructure reconstruction based numerical model, some electrochemical properties, such as electronic conductivity, ionic conductivity, ion concentration distribution in electrodes, electric potential distribution, and the capacity, are in real time obtained. By analyzing these properties, the effects of microstructure and interface topography on the energy storage in the electric double layer of the super lithium ion capacitor can be investigated.

References

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