SYNOPSYS®

Simpleware Software for Design of Energy Materials

Key Benefits

- Intuitive, User-Friendly Interface
- Quick and Accurate Segmentation
- Advanced 3D Image Processing
- Export High-Quality Meshes for Simulation
- Develop Automated Workflows
- Expert Technical Support

Key Features

- Import Images from Multiple Modalities
- Co-Register Image Data Sets
- Multiplanar Reconstruction (MPR)
- Measurements and Statistics
- Automated Multi-Part Meshing
- Export to FE or CFD Packages

Why Simpleware Software?

Simpleware™ software offers a fast, easy-to-use solution for generating models from 3D image data for the evaluation of energy materials. Rapidly inspect complex materials using image processing and measurement tools, and export watertight meshes for additive manufacturing and FE/CFD simulation. Use Simpleware software to characterize the form and function of energy materials and add speed and accuracy to the development of fuel cells and batteries.

Intuitive and Customizable

We pride ourselves on the ease-of-use of Simpleware software. Users new to the software can start processing image data within a short time frame, and very quickly visualize and identify regions of interest. Our range of fully automated, semi-automated and interactive segmentation and measurement tools allow even the most challenging image datasets to be processed efficiently. The software also offers scripting tools and plug-ins for users to customize the software and automate repetitive tasks without compromising on accuracy.

Dedicated Support and Training

Our expert technical support team are here to help you get the most out of the software, including step-by-step guidance and personalized support. We also regularly offer classroom training courses at our offices, or you can arrange customized training sessions online or at your site.

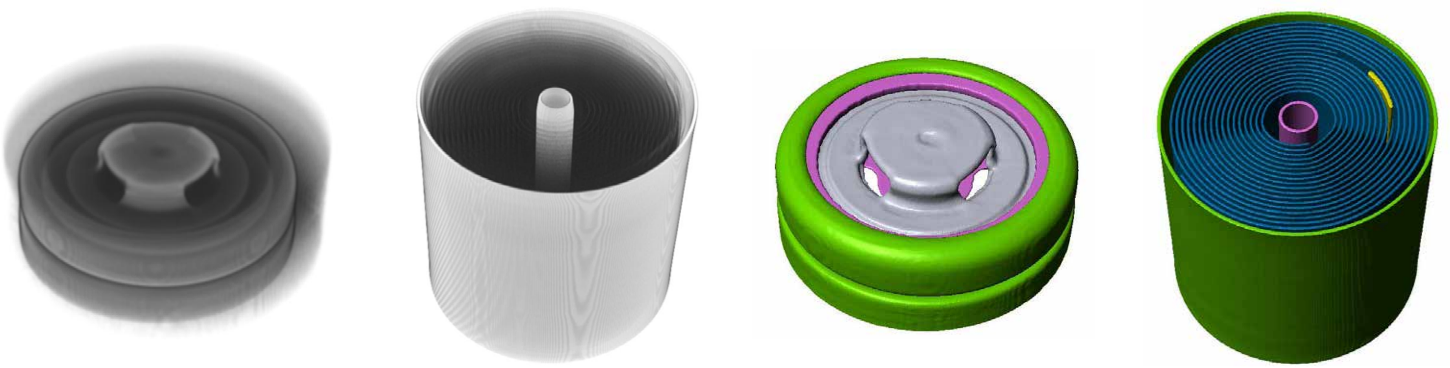
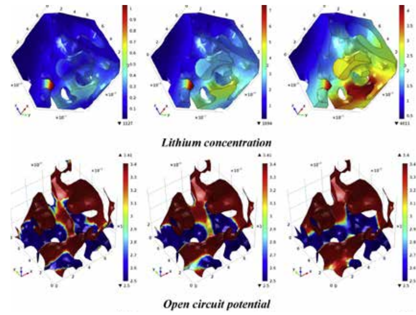


Image Based Modeling of Li-ion Battery Electrodes

University of Waterloo, Canada; University of Akron, USA; Carnegie Mellon University, USA; Indiana University Purdue, USA; Argonne National Laboratory, USA

The heterogeneous microstructure of lithium ion batteries (LIBs) remarkably influences performance by providing certain interfacial surface area, diffusion path, and active material connectivity. In this work, the LiFePO4 (LFP) electrode microstructure of a LIB is reconstructed based on the nano-XCT images in Simpleware software. The 3D model was then meshed and exported to COMSOL Multiphysics® for Finite Element Analysis. The results show that the electrode heterogeneity causes a wider range of physical and electrochemical properties compared to common homogenous models.

