INTERNATIONAL JOURNAL OF HYDROGEN ENERGY XXX (2014) 1–5

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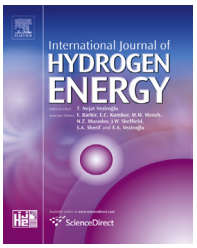

Short Communication

# On the tortuosity factor of solid phase in solid oxide fuel cell electrodes

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ARTICLE INFO

*Article history:*
Received 15 September 2014
Received in revised form
17 October 2014
Accepted 24 October 2014
Available online xxx

*Keywords:*
Tortuosity factor
Computational domain
Anisotropic property

ABSTRACT

Tortuosity factor $\tau$ of the solid phase is an important parameter for the accurate prediction of SOFC electrode conductivity. This work investigates the effect of computational domain on $\tau$. The results show that a computational domain with cross section area of $15d^{*}15d$ ($d$: particle diameter) is necessary for the calculation of $\tau$ when 15% deviation is allowed. The result also validates that the anisotropic property of $\tau$ shown in the previous literatures is caused by the insufficient sample size. This study builds a framework for the further study of $\tau$.

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## Introduction

Solid oxide fuel cell (SOFC) has attracted much attention in recent years for its expected high efficiency of power generation, broad fuel flexibility and environmental friendly effect [1]. An SOFC consists of three layers: porous anode, porous cathode, and dense electrolyte. In addition to material development, the ohmic loss of the electrolyte can be significantly reduced by decreasing the electrolyte thickness. It was reported by Andersson et al. [2] that only 10% of the total polarization occurred in electrolyte, while the left 30% was in cathode and 60% was in anode for an SOFC with 10 μm YSZ electrolyte and inlet gas temperature at 1010 K. As a result, it's more desirable to decrease the polarization losses in electrodes rather than electrolyte to improve the SOFC performance.

Three major kinds of polarization losses exist in SOFC electrodes: the activation polarization loss associated with electrochemical reactions, the ohmic polarization loss related to ion and electron transport and the concentration polarization loss caused by the concentration difference between electrochemical reaction sites and reference conditions. In many early modeling studies on SOFC [3,4], the electrochemical reactions were assumed to occur only in the electrode/electrolyte (E/E) interfaces and thus the ohmic

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http://dx.doi.org/10.1016/j.ijhydene.2014.10.111

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Please cite this article in press as: Zheng K, et al., On the tortuosity factor of solid phase in solid oxide fuel cell electrodes, International Journal of Hydrogen Energy (2014), http://dx.doi.org/10.1016/j.ijhydene.2014.10.111

**Nomenclature**

| | |
|---|---|
| $d$ | particle diameter, μm |
| $D_n$ | computational domain length |
| $j$ | current density, A/m$^2$ |
| $L_{vox}$ | voxel length, μm |
| *Greek letters* | |
| $\phi$ | electric potential, V |
| $\sigma_{eff}$ | effective conductivity, S/m |
| $\sigma^0$ | material intrinsic conductivity, S/m |
| $\tau$ | tortuosity factor |
| $\tau_{solid}$ | tortuosity factor of single phase electrode |
| $\tau_{ave}$ | average value of tortuosity factor in each case |
| $\Psi$ | volume fraction |

polarization in electrodes was ignored. However, it was found by Chen et al. [5] that the contribution of ohmic polarization to the total electrode polarization was actually significant, especially in the anode side. In SOFC, the effective conductivity ($\sigma^{eff}$) of solid phase in electrodes is very important for SOFC actual performance since ohmic polarization loss is mainly determined by the effective conductivity $\sigma^{eff}$. In addition, the effective conductivity $\sigma^{eff}$ also affects the reaction depth, which is a very thin layer from the E/E interface due to the low effective ionic conductivity in electrodes [6].

