Stochastic 3D microstructure modeling of one- and two-layer battery electrodes: a tool to investigate microstructure-property relationships

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Low rate performances and insufficient energy densities of batteries are a limiting factor for electromobility. This gives rise to the development of specific structuring concepts for electrode materials such as, e.g., blend electrodes with different active material particles, which lead to an increase in the volumetric energy density. In this contribution, we show how data-driven stochastic 3D microstructure modeling based on methods from spatial statistics and stochastic geometry supports the experimental optimization of structuring concepts. In particular, we generalize existing germ-grain models for electrode materials, which consist of active material particles, binder-additive material and pores. The shape of grains, representing the active material particles, is modeled by means of Gaussian random fields on the sphere. The binder-additive phase is modeled conditioned on the active material using morphological closing. This allows us to to generate digital twins of two-layer electrodes with differently sized active material particles in the two layers as well as digital twins of blend electrodes with an arbitrary mixing ratio of the contained types of active material particles. The parameters of the generalized stochastic 3D microstructure model are calibrated to 3D image data obtained by synchrotron tomography. This data-driven modeling approach enables us to statistically reproduce electrodes manufactured with different structuring concepts. By variation of model parameters, a large range of virtual, but realistic electrode microstructures can be generated which have not been manufactured so far. The virtual microstructures are used as an input for locally resolved electrochemical simulations in order to determine the behavior of lithiation as well as the energy density of the virtual electrode structures. The presented modeling and simulation workflow opens the possibility to provide structuring recommendations for optimized structuring concepts used for electrode design.

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