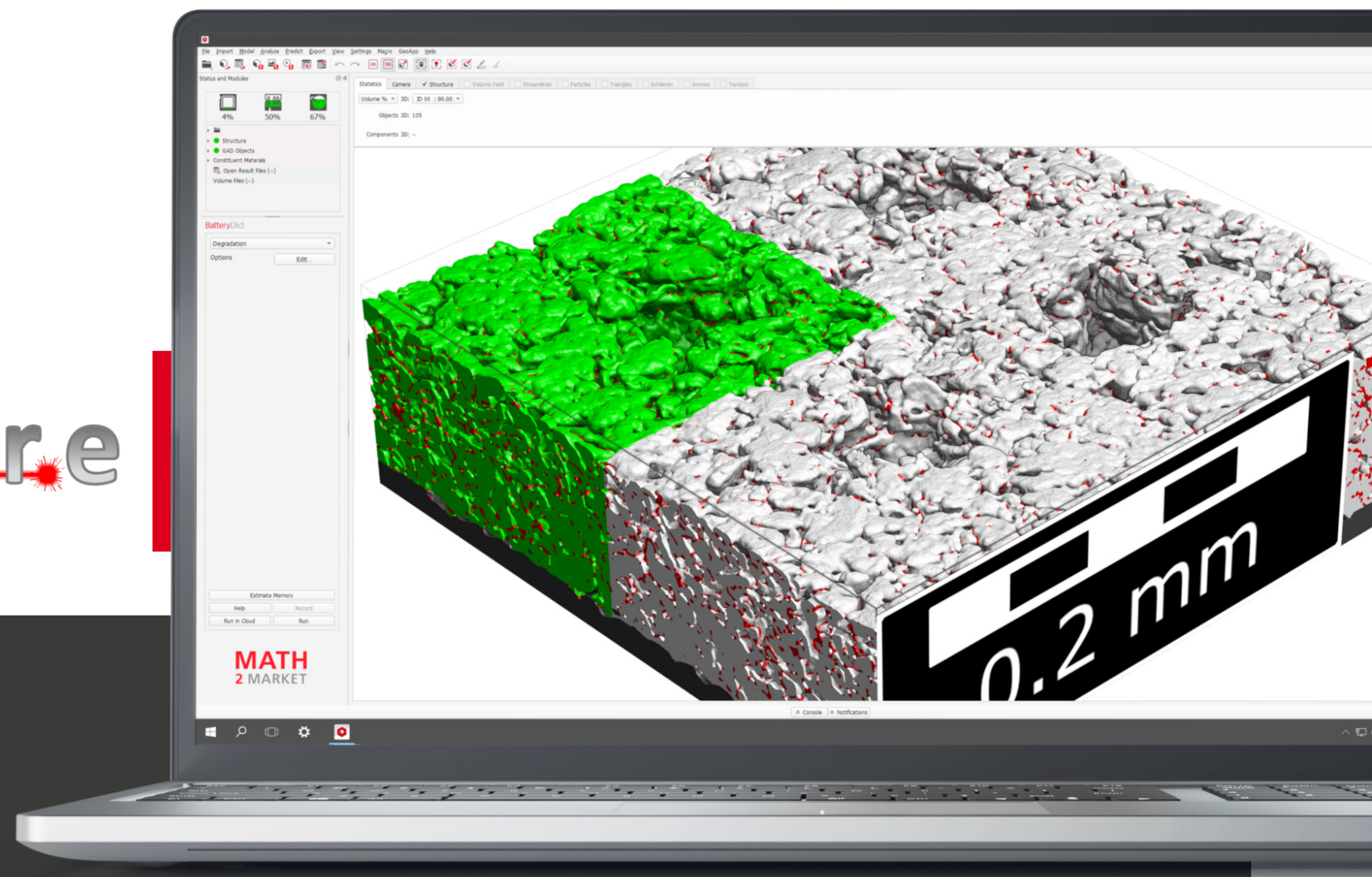
GeoDict

The Digital Material Laboratory

Electrode design booster using a statistical digital twin

structur.e



The microstructure of electrodes is key for better batteries. We understood and improved electrode materials in the structur.e project [1] by creating validated statistical digital twins of graphite anodes and running charging / de-charging simulations. The work leads to achieving fast-charging, long-lasting, sustainable, and cost-effective batteries. All Steps were done with the commercial software GeoDict.

