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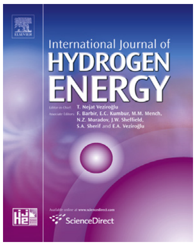

A review on micro-level modeling of solid oxide fuel cells

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ABSTRACT

Solid oxide fuel cells (SOFCs) are ceramic based electrochemical devices operating at high temperatures and generates electricity and useful heat energy utilizing various fuels at a high efficiency. The main structure of the cell comprises a dense electrolyte coated with two porous anode and cathode electrodes. The electrolyte is responsible for the transfer of oxide ion while the electrochemical reactions take place in the electrodes. The cell performance is limited by the number of reaction zones known as triple/three phase boundaries (TPBs). Therefore, the electrodes play a crucial role in achieving high power as well as long service life. When the requirements that SOFC electrodes should meet are considered, the most successful electrode materials seem to be composite ones, including ionic and electronic conductive phases with pores for the gas transport. However, this combination is not enough alone since the contiguous contact of these three phases within the electrodes is also necessary to obtain electrochemically active reaction zones. The number of these areas can be a useful metric for predicting the cell performance or provide a relationship between the performance and microstructure. The determination of the electrochemical reaction zones at the micro-scale and the microstructural parameters influencing their density are required to link the microstructure to the performance. Therefore, in this paper, micro-modeling studies of SOFC electrodes through advanced microstructural characterization are reviewed.

Introduction

A detailed analysis of the microstructure of SOFC electrodes is a critical and substantial for linking the processing of the electrode materials and related fabrication parameters to the microstructure and the microstructure to the electrode or the cell performance. Stereology is simply an analysis of the two dimensional cross sectional images obtained from three dimensional samples. It is advantageous in that it can be used to estimate the three dimensional properties of the material of interest. On the other hand, the accuracy of stereological methods is questionable if heterogeneous and complex microstructures like real SOFC electrodes are to be investigated.

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Nomenclature

L_{TPB}	Triple phase boundary length
R_{CT}	Charge transfer polarization resistance
R_{DA}	Dissociative adsorption polarization resistance
S_v	Pore surface area normalized per unit volume
d_i	Inner diameter
d_o	Outer diameter
i_0	Exchange current density
i_{reac}	Local reaction current density
j_s	Volume-averaged reaction current density
p_{H_2}	Partial pressure of hydrogen
p_{H_2O}	Partial pressure of steam
λ_{TPB}	Percolated TPB density
ρ_{elec}^{eff}	Effective electronic resistivity
ρ_{ion}^{eff}	Effective ionic resistivity
D	Diffusion coefficient
F	Faraday's constant
L	Thickness
R	Ideal gas constant
T	Temperature
t	Time
K	Permeability
S/V	Surface to volume ratio
j	Local current density
η	Overpotential
τ	Tortuosity

Moreover, these methods are inadequate to identify the phases and to determine the tortuosity, ionic or electronic transfer paths and the active TPBs accurately. Therefore, three dimensional reconstruction methods are essential to avoid these kind of limitations.

With the development in the visualization techniques and devices, it is now possible to observe the microstructure at the micro scale. Recently, focused ion beam – scanning electron microscopy (FIB-SEM) have been generally employed to collect a series of 2D SEM images as the specimen is sectioned via FIB. These images are then stacked together for the reconstruction of the real microstructure to be examined as a representative volume element for the entire domain of interest. The main emphasis in the reconstruction process should be given to the assignment of the phases. The reconstruction after some processes is then used to quantify the critical microstructural features of the electrode of interest such as volume fraction, particle size, pore size, closed and open porosity, tortuosity and length of three/triple phase boundaries. These parameters are generally used to link the microstructure to the electrochemical performance experimentally determined. Among them, the length of triple phase boundaries is one of the significant microstructural parameters since both the anode and cathode electrochemical reactions take place at these boundaries where the gas, ionic conductor and electronic conductor phases meet. However, contiguous electronic and ionic paths as well as a porous network to and from a TPB are essential to have electrochemically active TPBs. The examples of active and inactive TPB, electronic and ionic conductor phases in a typical Ni-YSZ SOFC anode are shown in Fig. 1.

Therefore; the number of active TPBs can be considered as an excellent indicator of the electrochemical performance of a SOFC electrode and it has a great importance to characterize them. This paper presents a detailed review of the recent efforts on micro-scale modeling of SOFC electrodes including the techniques involved, the equations defined, the determined microstructural parameters and some of the critical conclusions in a comparative way. The special emphasis is given to the 3D reconstruction of the electrodes via FIB-SEM. There can also be found other review articles on the microstructural characterization techniques of SOFC electrodes [1,2].

SOFC anode micro modeling

The first study on 3D reconstruction of SOFC electrode via FIB-SEM was published by Wilson et al. [3] who reported 3D reconstruction of Ni-YSZ anode with 6 × 5 × 3 μm dimensions to calculate significant microstructural properties including TPB length and volume fractions. The reconstructed structure is shown in Fig. 2 as an example of SOFC anode 3D reconstruction via FIB-SEM. They later presented their further results for 3D reconstruction of Ni-YSZ anode and initial results for LSM-YSZ and (La, Sr)CoO_3 SOFC cathode electrodes [4]. 3D reconstruction process for the anode was performed after the reduction of nearly dense NiO-YSZ. The assignment of the correct phases was achieved using 2D image contrast and each pixel was assigned to the correct phase together with accurate positioning of the phase boundaries. The structural data obtained from 3D reconstructed Ni-YSZ anode showed that Ni to YSZ volume ratio is 32:68 which was found to agree reasonably well with the initial anode composition of 35:65. The percentage of the pores, on the other hand, were 19.5%. The volume specific TPB length per unit volume was reported to be 4.28 μm^{-2} by analyzing the 3D anode map. However,

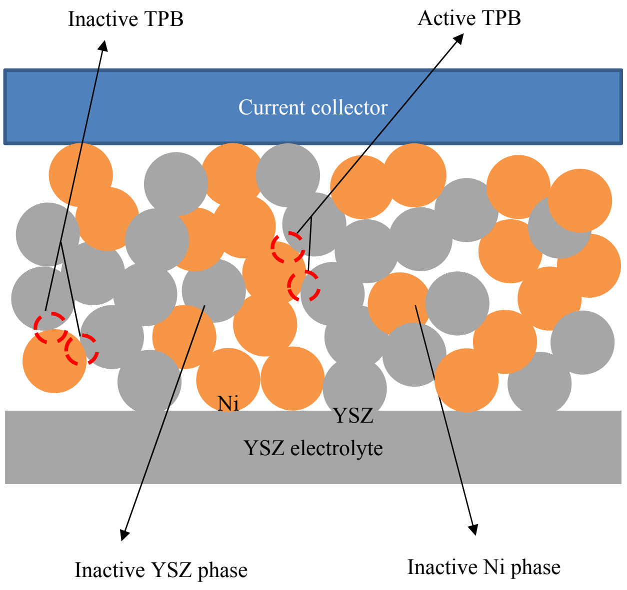

Fig. 1 – Possible formations of TPBs and phases in a SOFC electrode.