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Stochastic 3D microstructure modeling of differently compacted cathodes in lithium-ion batteries

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Lithium-ion batteries are one of the most promising technologies for storing electrical energy due to their preferable electrochemical properties. Thus, they are currently used in a large number of applications ranging from portable devices to electric vehicles. It is known that the electrode morphology strongly influences the overall battery performance. Therefore, a deeper understanding of the microstructure is an important task regarding the optimization of electro-chemical performance. Thus, the investigation of the manufacturing process and its impact on the microstructure is one main task in battery research. The 3D morphology of eight differently compacted cathodes has been obtained using synchrotron tomography. With the help of image processing techniques, as for example a marker-based watershed algorithm with extended regional minima, we obtain a phase-based as well as a particle-based segmentation, see Figure 1.

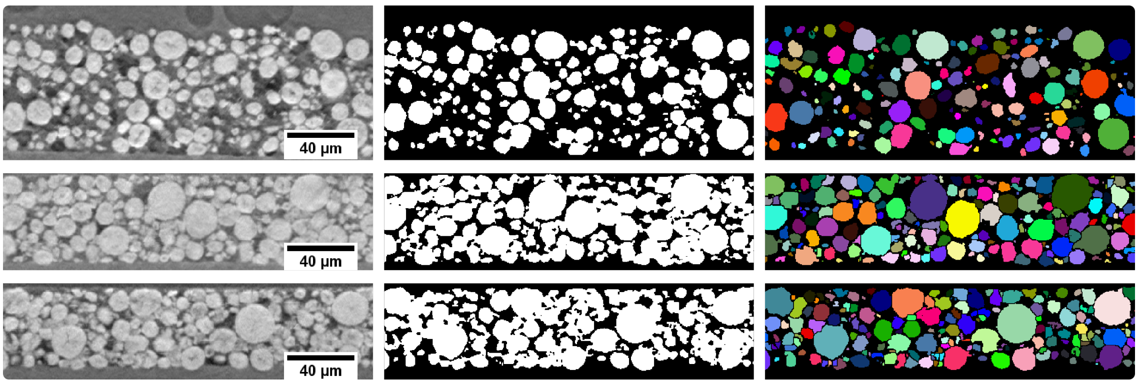

Figure 1: Through-plane cross sections of cathode microstructure for a compaction load of 0, 400 and 1000 MPa (from top to bottom). Left column: original 16-bit grayscale image. Middle column: Phase-based segmentation. Right column: Particle-based segmentation.

Thus, we are able to quantify the changes of the cathode morphology by means of numerous image characteristics. In addition, we are able to calibrate one and the same type of a parametric stochastic 3D microstructure model to all compaction loads. The goodness of fit is quantified by phase-based as well as particle-based image characteristics. A visual comparison between tomographic image data and a virtually generated cathode microstructure is shown in Figure 2. The utilization of a parametric model allows us to describe the complex 3D morphology of the cathode using only a few parameters. By least-squares regression analysis, we are finally able to predict the model parameters and hence the morphology of cathodes for arbitrary compaction loads. This can be used to provide a wide spectrum of virtual but realistic 3D microstructures as valuable input for numerical simulations of charge transport.

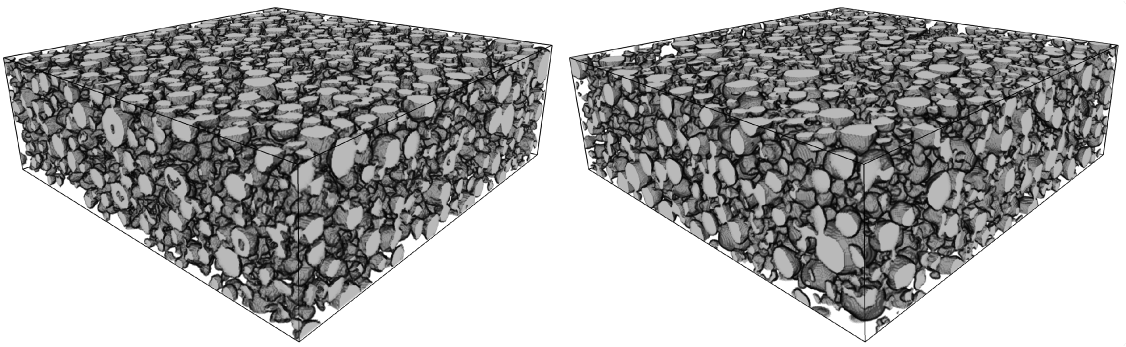

Figure 2: 3D rendering of tomographic image data (left) and virtually generated microstructure (right) for a compaction load of 0 MPa.