We used digital laser pinching to modify the digital twin of an anode structure and accurately predicted changes in key parameters. Our project partner then fabricated a laser-pinched electrode to confirm our predictions.

This showcase presents innovative approaches that can help drive the development of fast-charging batteries.

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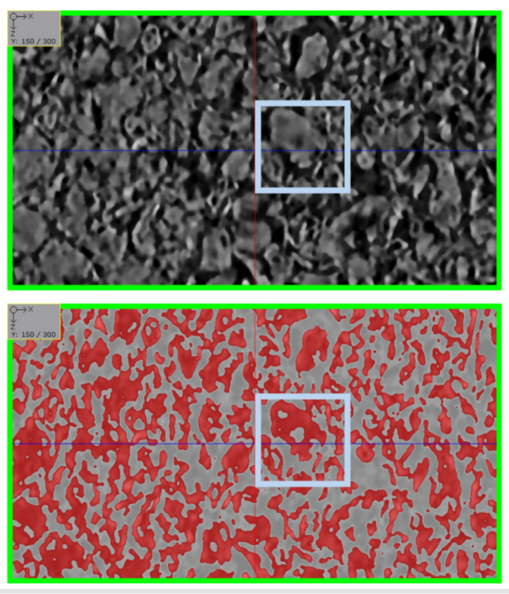


Import µCT Scan

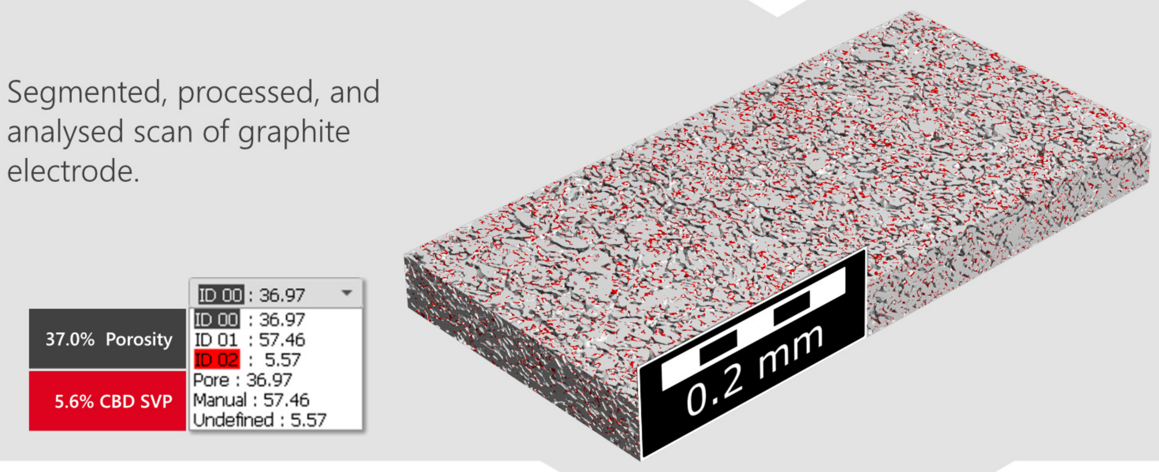
Our cutting-edge technology can transform 3D image data obtained by nanoCT into digital models with ease. We utilize AI routines provided by GeoDict to segment the grey value data and extract the solid part from the pore space.

