Reconstructing polycrystalline 3D grain architectures from 2D image data by combining stochastic 3D modeling and generative AI

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Abstract

This talk introduces a computational method for statistically reconstructing 3D grain architectures of (functional) materials from 2D image data using spatial stochastic modeling. We combine methods from generative adversarial networks (GANs) (1) with advanced stochastic geometry models, specifically random tessellation models (2). In particular, we use a generalization of Laguerre tessellations, namely, generalized balanced power diagrams (GBPDs) (3). The application of GBPDs in stochastic 3D models allows for a relatively low-parametric representation of 3D grain architectures, including those with curved grain boundaries. To achieve statistical reconstruction of 3D grain architectures from 2D image data, the parameters of the stochastic 3D models must be calibrated such that planar sections of the generated 3D grain architectures exhibit similar statistical properties to those observed in the 2D image data. The proposed calibration method uses convolutional neural networks, which act as so-called discriminators to differentiate between artificially generated and experimentally measured 2D image data. By tuning the parameters of the stochastic 3D model to make the generated planar sections indistinguishable by discriminators from the experimental ones, we obtain a statistically accurate reconstruction of the 3D grain architecture (3). In this talk, we apply the proposed method to reconstruct the 3D grain architecture of cathode particles in Li-ion batteries using 2D electron backscatter diffraction data. Furthermore, we combine the grain architecture model with a stochastic 3D model for the outer shell of non-spherical cathode particles. The latter model component, representing the outer particle shell, is calibrated using image data at a different length scale. Once calibrated, the stochastic 3D models can overcome the limitations of 2D imaging techniques by generating 3D morphologies that can be used as geometric input for spatially resolved numerical simulations of effective material properties (4). Additionally, by varying the model parameters, we can systematically explore different structural scenarios, creating a comprehensive database for establishing quantitative structure-property relationships (5). As a result, the presented method enables the generation of a wide range of virtual 3D morphologies, facilitating the identification of structures with optimized functional properties.

References

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