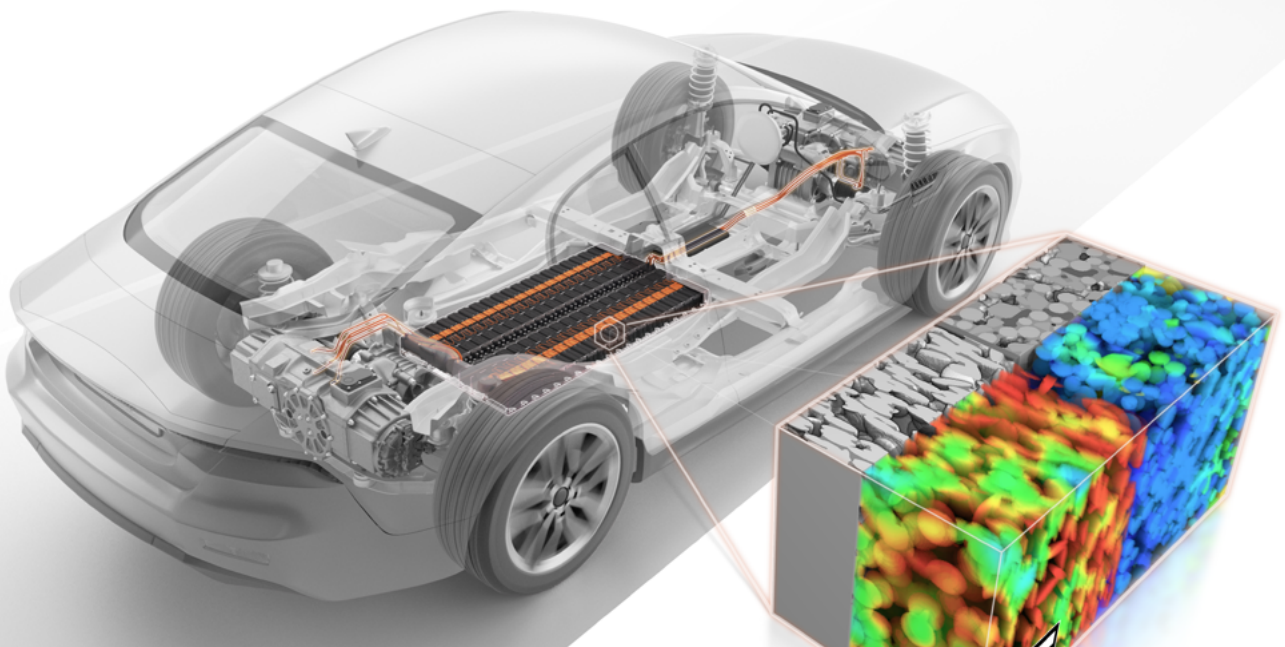


FAST CHARGING BATTERIES: MATERIALS DESIGN FOR THE MOBILITY OF TOMORROW

GeoDict® - Innovation through Simulation



Fulfilling the vast potential of electromobility and earning mainstream acceptance hinges on mastering the challenge of pairing fast charging batteries with high energy density. This task should not rely entirely on finding novel electrode material constituents with these conflicting and extreme technical pre-requisites, but must aim at solving this dilemma through the microstructural optimization of current electrode materials.

Ionic transport processes play a critical role on the microscale during charging and are mainly governed by the microstructure and texture of the electrode materials.

An experimental optimization by trial-and-error is time consuming, costly, and excludes the possibility of assessing the impact of single parameters on the complex battery system.

Addressing this challenge, the advanced simulation software GeoDict® has been built for import and segmentation of CT scans of electrode materials or virtual generation of realistic 3D-microstructures with a representative volume (REV). This easy-to-use software is applied to improve the microstructure of electrode materials and drive genuine innovation in battery research.