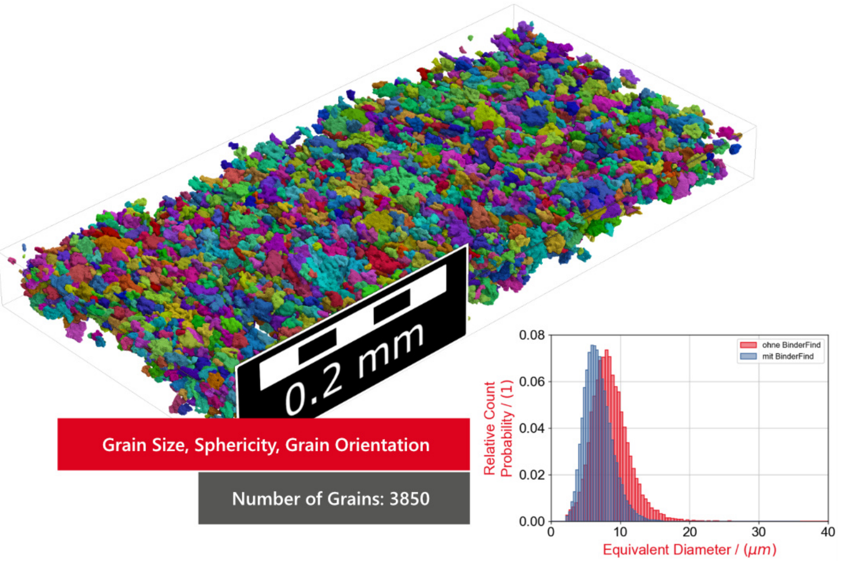
Our advanced GrainFind AI module is specifically designed for graphite electrode structures, allowing us to segment the binder from the graphite grains with precision.

Processing | Segmenting | Analysing

ImportGeo-Vol

Segmented, processed, and analysed scan of graphite electrode.

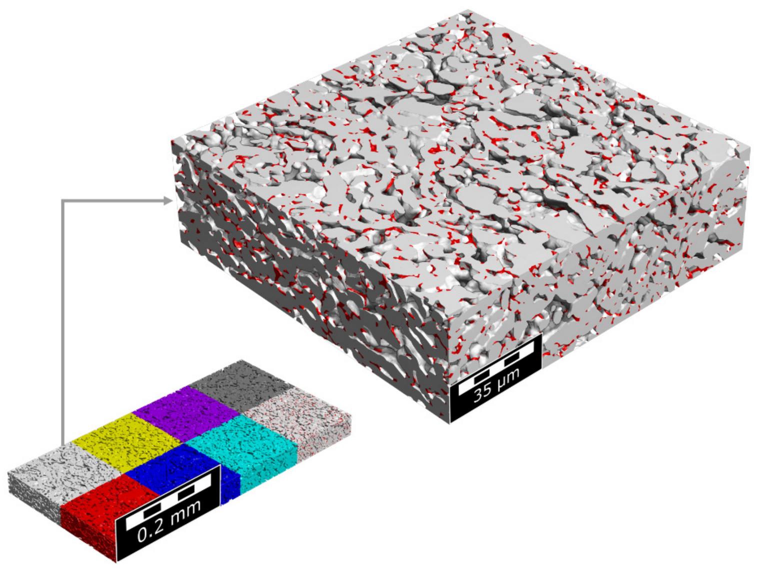




Create Statistical Digital Twin

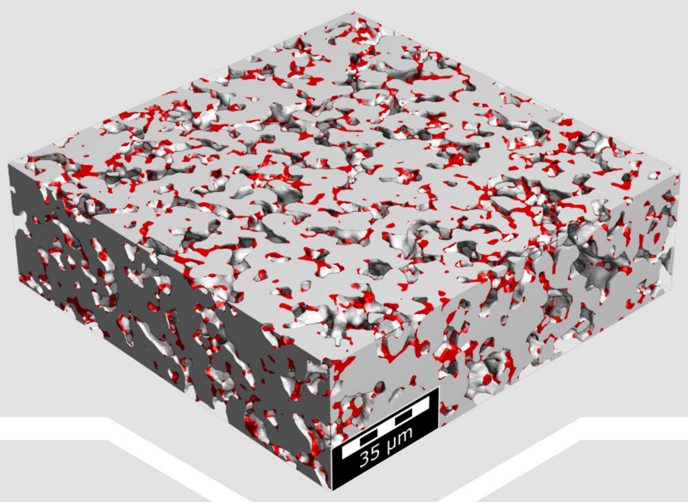
Analyzing digital models of electrodes is easy with our advanced techniques. We use a water-shed algorithm to identify graphite grains, measure their size and orientation, and determine volume fractions of different phases.

