Methods from machine learning and spatial stochastic modeling for the characterization of complex microstructures

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Microscopy techniques like scanning electron microscopy (SEM) or X-ray computed tomography (CT) can provide detailed image data of electrode particle microstructures in lithium-ion batteries. Followed by a quantitative structural characterization such data allows for the investigation of structure-function relationships, i.e., the influence of an electrode particle's microstructure on its properties like its mechanical or electrochemical behavior. However, for the structural characterization by means of image data nontrivial processing tasks are often necessary. In this talk, several applications of methods of spatial stochastic modeling and machine learning are presented for the characterization of the inner (polycrystalline) grain architecture and outer shell of individual active particles in cathodes of lithium-ion batteries imaged by SEM, CT and 3D FIB-EBSD tomography. In particular, it is shown how convolutional neural networks can be used to achieve a grain-wise segmentation of FIB-EBSD data of NMC particles [1]. In the next step, the segmented image data serves as a basis for structural multi-scale modeling of cathode particles to overcome limitations of different imaging techniques, see Figure 1. Therefore, a stochastic geometry model, namely a mixture of Gaussian random fields on the unit sphere, is calibrated using CT data depicting the outer shell of cathode particles. The grain architecture is modeled by a random Laguerre tessellation which has been calibrated to FIB-EBSD data [2]. The model can be exploited to perform structural scenario analyses, i.e., to generate arbitrarily many digital twins with statistically similar shape and grain architecture as the particles observed in the image data. These digital twins are then used as input for numerical charge simulations to investigate their degradation behavior [3]. Moreover, a generative adversarial network (GAN) is deployed to perform super-resolution on SEM-images of cycled cathode particles such that fine features like cracks within particles can be more reliably characterized to quantify the state of degradation [4].

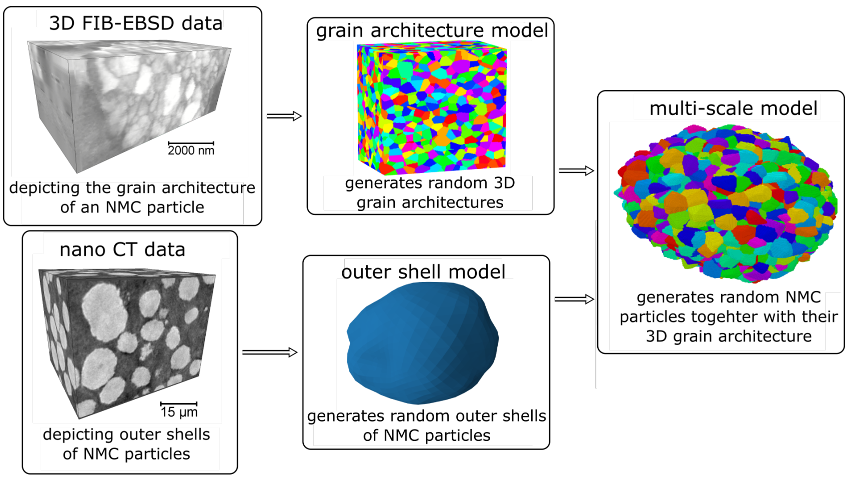

Figure 1: Workflow for stochastic modeling of polycrystalline particles, using random tessellations and random fields on the unit sphere.

References

[1] O. Furat et al., 2021.*Journal of Power Sources*, 483:229148.

[2] O. Furat et al., 2021 *npj Computational Materials*, 7:105.

[3] J. Allen et al., 2021. *Journal of Power Sources*, 512:230415.

[4] O. Furat et al., 2022. *Journal of The Electrochemical Society*, 169:100541.