Experimental Approach



Simulation and Digital Design with **GEODICT®**

The Challenge

- High-energy anodes for fast charging
- Optimization of anode kinetics
- Targeting of microstructure and texture

Lithium-ion batteries are still limited regarding energy density, fast charging and costs. High-performance electrode materials are needed to overcome the current limitations of electromobility. Currently, the unification of fast charging and high energy density is consistently pursued.



If high-energy anodic materials are charged, the transport pathways for the Li-ions are often restricted. This leads to irreversible accumulations of reactive metallic lithium that result in reduced cell capacity, high inner resistances, shortcuts and, finally, safety issues.

Due to a lack of systematic approaches, the key parameters determining anode kinetics are particle size, shape, and distribution, together with tortuosity and porosity. Their experimental optimization is currently attempted by time consuming and costly trial-and-error due to a lack of systematic approaches in R&D.

With this experimental method, the impact of one single parameter on a complex battery system is often elusive.

Solutions through Simulation

GeoDict® substitutes and complements this experimental approach by providing powerful software tools to simulate battery cycling as well as geometric and transport properties on realistic microstructures and to optimize the performance of the anodic material. Math2Market GmbH offers GeoDict® as the optimal simulation solution and is ready to help in developing electrode materials enhanced for fast charging.

- GeoDict® modules for this solution are: ImportGeo, GrainFind, DiffuDict, PoroDict, GrainGeo, FiberGeo, and BatteryDict
- GeoDict® runs detailed 3D simulations of complex battery systems, starting from the microstructure of the electrodes up to charging of the virtual battery.
- GeoDict® simulations reveal the impact of single parameters on the battery performance

Rounded off with individualized training and support, the modular GeoDict® software is perfectly designed to adapt to any R&D workflow:

1. Importing and analyzing of 3D-scans of electrode materials with ImportGeo and GrainFind. Identifying active material, binder and carbon black, as well as electrolyte on the microscale and assigning their physical properties (e.g. ionic conductivity) manually or by using the editable Material Database.
2. Computing of specific active surface, ion diffusivity and tortuosity with DiffuDict and PoroDict to e.g. identify bottlenecks for the lithium intercalation, which lead to Li plating.

3. Simulating with BatteryDict the fast charging of a virtual battery consisting of electrodes with:

- Calculation of cell voltage, local ion concentration and potential distribution, ionic and electric currents, overpotentials, heat sources, etc.
- Detection of Li plating by monitoring the overpotential at the interface between active material and electrolyte.

4. Generating statistical variations in the material, with the GrainGeo and FiberGeo modules, while preserving the microscopic (e.g. particle size distribution) and macroscopic (e.g. tortuosity, porosity) properties of the anodic material. Generating a Digital Twin of the real electrode material, that exhibits identical properties and performance until the desired properties are matched.

5. Solving the optimization challenge by generating a matrix of 50.000+ instances of the electrode material with GeoDict® and varying a single parameter at a time. The most promising solutions are identified regarding conductivity, diffusivity, tortuosity, and charging behavior through fast BatteryDict 3D charging simulations.

- Reduce Li plating during charging to a minimum: e.g. by changing the particle size distribution, binder content, etc., until the fast charging simulation converges to an ideal behavior.

6. Finding the superior digital prototypes and formulation of new practical design guidelines to boost innovation in battery technology.

Integrating Simulations in R&D

How can GeoDict® be integrated into an established R&D workflow?

Math2Market joins in your efforts and helps in applying GeoDict® to tackle specific issues. In a tailored evaluation project, we train you in using GeoDict® optimally for modelling of microstructures, simulation and prediction of properties, as well as visualization and interpretation of simulation results.

GeoDict® supports a variety of import and export file formats (e.g. MATLAB®, Microsoft Excel®), and can mesh and export the generated structures. In this way, GeoDict® can be seamlessly integrated into an existing workflow with other software tools. Besides, GeoDict® can be controlled and run through user-created python macros and scripts.

After the training, the professional support of Math2Market focuses on keeping the user in the road to success. Yearly software updates guarantee that GeoDict® remains at the forefront of scientific developments in material microstructure design.