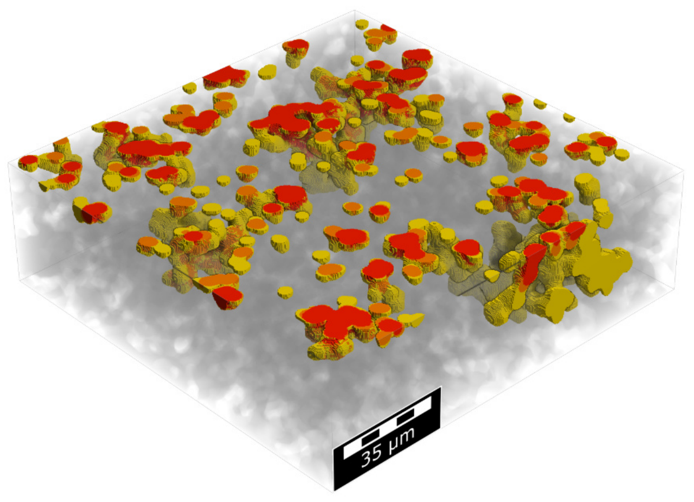
Our GrainGeo structure generation modules create a synthetic statistical digital twin of the anode, which can be enhanced with binder data for a more comprehensive analysis.



Statistical Digital Twin

Synthetically created digital twin of graphite anode.





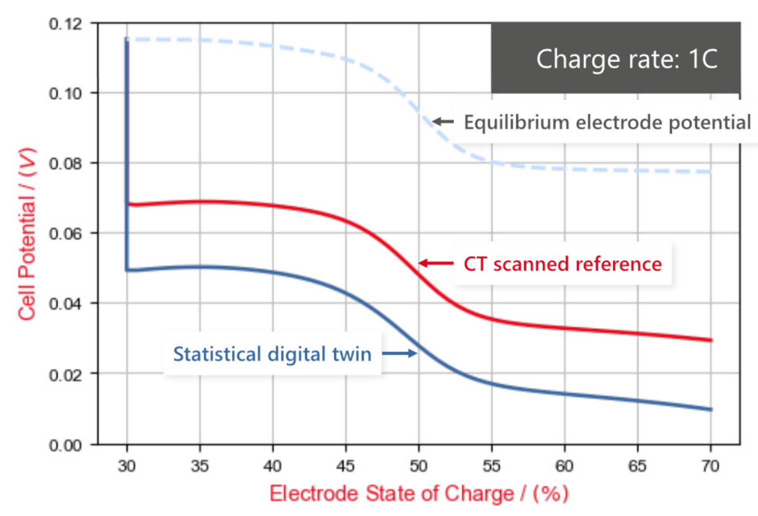
Recognized pores in SDT larger than D50

Validating Digital Twin

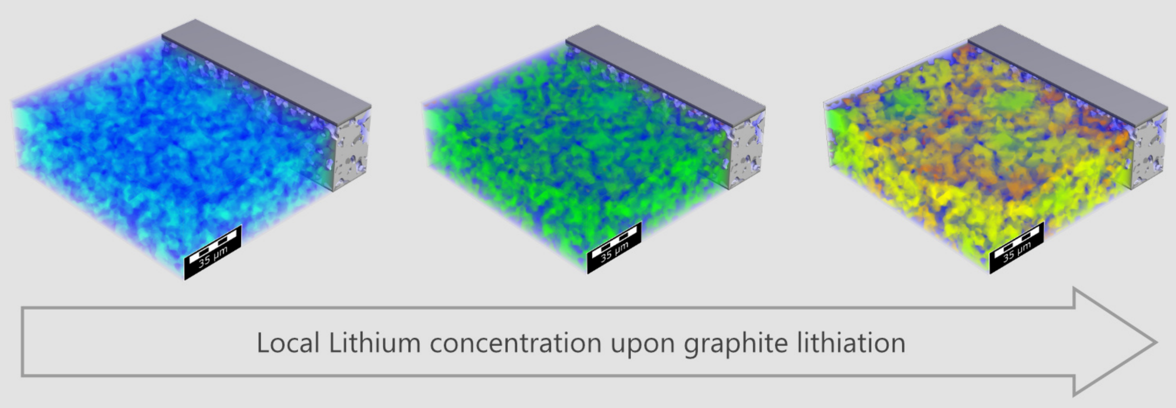
We compared properties of the statistical digital twin with the scanned electrode, focusing on porosity, tortuosity, and diffusivity. Deviations were below 6%.

