Artificial generation of representative single Li-ion electrode particle architectures from microscopy data

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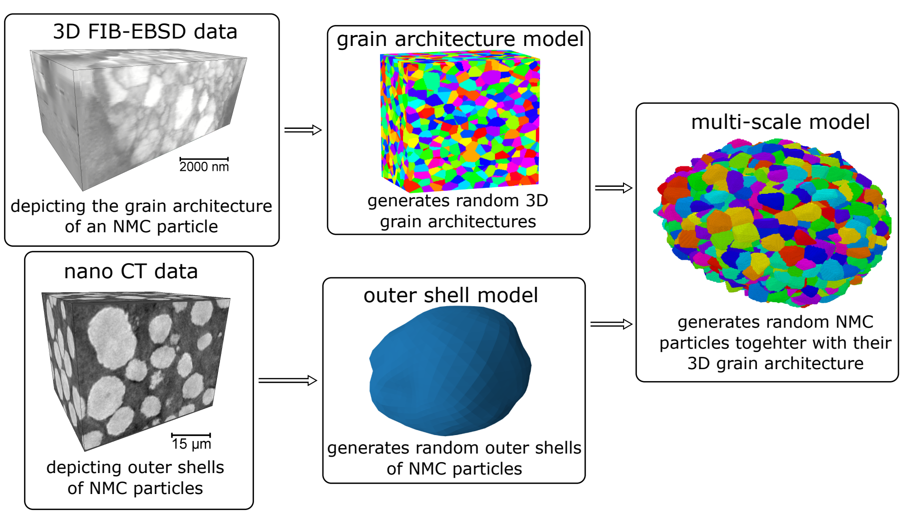
Accurately capturing both the shape and intergranular architecture of single lithium-ion electrode particles in 3D is essential for quantifying their influence on material properties, like, e.g., degradation mechanisms. Microscopy techniques like X-ray nano-computed tomography (CT) and focused ion beam (FIB) - electron backscatter diffraction (EBSD) can provide representative 3D image data of the particles shape (outer shells) and their grain architecture, respectively. However, it can be quite time-consuming and costly to rely solely on imaging techniques for generating a sufficient amount of data for the analysis of structure-property relationships. In this talk, we present an alternative approach using stochastic geometry models. More precisely, using parametric stochastic geometry modeling, we leverage data from both nano-CT and FIB-EBSD to generate artificial but representative single particle architectures completed with grain morphological details. Therefore, a random Laguerre tessellation model is fitted to the grains depicted in FIB-EBSD data from which we can generate virtual, but statistically representative grain architectures. Analogously, we utilize nano-CT data depicting the outer shells of numerous particles to derive a random outer shell model, using mixtures of Gaussian random fields on the sphere. By combining both models, we can generate a large number of virtual particles with statistically representative shapes and grain morphologies. Moreover, by systematic variation of model parameters, even further virtual particles covering a broad range of structural scenarios can be generated. Then, such virtual particles can be used as input for numerical simulations, i.e., for virtual materials testing to study the influence of a materials geometry on its physical properties in the search for improved particle architectures of high energy- or power-density cells.



Modeling approach: FIB-EBSD data is used to calibrate a grain architecture model (top). From nano-CT data an outer shell model is fitted (bottom). By combining both models, we can generate representative particle architectures (right).