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3D Model for the Dynamic Simulation of SOFC Cathodes

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Abstract

A fuel cell is an electrochemical system, which converts chemical energy into electricity by a controlled reaction of hydrogen and oxygen. It consists of two electrodes (anode and cathode), which are separated by a gastight electrolyte. As oxygen electrode (cathode) material, porous mixed ionic / electronic conducting (MIEC) materials like LaSrCoFe (LSCF) are qualified for the application in intermediate temperature (T = 600 ... 800 °C) Solid Oxide Fuel Cells (SOFCs). The performance of the electrode is likewise determined by its material and the microstructure.

We present a dynamic time-dependent 3D cathode model based on a formerly published stationary model [1] which includes the main processes occurring in the SOFC cathode:

i) gas diffusion in the pores,

ii) oxygen exchange between the gas phase and the mixed conductor,

iii) oxygen ion diffusion in the mixed conductor

iv) charge transfer at the MIEC-cathode/electrolyte interface.

The simulations were performed directly on reconstructions of real electrodes (Figure 1), obtained from focused ion beam (FIB) tomography [2].
A finite element method (FEM) mesh for the simulations is generated by using the commercial software Simpleware.

The gas diffusion in the pores is implemented by defining the equations of the Dusty-Gas-Model in the 'PDE application mode'. For the oxygen ion diffusion in the MIEC phase the 'Transport of Concentrated Species' interface provides a detailed description of the physical processes. Finally the oxygen ion transport in the homogenous electrolyte is taken into account by using the 'Electric Currents Interface'.

We automatized the simulations for a wide parameter range with MATLAB script including the evaluation and post-processing of the results (Figure 2). For experimental analysis of the loss mechanisms in the SOFC cathode, Impedance Spectroscopy is an established method the analysis of complex electrochemical systems such as the SOFC [3].

The presented time-dependent model is able to calculate the impedance spectrum of a MIEC-cathode (Figure 3) from a simulation of the current response due to a sinusoidal voltage stimulus at different frequencies or an appropriate voltage step.

By disabling the loss contribution of individual processes in the model their impact on the impedance spectra can be evaluated for various MIEC cathodes differing in microstructure.

The model is discussed in detail and actual limits and problems during the implementation are shown. Last but not least an outlook will be given on how this flexible model approach can be extended, e.g. by including diffusion modelling in the frequency domain.

Reference

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