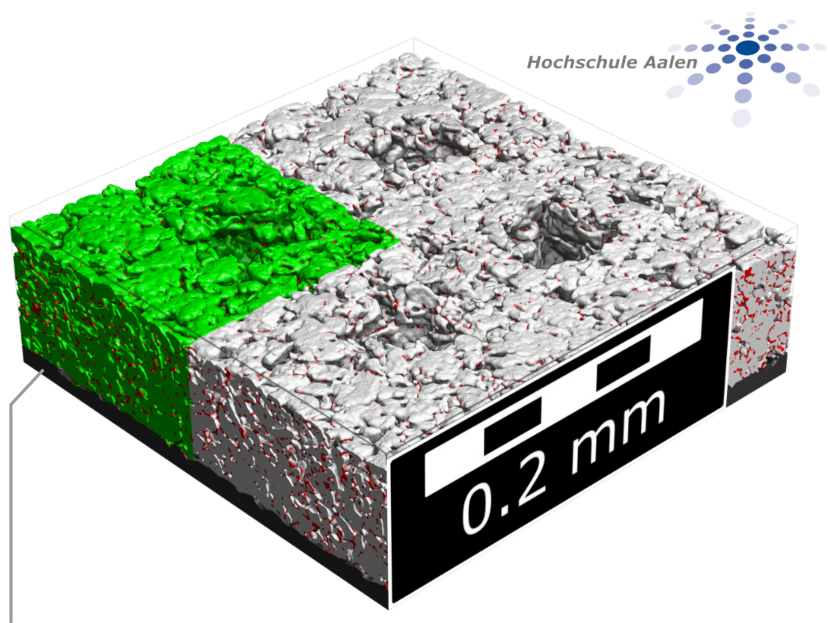
The surface loading determined from the CT scan was 1.83 mAh/cm², while the digital twin yielded a slightly higher value of 1.85 mAh/cm², resulting in a deviation of less than 0.5%.

With our validated digital twin, it is easy to create structures with modified parameters and check their influence on cell performance.



Physical Simulation





CT scan of experimentally fabricated laser pinched graphite electrode.

