Random set models for hierarchically structured battery cathodes

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A stochastic 3D modeling approach for the morphology of hierarchically structured battery cathodes is presented. In the first part of the talk, we present a parametric random set model for the 3D morphology of nanostructured active material particles based on excursion sets of χ^2-fields. Parameter estimation is performed based on analytical formulas relating the covariance function of the random field to the so-called two-point coverage probability functions, which can be estimated from 3D image data. In the second part, we consider the nanoporous binder-conductive additive phase surrounding the active materials particles in the cathode. The morphology of the latter consisting of carbon black, polyvinylidene difluoride binder, and graphite particles is also modeled by means of parametric random closed sets. For this part of the cathode, we propose a three-step approach. To begin with, the graphite particles are described by a Boolean model with ellipsoidal grains. Then, the mixture of carbon black and binder is modeled by an excursion set of a Gaussian random field in the complement of the graphite particles. Finally, large pore regions within the mixture of carbon black and binder are described by a Boolean model with spherical grains. A method for parameter estimation based on 3D image data is presented. Both random set models are validated by comparing 3D image data and model realizations in terms of morphological descriptors that are not used for model fitting. The developed stochastic 3D models are used for so-called virtual materials testing. Virtual, yet realistic structures are generated on the computer. In doing so, a large database of nanostructures is created which allows us—in combination with numerical simulation of physical properties—to efficiently study quantitative relationships between the manufacturing process, the morphology, and effective macroscopic properties of the considered battery cathodes. This talk is based on joint work with Phillip Gräfensteiner and Volker Schmidt.