University of Fribourg / Faculty of Science and Medicine / Department of Physics

# Digital Materials Design of Solid Oxide Fuel Cell Anodes

Philip Marmet

The storage and efficient conversion of energy is one of the key issues for a successful transition to renewable energies. Solid oxide fuel cell (SOFC) technology is a promising solution for the on-demand supply of electrical energy using synthetic gas or biogas (or natural gas) as input. To significantly improve on the unavoidable degradation of state-of-the-art anodes like Ni-YSZ, we elaborate on new nickel-free electrode concepts, which are based on mixed ionic and electronic conductors (MIEC) like doped ceria and perovskite (e.g., titanate) materials. The challenges associated with the complex physico-chemical processes involved in these electrodes are addressed in this thesis in two ways.
First, a Digital Materials Design (DMD) framework for the systematic and model-based optimization of MIEC SOC-electrodes is elaborated. In our DMD approach we combine stochastic microstructure modeling, virtual testing of 3D microstructures and a multiscale-multiphysics electrode model to explore the available design space by performing parametric studies. The basis for the DMD process is a set of fabricated solid oxide cells. Their real microstructures are reconstructed using FIB-SEM tomography. Stochastic digital microstructure twins with matching microstructure properties are then constructed for each real structure using a pluri-Gaussian method. On that basis, the microstructure can be virtually varied for a large parameter space in a realistic way. The real and subsequently the virtual 3D structures need to be characterized quantitatively by means of image analysis and numerical simulations. Hence, a standardized and automated microstructure characterization has been developed, which enables the fast determination of an extensive set of microstructure properties relevant for SOC electrodes. A multiphysics continuum simulation model is then used to predict the impact of the microstructure variation on the electrode performance, using the previously determined microstructure properties as an input. In addition, the kinetic reaction parameters of the model are calibrated to the experimental performance characterizations of the cells (e.g., EIS results). This model-based performance prediction enables to establish the relationship between materials choices and compositions, fabrication parameters, microstructure properties and cell-performance. This approach is thus capable to explore a much larger design space than it would be possible with experimental methods only.
Second, this DMD workflow is applied for the optimization of titanate based LSCT-CGO SOFC-anodes with a noble metal catalyst impregnation. Based on the performance and microstructure characterization of fabricated cells, several DMD studies are performed. Thereof, design guidelines for titanate-CGO anodes with an improved electrode performance are provided.

Jury:
Prof. Dr. Joseph M. Brader (thesis supervisor)
Dr. Lorenz Holzer (external thesis co-supervisor)
Prof. Dr. Thomas Hocker (external thesis co-supervisor)
Dr. Andreas Nenning (external co-examiner)
Prof. Dr. Robert Steinberger (external co-examiner)
Prof. Dr. Christian Bernhard (internal co-examiner)
Prof. Dr. Guillermo Pedro Acuna (president of the jury)