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Reconstruction of solid oxide fuel cell electrode microstructure and analysis of its effective conductivity

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Abstract The effective conductivity (σ_{eff}) of solid oxide fuel cell (SOFC) electrode is an important parameter for predicting the ohmic loss in SOFC. This paper investigates the effective conductivity of SOFC electrodes reconstructed numerically by packing spherical particles in a computational domain, followed by a dilation process to simulate the sintering procedure. The effects of various parameters on the effective conductivity of the electrodes are investigated, including material composition, porosity, particle size and contact angle. Results show that the effective conductivity ratio (σ_{eff}/σ_0) of the computed conducting phase is mainly affected by its total volume fraction (VF) in electrode (including the porosity). The effective conductivity can be improved by increasing the VF, electrode particle size or the contact angle between electrode particles. Based on the numerical results, the conventional percolation model for the calculation of σ_{eff} is improved by adjusting the Bruggeman factor from 1.5 to 2.7. The results are useful for understanding the microstructure properties of SOFC composite electrode and for subsequent electrode optimization.

Keywords Fuel cell · Electrode · Conductivity · Modeling · Random particle packing

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1 Introduction

Solid oxide fuel cell (SOFC) has received much attention for its potential in clean power generation field [1]. An SOFC basically consists of three components: the porous anode, the porous cathode and the dense electrolyte. With the development of material processing technology, the ohmic loss in the electrolyte has been greatly decreased by fabricating thin film electrolyte with a thickness of about only 10 μm [2]. As a result, the electrode especially the cathode plays a more important role in determining SOFC actual performance, particularly at an intermediate temperature.

As known to all, the electrode performance is mainly determined by three kinds of losses: the activation loss due to local electrochemical reactions, the concentration loss due to gas transport and the ohmic loss due to ion/electron transport. Under typical operating conditions, the activation loss and the ohmic loss of an electrode are usually much higher than the concentration loss, and thus they are the key for improving the SOFC performance. The effective conductivity (σ_{eff}) is a key parameter which determines the ohmic loss in SOFC electrodes. If the σ_{eff} can be improved, the electrochemical active thickness will be significantly increased [3], which means more potential triple-phase boundaries (TPBs) can be activated under operating conditions.

The σ_{eff} is determined by the intrinsic conductivity of electrode material and electrode microstructure parameters (such as porosity and electrode particle size). Therefore, in addition to the development of electrode materials with high conductivities, an alternative way to improve the electrode effective conductivity is to optimize the electrode microstructure, which relies on a clear understanding of the relationship between electrode microstructure parameters and its effective conductivity.

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Great efforts have been devoted to linking the σ_{eff} with electrode microstructure parameters [4–19]. Previous numerical studies in this field can be mainly classified into three kinds: (1) numerical modeling based on the reconstructed actual electrodes using experimental methods, such as the focused ion beam scanning electron microscope technique [4–7]; (2) numerical modeling based on the constructed electrodes using numerical methods (for example, the random particle packing procedure [8, 9]); (3) analytical works based on the percolation theory [10–16]. The research approach based on experimental techniques provides a microstructure characterization of the actual electrode; however, it does not have any predictive ability and may be more suitable to be used to adjust and verify the developed relationship between electrode microparameters and electrode effective properties. In addition, this approach relies on both of the experimental technique and image processing technique, which may also cause some uncertainty [14, 19]. In comparison, the particle packing electrode construction method only presents a simplified electrode structure [14]; however, it is comparably easy to be accomplished [16] and thus more suitable to conduct detailed parametric analysis between σ_{eff} and its affecting factors. Furthermore, the particle packing procedure can simulate the actual electrode fabrication process and thus makes it possible to investigate the fabrication parameter (for example, the sintering process) effect on σ_{eff} [16, 20, 21]. The percolation model can be regarded as an extended theory of the particle packing electrode construction method, and it mainly includes two parts: the relationship between electrode microparameters and the coordinate numbers and the relationship between coordinate numbers and electrode effective properties [10, 14, 16]. Although percolation model cannot show a specific electrode microstructure and can only reflect an averaged situation of an SOFC electrode, it is easy to be incorporated into a high-level model to establish a complete relationship between electrode microparameter and SOFC cell performance [16].

However, present information is still not enough to build a clear and reliable relationship between σ_{eff} and its affecting factors. Most of works in literatures were based on certain electrode structures and investigated the effect of electrode porosity and composition on σ_{eff}, while rare study considered the effect of the electrode particle size and the contact angle among electrode particles (mainly related to the sintering process). Besides, although the percolation models describe the relationship between the electrode microparameters and coordinate numbers were well developed [11, 12] and improved [10, 14, 15], the effects of porosity and contact angle on the average coordinate number (Z_{ave}) still need more investigation. Bertei et al. [16] studied the sintering effect on Z_{ave} in random packing structures. However, the porosity effect is examined by adding additional pore-former particles into the rigid particle packing structures (8° contact angle among particles), and the minimum porosity considered is 0.41 (without pore-former). In addition, the electrode porosity decreased from 0.404 to 0.329 as the contact angle increasing from 30° to 46° in their study, and thus it is not reasonable to conclude that large contact angle leads to large Z_{ave}, which also might be caused by the low porosity. Furthermore, the commonly used percolation model describes the relationship between the coordinate number and σ_{eff} is still unconvinced (as shown in Eq. (1) [10], Eq. (2) [15]). While other parameters involved in the relationship possess clear physical meanings and are easy to be accessed, the Bruggeman factor μ is experimentally assumed as 1.5, which is doubted to be too small to overestimate the σ_{eff} [22].

$$\sigma_{\mathrm{eff},i} = \sigma_{0,i}\left[(1-\varepsilon)\psi_i P_{\mathrm{erco},i}\right]^{\mu}, \quad i = \mathrm{el\ \ or\ \ io}, \tag{1}$$

$$P_{\mathrm{erco},i} = 1 - \left(\frac{4.236 - Z_{i,i}}{2.472}\right)^{3.7}, \quad i = \mathrm{el\ \ or\ \ io}, \tag{2}$$

where σ_{eff} and σ_0 refer to the effective conductivity and material intrinsic conductivity of the i-conducting phase, (S/m); ε is the electrode porosity; Ψ is the volume fraction of the i-conducting phase; P_{erco} is the percolation probability; $Z_{i,i}$ is the coordinate number among the i-conducting particles.

Consequently, a more comprehensive study was conducted in this work to investigate the σ_{eff} of SOFC composite electrode via numerical simulation. The microstructure of porous electrode is constructed numerically by randomly packing spherical particles in a computational domain, followed by a geometrical dilating procedure to simulate the sintering process [21, 23]. The effects of various parameters (particle size, contact angle, material composition and porosity) on σ_{eff} are investigated. After that, the percolation model for the calculation of σ_{eff} is improved based on the numerical results. This work provides further insight into the relationship between electrode microstructure and its effective conductivities.

2 Methodology

2.1 Electrode construction

A typical composite electrode is fabricated from a mixture of ion-conducting particles and electron-conducting particles, followed by a sintering process to generate penetrated networks of different conducting phases [24–26]. The approach used in this work to construct SOFC electrode is briefly introduced as following (implemented by MATLAB ®):