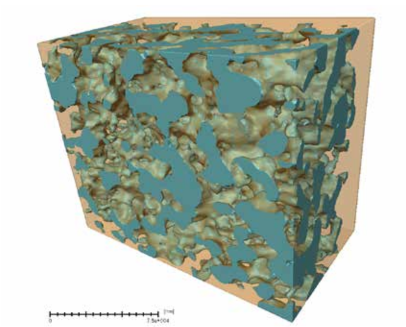


Distribution of lithium concentration and open circuit potential during discharge at c-rate = 1 for different SOCs

Improving Degradation of Solid Oxide Fuel Cells

Imperial College, UK; University College London, UK

The lifetime and degradation of solid oxide fuel cells (SOFCs) are affected by stresses generated within different layers of a device. While macro-scale modelling of stress in fuel cells can be used for homogeneous studies, more accurate stress analysis can be made of heterogeneous multiphase porous layers within electrodes on the micron and sub-micron scale using Focused Ion Beam (FIB) tomography and Finite Element modelling. By combining microstructural characterization of a porous SOFC with volume meshing in Simpleware software, researchers were able to perform a 3D FE stress analysis of the individual phases and boundaries of a fuel cell electrode, developing a better understanding of fuel cell failure.

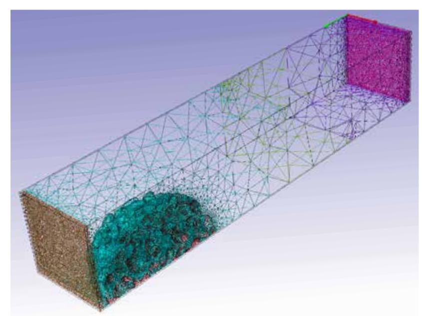


3D reconstruction of a solid oxide fuel cell (pores green and ceramic transparent)

Influence of Single Particle Structure on LIB Performance

L. Nowack • T. Bunjaku • M. Luisier • V. Wood, ***ETH Zurich, Switzerland***

Lithium ion diffusion in the active material is one of the limiting factors in lithium ion batteries (LIBs). The rational structuring of materials enables optimal function within the LIB. Single particle simulation gives an insight into how particle size and porosity influence the charging and discharging behavior of single LIB particles in dependence of the energy density. The research determined a nanoporosity of 25% to be an optimal strategy for usual battery operation. Higher porosity or larger pores only limited the volume energy density of the battery. Defined hierarchical internal structures were created by spray drying to compare experimental results with the simulation, which gave very comparable results on 2D and 3D structures.

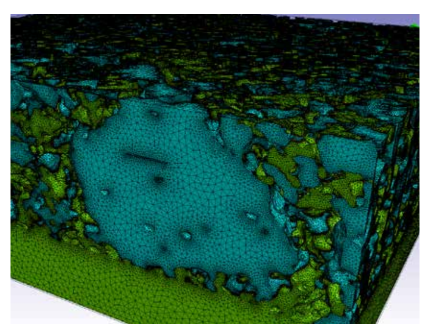


A quarter of a meshed structure in Simpleware FE which is transferred to COMSOL Multiphysics®

High-performance Computation of Local Electrochemistry in Solid Oxide Fuel Cell Electrodes

T. Hsu, ***Carnegie Mellon University, USA***

This study quantifies local distributions of electrochemical properties in heterogeneous SOFC microstructures, with an emphasis on the workflow to scan, mesh, and model complex SOFC microstructures over large scales. In Simpleware software, FIB-SEM image data of a commercial cell cathode was converted into multi-domain FE meshes that preserve surface morphologies in three-phase SOFC electrodes. Large-scale simulations regarding distributions of local electrochemical parameters were performed and analyzed for five different microstructure types using the MOOSE FE framework on high-performance supercomputers.



Large scale meshing (30 x 30 x 30 μm, 130 million mesh elements) in Simpleware FE

For more information on Simpleware Software Solutions go to www.synopsys.com/simpleware

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