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Electrode Design Booster Using a Statistical Digital Twin

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Highly performing Li-ion batteries are needed as part of reliable energy storage systems to successfully master the transition to renewable energies. To meet this challenge, batteries must be fast-charging, long-lasting, sustainable, and cost-effective to manufacture, while also offering high storage capacity. One essential piece of this highly challenging puzzle resides in improving the microstructure of the electrodes, i.e., on a length scale of a few nanometers to a few hundred micrometers.

The use of direct experimental approaches is difficult at this scale - even sometimes impossible –and also expensive and time-consuming. Alternatively, running simulations to specifically improve batteries at these scales is extremely useful. Simulations provide data to be used as reference for the microstructure of the electrode and help to determine the critical parameters for performance improvement. Our work is carried out on a complete commercial software environment called GeoDict, which is suitable to perform all necessary steps.

A starting point to improve the microstructure is to reliably reproduce the original material with a model. We call this model a statistical digital twin when the performance parameters match those of the original material, and at the same time the geometric properties on the micro-scale match those of the original material in a statistical sense.

This talk will show how to create a digital twin of an electrode material. Starting from a microCT scan, all steps up to the validation of the resulting properties will be explained.

All starts with an image stack of an anode material and performing image processing to improve image quality. Then, the material phases are segmented and the 3D structure is reconstructed. Subsequently, the statistical properties of this imported 3D structure are calculated, such as open and closed porosity, tortuosity, or diffusivity. Using this data and starting from grains with a certain shape and size distribution, the volume fraction of these grains is determined and their shape is adjusted to create an statistical digital twin of the original 3D structure. Finally, the binder-carbon black (CBD) is added at a certain contact angle to the structure.

The resulting statistical digital twin is validated by comparing its porosity, tortuosity, and diffusivity to the same parameters of the originally imported 3D structure. To finely adjust the result, an automatic structure generation iteration may be scripted using GeoPy, the Python interface in GeoDict.

As application example, we show a case study that displays how batteries may be improved by 3D microstructuring approaches. We simulate the structuring of a graphite anode with a laser and describe how these changes affect crucial parameters of the material, such as tortuosity and diffusivity. This work was performed during the structur.e project of the BMWK [1]. In this project, laser perforated electrodes are manufactured and studied experimentally and via simulations to elaborate design principles for fast-charging anodes. Additionally, this project tested alternative design options, like laser ablation of the CBD-phase and using a graded grain size distribution in the electrode.

Participation

In-Person

References

[1] https://math2market.com/math2market/publicly-funded-projects/structur-e.html

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