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Site specific 3D pathway analysis of functional energy materials

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Site specific 3D pathway analysis of functional energy materials

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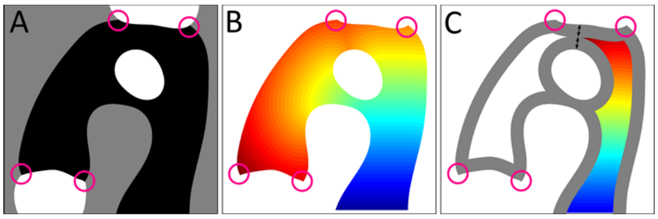
Introduction

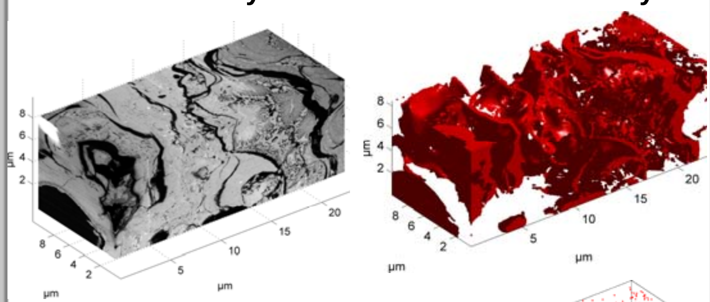
Energy devices such as solid oxide fuel cells (SOFC), electrolysis cells and batteries are promising technologies for conversion and storage of energy in a future based on sustainable energy. Common two the materials is that the chemical reactions occur a specific sites, such as the interface between pores and solids or triple phase boundaries where ion conduction, electron conduction and gas transport is available. The performance of these devices is dependent on both the density of these sites and on how easily ions, electrons, reactants and products can be transported to and from them.
The accurate geometrical characterization of the pathways to and from the electrochemically active sites is thus a strong tool for optimizing production recipes, troubleshooting microstructure related issues and linking the electrochemical performance to the microstructure morphology.

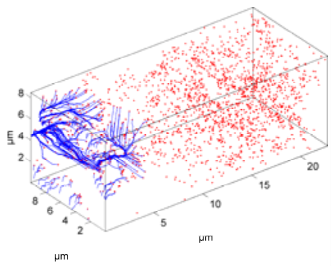
Site specific pathway analysis



The method for analyzing the pathways is straight forward. First the active sites are identified, illustrated by the TPB sites in (A) circled in pink. Next, a 3D distance map is calculated from the source through the phase of interest to all sites (B). This makes it possible to extract distributions of distance to each site through each phase. Finally, the phase of interest is gradually eroded while keeping track of the connectivity of each active site (C). This makes it possible to determine the critical pathway thickness of each site corresponding to the diameter of the largest sphere that can be passed through the structure to reach the site.

Pore Connectivity of a Ni electrode for electrolysis

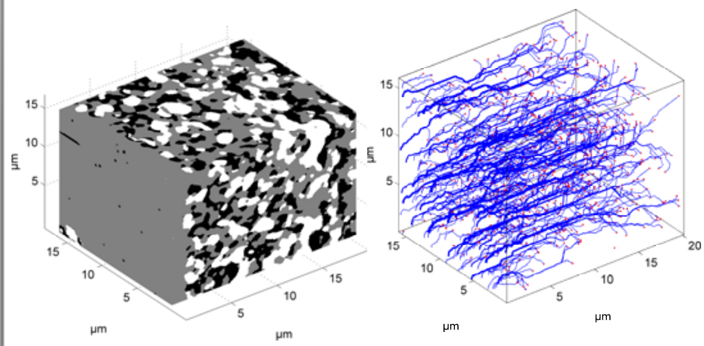




The pore network of a Ni electrode for hydrogen electrolysis in KOH is investigated. (top) The gray level intensities in the raw reconstructed image data. (upper right) Surface rendering of the pore network. (right) Pathway analysis from surface sites to the electrode surface. Red dots are 2000 randomly selected surface sites on the inside of the pores. Blue lines show the shortest pathway from each site to the surface of the electrode (the leftmost plane).

These preliminary results highlight the general structure of the large pores in the structure. The pores can be seen to form plane like structures parallel to the surface of the sample. The pathway plot shows that only pore/interface sites (red dots) close to the surface have a connected pathway through the large pores. It is however likely that pore transport can be facilitated through pore connections in the large pores on a larger scale (outside the reconstructed volume) or that transport of KOH can occur through nanosized pores below the resolution of the dataset.

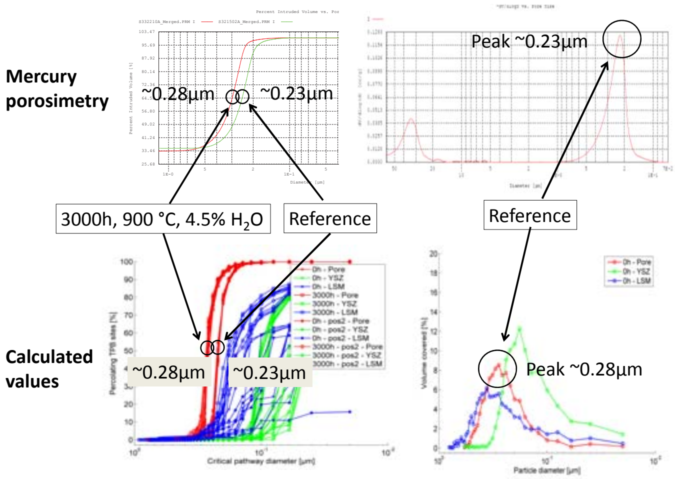
Triple phase boundary pathways in Ni/YSZ fuel cell electrode



A solid oxide fuel cell Ni/YSZ electrode is investigated. The image data is segmented into the three phases: pore (black), YSZ (gray) and Ni (White). The red dots are 1000 randomly selected sites on the triple phase boundaries (TPB) between pore, YSZ and Ni. The blue lines are the shortest pathways from the TPBs to the start of the electrolyte, seen as the part of the structure that is dense in the YSZ phase to the left in each figure. The thickness of the blue lines is proportional to the number of TPB pathways that use it.

The plot shows that almost all TPB sites are percolating in the YSZ phase. The YSZ furthermore have low tortuosity as seen by the almost straight main pathways that the individual TPB pathways gather in.

Comparison to mercury porosimetry on a LSM/YSZ fuel cell electrode



Mercury porosimetry was performed on two LSM/YSZ solid oxide fuel cell electrode samples, one tested for 3000h and one reference (not tested). Two 3D reconstructions were performed on the same samples. Excellent agreement was found between the calculated distribution of the critical pathway diameters and the mercury porosimetry intrusion curves. The calculated pore size distribution however showed some discrepancy when compared against the mercury porosimetry curve, illustrating the intrusion curves inability to measure wide pores connected through thinner pores.

Acknowledgements

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