Results

The effective ionic diffusivity in the electrolyte is a key parameter to optimize electrode materials for fast charging. It depends critically on the tortuosity τ , which is a measure of the curvature of the ion transport pathways due to the microstructure of the electrode. A lower tortuosity leads to higher diffusion of the Li-ions.

$$D_{eff} = \frac{\varepsilon}{\tau} D_{el}$$

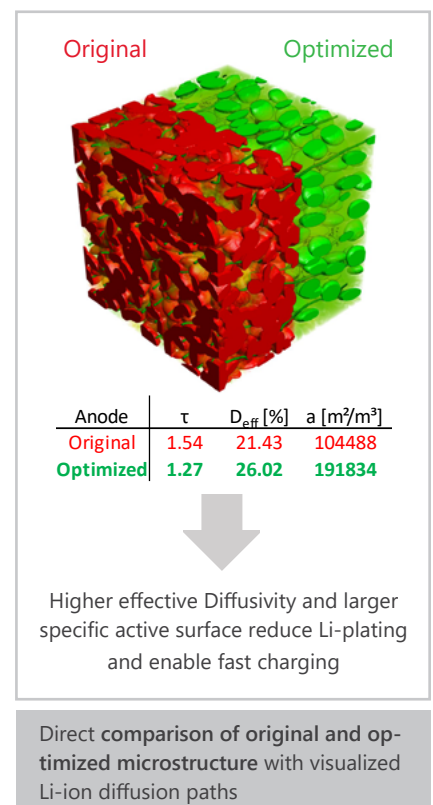
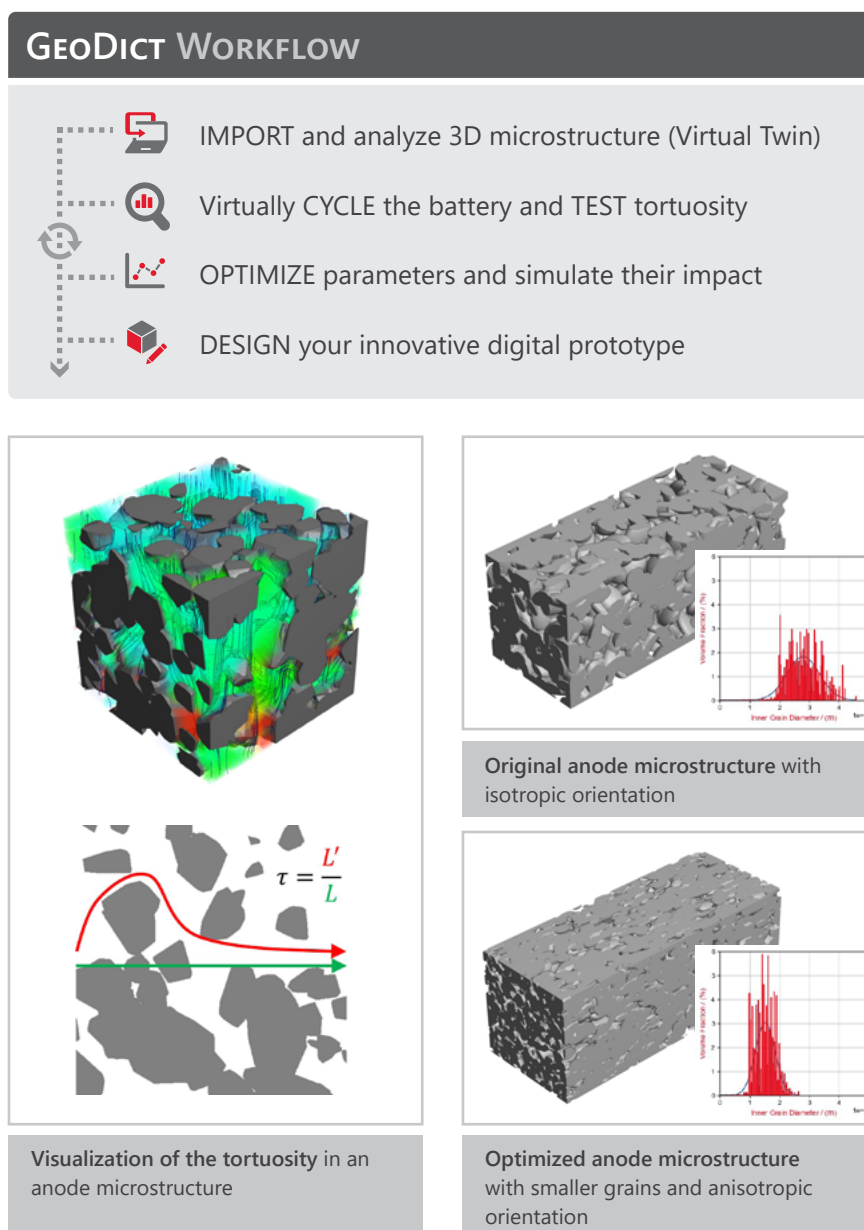
The critical parameter for the active particles in the electrode is the specific active surface, which must be maximized to offer sufficient electrochemically active sites for ion transfer.