In SOFC modeling studies, $\sigma^{eff}$ is usually calculated as follows (for both ionic conducting phase and electronic conducting phase) [7–9]:

$$\sigma^{eff} = \sigma^0 \frac{\Psi}{\tau} \quad (1)$$

where, $\sigma^0$ is the material intrinsic conductivity (S/m); $\Psi$ is the volume fraction of the conducting phase (pore phase is included in calculation); $\tau$ is the tortuosity factor of the conducting phase. Unlike $\sigma^0$ and $\Psi$, $\tau$ is difficult to obtain experimentally and is often directly assumed or used as an adjustable parameter in SOFC modeling studies [10,11]. However, $\tau$ plays an influential role in SOFC performance prediction: Andersson et al. [2] examined the effect of the tortuosity factor of electrode ionic conducting phase ($\tau_{io}$) on the cell performance with a complete SOFC model and revealed that the current density increased from 3000 A/m$^2$ to 4050 A/m$^2$ as the $\tau_{io}$ decreased from 10 to 5.

In spite of the significance of $\tau$, studies in this field are limited [12–17] and the values reported in the literatures vary significantly (as shown in Table 1). Iwai et al. [13] reconstructed a Ni/YSZ anode using the focused ion beam scanning electron microscope (FIB-SEM) technique, followed by calculation of $\tau$ using random walk method and by solving the steady state diffusion equation in the conducting phase. The volume fraction of their constructed anode was gas/Ni/YSZ = 49.6%/25.3%/25.1% and the reported $\tau$ of Ni and YSZ (in the Y direction) were 29.45 and 14.82 respectively. By comparison, the $\tau$ of Ni reported by Vivet et al. [17] was only 10.11 with a similar volume fraction of 26%. Since the Ni phases and YSZ phase are of the same proportion in Refs. [13,17], it is expected that the $\tau$ in each phase should be similar. The large variation of the reported $\tau$ was attributed to the insufficient sample size [13,14], yet without any validation. It should be noted that the unexpected anisotropic property of $\tau$, as another possible consequence of the insufficient sample size was also found in most studies [12–17].

This short communication aims to investigate the effect of the computational domain on $\tau$ calculation and its anisotropic property. The three-dimensional (3D) microstructure of conventional binary composite electrode is numerically constructed by a well-validated sphere packing algorithm [18] for its good predictive ability and cost effective property. Finally, $\tau$ is obtained by solving charge conservation equations in the conducting phase.

**Table 1 – Main results in the literatures.**

| | [12] | [13] | [14] | [15] | [17] |
|---|---|---|---|---|---|
| Microstructure construction | FIB-SEM | FIB-SEM | FIB-SEM | particle packing | FIB-SEM |
| Methodology | Random walk method | Random walk method<br>Diffusion method | Diffusion method | Diffusion method | Diffusion method |
| Computational domain | Sample A:<br>X: 9.12 μm<br>Y: 4.75 μm<br>Z: 4.08 μm | X: 18.6 μm<br>Y: 8.432 μm<br>Z: 6.2 μm | X: 18.1 μm<br>Y: 9.72 μm<br>Z: 9.97 μm | X: 3.3 μm<br>Y: 3.3 μm<br>Z: 3.3 μm | Sample A4:<br>X: 9.12 μm<br>Y: 6.56 μm<br>Z: 5.84 μm |
| Voxel | 0.011 μm | | X: 0.035 μm<br>Y: 0.035 μm<br>Z: 0.062 μm | | 0.01 μm |
| Composition | gas/LSM: 42.5/57.5 | gas/Ni/YSZ: 49.6/25.3/25.1 | gas/Ni/YSZ: 36.1/34.2/29.7 | | gas/Ni/YSZ: 41/26/33 |
| Particle diameter | 0.73 μm | | Ni: 2 μm<br>YSZ: 1.4 μm | 0.6 μm | |
| Tortuosity factor | Sample A:<br>gas/LSM:<br>X: 1.398/2.38<br>Y: 1.43/2.56<br>Z: 1.89/3.94 | gas/Ni/YSZ:<br>X:2.03/21.68/27.66<br>Y:2.06/29.45/14.82<br>Z:1.83/6.94/9.84 | gas/Ni/YSZ:<br>X: 3.48/4.91/7.93<br>Y: 3.04/3.43/5.63<br>Z: 2.64/3.79/5.39 | | Sample A4:<br>Ni:<br>X: 9.24<br>Y: 10.11<br>Z: 39 |

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