concentration	hydrostatic strain	von Mises strain
0.009	0.007	0.006
0.012	0.011	0.018
0.015	0.015	0.030

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BATTERY SIMULATION TOOL BEST – NEW EFFICIENT SOLVERS AND INTEGRATION IN GeoDict

1 *Lithium Ion concentration (mol/cm³), hydrostatic strain, and von Mises strain simulated with BESTmicroFFT for a realistic, stochastic electrode structure (structure generation: Inst. of Stochastics, Univ. Ulm)*

Electric mobility places a high demand on the energy storage systems – mainly lithium-ion batteries. Computer simulations can help in evaluating the performance of new battery cells, in understanding the microscopic reasons for the observed behaviour, and in optimizing the design. Several years ago, ITWM started the development of BEST (Battery and Electrochemistry Simulation Tool), which is continuously updated in public and private industrial projects.

Interesting problems range from design issues at the macroscopic battery cell scale (BESTmeso) to the effects of the microscopic design of electrodes (BESTmicro) on the electric, thermal, and mechanical characteristics of the cell. Two different software components are used to account for these multiscale aspects: BESTmeso and BESTmicro.

BESTmicroFFT reduces computing and storage costs
Simulations that account for the three dimensional microstructure of electrodes are very expensive because of the fine spatial discretization required. BESTmicro can sometimes take several days of computing time on common work stations. In many standard cases, the recently developed BESTmicroFFT software-module provides the remedy. Similar to ITWM's mechanical solver FeelMath, the new solver is also based on a Fourier method (FFT) and requires significantly less computing and storage effort for simulations. The user can now decide between the two micro-solvers depending on the current requirements.

BatteryDict as new GeoDict component
The BESTmicro and BESTmicroFFT solvers are fully compatible with the structure generators in the GeoDict software from Math2Market (M2M). In the area of battery simulation, we began collaborating with M2M last year on the joint development of the new GeoDict module BatteryDict. The new module is now commercially available in the GeoDict2018 release and offers BESTmicroFFT-based battery simulation in a fully integrated GeoDict workflow. The GeoDict2019 version has been expanded to provide for electrodes made from different active materials (electrode blends) and additional material classes (conductive additives).