Multi-Scale Image-Based Modeling of Effective Mass Transportation in a Novel-Fabricated Porous Solid Oxide Fuel Cell Anode

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Summary: This study uses multi-scale imaging and simulation to investigate the electrode with microstructure sizes spanning over 2 orders of magnitude. Parametric study reveals the effect of porosity on both local and global mass transport properties. Electrochemical simulation based on CT data is indicative for fabrication optimization.

1. INTRODUCTION

Solid Oxide Fuel Cells (SOFC) are promising electrochemical devices for future energy systems since they are energy efficient and environmental-friendly. Great efforts have been made in the past years to optimise their micro-structure for better electrochemical performance. Mass transportation of the reactants and products significantly determines the efficiency of the electrochemical energy conversion, because of which most of the cathodes and anodes are fabricated with high porosity [1]. However, we still have poor understanding on how the effective mass transport properties change with the porosity locally and globally.

Mass transport properties are critical in determining the electrochemical performance of Solid Oxide Fuel Cells (SOFCs), particularly when operating at high current densities. Tortuosity, porosity and permeability are the main microstructural parameters impacting the mass transport. For porous materials with pore sizes spanning over two orders of magnitude, measuring these microstructural parameters is challenging using image-based techniques (e.g. X-ray computed tomography) due to the trade-off between field-of-view and resolution. Pioneering steps have been made in this study to extract these microstructural parameters using multi-length scale imaging and modeling techniques. A tubular SOFC anode, composed of self-organized micro-channels and sponge-like regions, fabricated using a phase inversion technique [2], is used to illustrate this approach.

2. EXPERIMENTAL METHOD

The experiment was conducted at Electrochemical Innovation Lab (EIL), UCL, London. Micro-CT (Zeiss Xradia Versa 520) and nano-CT (Zeiss Xradia Ultra 810) were used to extract the materials at two length scales. The voxel sizes are 1.07 μm and 0.032 μm respectively. Polychromatic beam at 140 kV and monochromatic beam at 35 kV were used. The reconstructed data were segmented in Avizo V9.2 (FEI, Bordeaux) and imported to Star-CCM+(CD-adapco Inc.) for thermal flux and gas flow simulation. The reconstructed volume was then imported into Comsol Multiphysics for electrochemical simulation.

3. RESULTS

The results conclusively show that embedding finger-like micro-channels into the spongy anode can improve the effective mass transport by 250 % and the permeability by 2 to 3 orders of magnitude compared with a conventional tubular SOFC anode. Parametric study shows that 10 % is the threshold of a good percolation and thus the mass transport property; the increase of the porosity in the spongy layer enhances the effective mass transport parameters (i.e. tortuosity factors, permeability) of the spongy layer at an exponential rate (2.33), but linearly (0.75) for the full anode. The measured permeability was used for image-based electrochemical simulation for the first time on this novel-structured tubular SOFC. The conceptual multi-length scale techniques

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demonstrated in this study for the first time to correlate the microstructure with the local and global mass transport property, which can be significant for the optimization of SOFC electrode fabrication.

References

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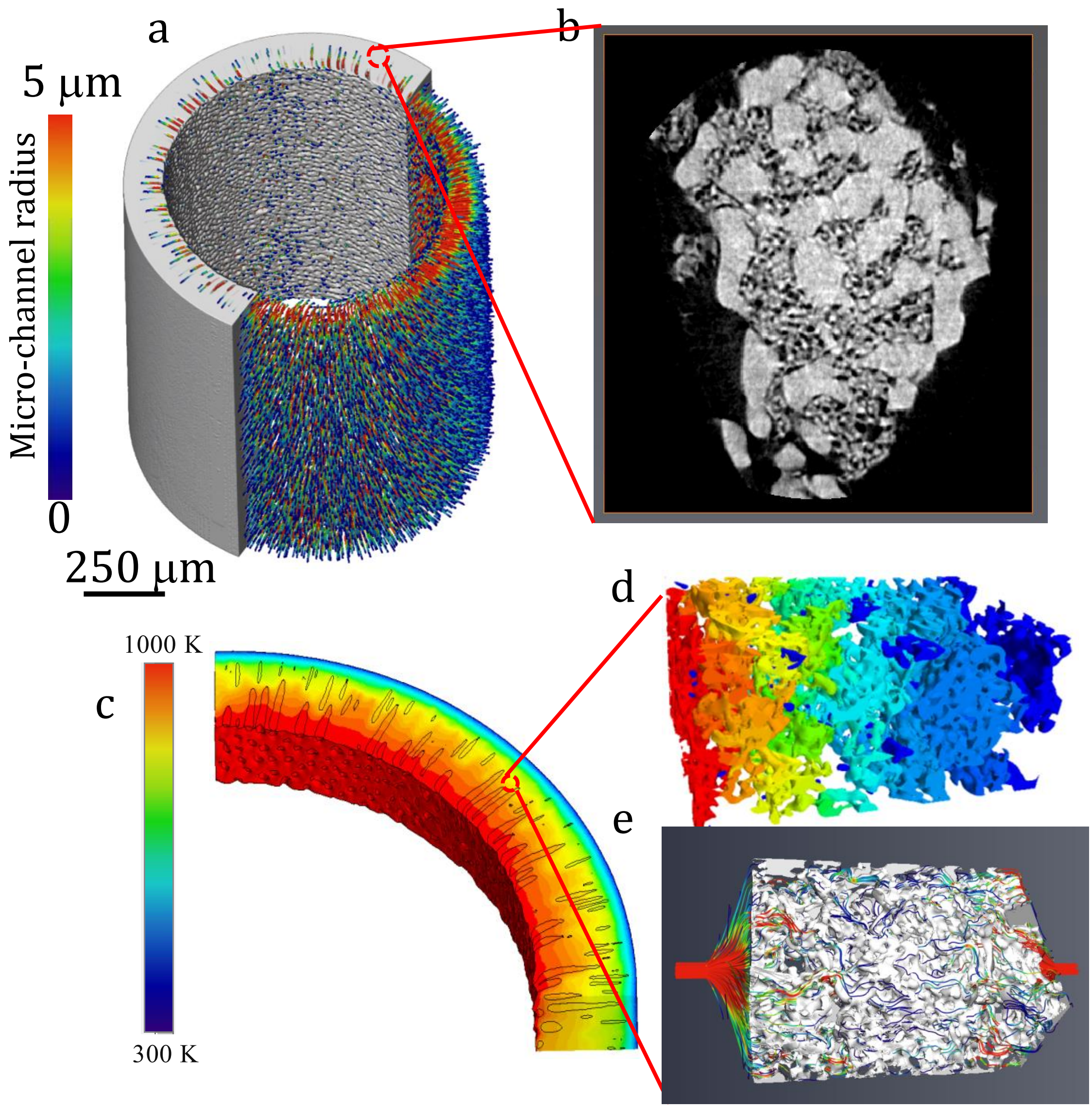

Figure 1. (a) 3D volume rendering from a low resolution scan shows the anode and the diameter variation of the micro-channels; (b) virtual orthoslice of the spongy layer extracted from the anode. The white phase is YSZ, grey phase is Ni. Highly porous Ni is observed; (c) a full-thickness anode simulation to extract the effective transport properties globally with varying porosity in the spongy layer (solid region). The spongy layer in the model was defined based on the effective transport properties (i.e. tortuosity factor, porosity and permeability) obtained from high resolution scan of the spongy layer (i.e. panel (d) and (e)).