Stochastic 3D Microstructure Modeling and Structure-property Relationships for Polymer-based Electrodes

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Abstract

Polymer-based batteries represent a promising candidate for next-generation batteries due to their high power densities, decent cyclability and environmentally friendly synthesis. However, the performance of these batteries essentially depends on the complex multi-scale morphology of their electrodes. In this contribution, we present a comprehensive investigation of the complex relationship between the three-dimensional (3D) morphology of polymer-based battery electrodes and their effective transport properties [1]. In particular, focused ion beam scanning electron microscopy (FIB-SEM) is used to characterize the 3D morphology of three different polymer-based electrodes. The subsequent segmentation of 3D image data into active material, carbon-binder domain and pore space (see Figure 1 for 3D renderings) enables a comprehensive statistical analysis of the electrode structure. Moreover, spatially resolved numerical simulations allow for computing effective ionic and electronic transport properties. The obtained results are used for establishing quantitative structure-property relationships. Their robustness can be increased via stochastic 3D microstructure modeling, which is a powerful tool to overcome the limitations of tomgographic imaging by generating a large number of virtual but realistic structures just at the cost of computer simulations. In particular, excursion sets of Gaussian random fields are used to calibrate a stochastic model to 3D image data of three electrode samples [2]. The low number of interpretable model parameters can be varied systematically to generate electrodes structures that have not yet been manufactured.

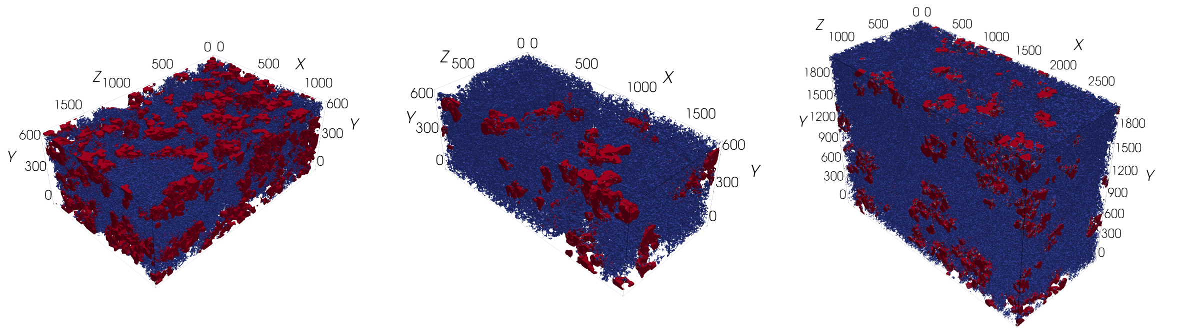

Figure 1: Visualization of the segmented 3D FIB-SEM image data. The active material is shown in red, the carbon-binder domain is shown in blue and the pore space is kept transparent.

References

1. B. Prifling, L. Fuchs, A. Yessim, M. Osenberg, M. Paulisch-Rinke, P. Zimmer, M. Hager, U.S. Schubert, I. Manke, T. Carraro and V. Schmidt. Correlating the 3D morphology of polymer-based battery electrodes with effective transport properties.*ACS Applied Materials & Interfaces* **16**, 66571-66583, 2024.

2. B. Prifling, L. Dodell, A. Yessim, M. Osenberg, A. Hilger, P. Zimmer, M. Hager, U. S. Schubert, I. Manke, T. Carraro, and V. Schmidt, Stochastic 3D nanostructure model for quantifying the impact of electrode morphology in polymer-based batteries on diffusive charge transport. Working paper (under preparation).