# Investigating the aging behavior of SOFC anodes and predicting their 3D microsrtucture from 2D SEM-images using stochastic 3D modeling and CNNs

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The 3D microstructure of solid oxide fuel cell (SOFC) anodes plays a crucial role in determining their electrochemical performance and long-term stability.
In the first part of the presentation, we focus on the microstructural degradation of SOFC anodes during long-term operation. Understanding and predicting these complex aging processes typically requires repeated 3D imaging via focused ion beam scanning electron microscopy (FIB-SEM) at different degradation stages, which is experimentally demanding. To overcome this limitation, we combine physics-based phase-field simulations with data-driven stochastic 3D microstructure modeling. More precisely, an excursion set model based on $\chi^2$- and Gaussian random fields with a set of six interpretable parameters is used [1]. The temporal evolution of these parameters is modeled analytically, enabling predictive simulations of microstructural aging. Validation using physics-based aging confirms the quality of the model through quantitative comparison of geometric descriptors.
In the second part, we would like to bypass the necessity of 3D imaging. Imaging using 2D scanning electron microscopy (SEM) is much more accessible, but the information required for quantitative 3D characterization is typically lacking. This motivates our approach for predicting the 3D microstructure of SOFC anodes based on 2D SEM images via a convolutional neural network (CNN) [2]. The main idea for generating training data is to use the above parametric stochastic 3D microstructure model. By doing so, a large number of 3D microstructures can be generated by systematic variation of the model parameters just at the cost of computer simulations. Next, virtual but realistic 2D scanning electron microscopy images are generated via the physics-based simulation tool Nebula [3], using the simulated 3D geometries as structural input. Thus, the convolutional neural network can be trained on pairs of 2D SEM images and the corresponding parameters of the 3D microstructure model, where the latter enable a low-parametric, interpretable representation of complex 3D structures. The prediction accuracy of the CNN is evaluated with regard to the model parameters as well as with regard to various geometrical descriptors of the 3D microstructure.

## References

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[3] L. van Kessel, C. Hagen, Nebula: Monte Carlo simulator of electron–matter interaction, SoftwareX 12 (2020) 100605.