Fakultät für Mathematik und Wirtschaftswissenschaften

universität ulm

Mathematisches Kolloquium

Data-driven stochastic 3D nanostructure modeling for virtual materials testing of battery

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Based on 3D image data, a parametric stochastic model is developed for the simulation of differently manufactured nanoporous particles, which *are used as active material in battery electrodes. Functional properties of these particles, like effective diffusivity, depend on the 3D morphology of the nanopores, which, in turn, are influenced by the underlying production parameters. In order to study relationships between the pore morphology and effective properties influencing the performance of the electrode, data-driven stochastic 3D modeling is a powerful tool. It enables for the generation of a large range of virtual, but realistic nanostructures on the computer, which vercomes limitations of time-consuming 3D imaging. For the virtual structures, morphological descriptors as well as effective properties can be determined, in order to statistically quantify relationships between them. We call this virtual materials testing. The stochastic 3D nanostructure model is based on tools from stochastic geometry. The solid phase of aggregate particles is modeled by an excursion set of a certain class of chi-square random fields. Model fitting is performed using analytical relationships between the covariance function of the chi-square field and two-point coverage probabilities, where the latter can be directly estimated from 3D image data. After having fitted the model parameters to image data, model validation is performed by comparing morphological descriptors (not used for model fitting) of simulated and experimental image data.*

Der Vortrag ist für ein breites Publikum geeignet