Optimizing tortuosity and specific active surface will prevent bottlenecks for Li-ion transport and intercalation and, therefore, restrict Li-plating. The calculation of the microstructure's tortuosity and the effective diffusivity in the electrolyte is carried out using the DiffuDict module. The specific surface area of the active particles is determined within the GrainFind module.

In the next step, structural parameters like solid-volume-percentage, porosity, and size distribution, shape, and orientation of particles are optimized in the GrainGeo module. A charging simulation with BatteryDict then proves the reduction of Li-plating.

The Volkswagen Group Innovation is investigating the design guidelines for fast charging anodes using this workflow:

- Increasing active graphite surface by e.g. smaller particle size
- Increasing effective electrolyte diffusion by e.g. particle orientation
- Orienting the particles to expose the prismatic surfaces for Li-ion exchange



Conclusions

- + Reaching the goal of unifying high energy density, low cost, a superb lifetime and fast charging for batteries starts with understanding and fine-tuning the materials at the microscale.
- + The simulation software GeoDict® constitutes a true digital material laboratory, enabling the digital characterization and design of innovative battery materials for the mobility of tomorrow.
- + GeoDict® is the ultimate R&D toolkit to analyze and optimize the battery microstructure and can be easily integrated into any workflow.
- + Math2Market provides strong and competent scientific support to tackle specific R&D challenges and is proud of assisting its clients to succeed in their development goals.
- + Example of simulations result: Simulate and optimize transport properties, such as effective ionic diffusivity, geometric properties like tortuosity, and the specific surface of the active particles to prevent Li-plating in anodes.
- + Volkswagen has successfully integrated GeoDict® into its Group Innovation processes to investigate electrode microstructure while developing design guidelines for high energy electrodes, fast charging, and other research projects.



GeoDict® is a powerful design and simulation software to virtually recreate and process complex electrode structures in 3D. The analysis of morphology, size distribution and orientation of the active particles on the microscale provides deep insights into the properties of the macroscopic battery cell behavior. Thus, GeoDict® stands for a truly new design guideline and is the first choice for the digital optimization of energy materials. Contact us to get inspired!

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Math2Market - The Company

Math2Market GmbH was founded in September 2011 by three members of the GeoDict® software development team as a spin-off from the Fraunhofer Institute for Industrial Mathematics (ITWM, Institute für Techno- und Wirtschaftsmathematik) in Kaiserslautern, Germany. Some of the founders had been working on the software since its inception in 2001.

Today, Math2Market is one of the worldwide leading providers of digital solutions in the field of materials research and development. Over 150 large companies from various industry sectors, universities, and research institutes worldwide simulate with GeoDict® to develop innovative materials and optimize their material development processes.

With our unique pool of top mathematicians, physicists, geologists, engineers, and computer scientists, we believe in making available to our clients the benefits of cutting-edge, university-level research that can be utilized by non-experts using our software GeoDict®.