Material Design: Modify Digital Twin by Laser Pinch

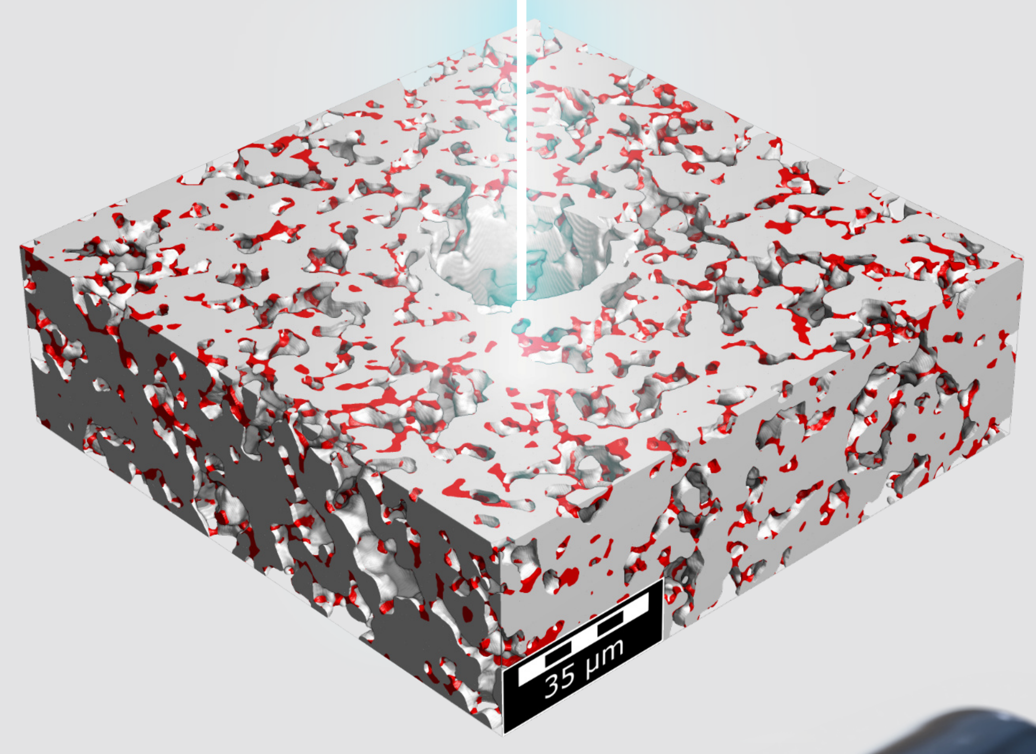
Our Python script makes it easy to modify the digital twin of the graphite anode by simulating a laser pinch process. This process creates a structured electrode that can improve transport properties at high charge rates, as evidenced by a 9% decrease in diffusion tortuosity.

Our simulations also revealed an increase in effective diffusivity, indicating a significant performance boost.

	Statistical digital twin	Statistical digital twin laser pinched	Change
Porosity	36.1%	38.4%	+6%
Geodesic Tortuosity	1.12	1.10	-2%
Diffusion Tortuosity	1.89	1.72	-9%

Laser Pinched Digital Twin

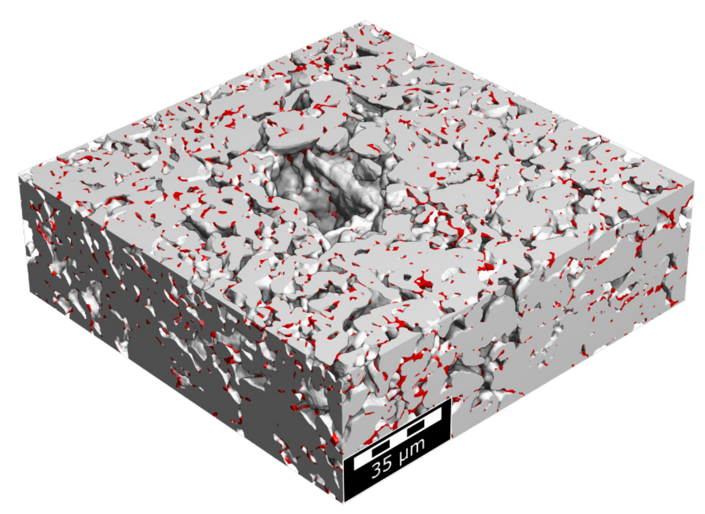
Laser Pinching of digital structure by Python script.



Validation by Comparison with Experiment

We validated the predicted changes in transport properties resulting from digital material design by comparing our results with CT-scans of a laser pinched electrode fabricated by our partners at Aalen University of Applied Sciences.

The tortuosities in the scans differed by less than 1% from the digital twin, confirming the accuracy of our simulations. However, the porosity differed by 18%, likely due to the simplified simulation of the laser pinching process, which only created a simple hole in the structure.



Segment of scan with same size as digital twin.

The materials of the future are within reach, and GeoDict helps you develop them faster. This is innovation through simulation.

Our digital material design approach allows for efficient and cost-effective development of high-rate compatible anodes.

By creating a digital twin of a graphite anode and performing physical simulations, we achieved similar effective properties as the scanned electrode.

We further improved transport properties by simulating the structuring of the electrode through laser pinching, resulting in a significant increase in effective diffusivity.

These results were confirmed through experimental fabrication of electrodes.

Our approach saves time and resources by efficiently utilizing experimental capabilities, making it a promising solution for developing high-rate compatible anodes.

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

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