Investigating Solid Oxide Cells degradation via advanced 3D microscope reconstructions analysis: from image segmentation to microstructural characterization.

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Context

Thanks to their high efficiency, large fuel flexibility, and reversibility between fuel cell and electrolysis operations, Solid Oxide Cells (SOC) have great potential for becoming a key technology in the ongoing energy transition. Indeed, the same device can alternatingly be used to produce hydrogen/methane from excess green energy, and *vice-versa*, power and heat from hydrogen/methane, when and where they are needed. Besides, thanks to its low cost (no expensive catalysts like platinum are required), and customizable power (cells are stacked to reach any target), reversible SOC can be the answer for a very wide range of applications from residential and industrial to transportation sectors.

The microstructure of porous SOCs plays a key role in both their performance and durability. For example, the electrodes should provide a high density of active electrochemical sites, i.e, lines of contact between the ionic (ceramic) and electronic (metallic or semi-conducting) conducting phases with porosity. These phases should also exhibit low tortuosity and high percolation for a good charge conduction and gases diffusion. These desired features can be reached by optimizing and tuning the cell manufacturing techniques. However, the cell layers undergo some morphological (e.g. grain growth) and compositional (e.g. secondary phase formation) alterations over operation-time, especially under harsh conditions (e.g., high temperature, steam content, overpotential, etc.). In order to investigate these microstructural evolutions, several imaging techniques can be used to reconstruct the 3D microstructure of the different layers, and image analysis is performed to extract the metrics that allow a better understanding of the complex medium degradation. This work is very important to improve SOC durability which represents its main weakness towards being a competitive technology in the energy conversion landscape.

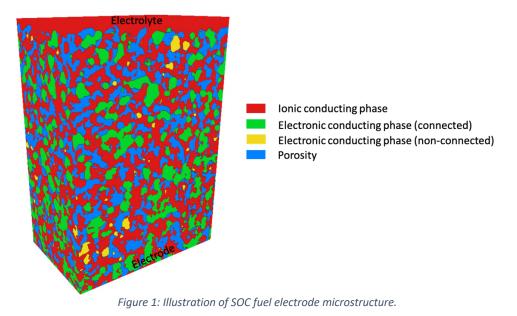
Objectives

The objective of this work is to quantify the electrode microstructural evolutions via advanced characterization techniques [1]. For this purpose, 3D raw reconstructions acquired via scanning electron microscopy coupled with focused-ion-beam (FIB-SEM), and energy dispersive X-ray (EDX) spectroscopy will be provided. The workflow is divided into two sections:

1. Image segmentation: first, the raw gray-scale data will be pre-processed by using adapted filtering tools. This initial step helps enhancing the contrast between the phases and homogenize the gray-scale level within each phase. As the reconstructed volume contains several phases with very close gray-scale level, the classical segmentation with simple thresholding is not adapted to accurately retrieve the different phases. Machine learning is then used as a powerful tool to separate the phases. For this purpose, several image processing softwares can be used (e.g., ImageJ, Ilastik, or Matlab). The challenge here is to select the most relevant training features for an optimal ratio of phase-separation/computational-time. The last step is

image post-processing, which consists in artefacts corrections due to the numerical segmentation.

2. Microstructural properties extraction: This second section consists in computing the morphological properties of the segmented 3D image. These include the phase volume fractions, interfacial surface areas, triple phase boundary lengths (connected/non-connected), tortuosity, percolation, etc. Furthermore, physical properties, namely the porous medium diffusivity and effective charge conductivity, can be extracted by using an available Matlab model. These geometrical and physical parameters are finally used to gain valuable insights into the SOC degradation mechanisms.



[1] H. Moussaoui, A. Nakajo, G. Rinaldi, M. Hubert, J. Laurencin and Jan Van herle,

"Modeling Nickel Microstructural Evolution in Ni-YSZ Electrodes Using a Mathematical Morphology Approach" 2021 ECS Transactions (103) 997. doi.org/10.1149/10301.0997ecst