Electrochemical Simulation of Solid Oxide Fuel Cell Electrodes: an Integrated Approach to Address the Microstructure-Performance Correlation

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Understanding the complex interplay between electrode microstructure and electrochemical performance is one of the key aspects for the optimization of Solid Oxide Fuel Cells (SOFC). Physically-based modelling, at different levels of sophistication, can provide a valuable insight in order to help the interpretation of experimental data and provide design indications to improve electrode stability and performance.

In this contribution we summarize the different modelling approaches used in our group, ranging from physically-based equivalent circuits, continuum conservation models and 3D models solved within the reconstructed electrode microstructure. When necessary, these models are coupled with percolation theory, packing algorithms and tomographic techniques. Special focus is given to the application of the models to interpret impedance spectra and their thorough validation under different conditions. Examples include the application of the models to electrodes with different microstructures, the study of the degradation mechanisms of Ni-infiltrated anodes as well as impedance simulations in real microstructures (Figure 1).

Results reveal that coupling physically-based modelling, impedance spectroscopy and 3D tomography is a promising approach to gain a fundamental understanding of the phenomena occurring at different length scales in SOFC electrodes, allowing for interpreting and planning experiments as well as to design more stable and more efficient electrodes.

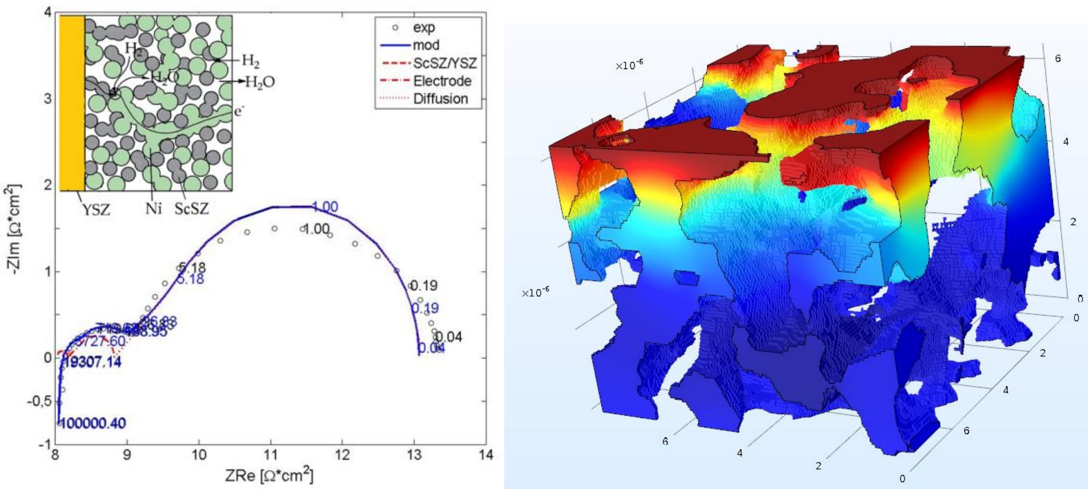

Figure 1. Examples of physically-based impedance simulation and 3D modelling of gas transport