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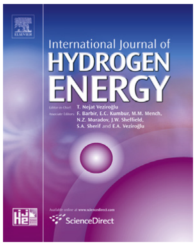

Simulation-based microstructural optimization of solid oxide fuel cell for low temperature operation

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ABSTRACT

Despite immense potential, the widespread application of solid oxide fuel cells (SOFCs) is hindered by high operating temperatures. Successfully tailoring the microstructures of SOFC electrodes can offset adverse effects of lowering operating temperatures. Our previous work considered functionally graded anode, however, further investigation needs to be done on the cell level optimization of SOFCs considering both anode and cathode to lower cell operating temperature. In this paper, a complete cell level multi-scale polarization model has been developed assuming the electrode particles to be randomly packed spheres. Micro- and macro-models are developed separately and then integrated to establish a cell level model. Suzuki's model is adopted for micro-modeling with ionic-electronic particle size ratio limited from 0.1547 to 6.646. The results of this modeling work closely match the referenced literature. Simulation results show that the performance of SOFCs can be improved with tailored microstructures. The power output of SOFC with nonlinearly graded electrodes shows 28% improvement compared to SOFC with linearly graded electrodes. Moreover, the combination of nonlinear particle-size- and porosity-graded electrodes enable SOFCs to operate at a reduced temperature (as low as 873 K) while maintaining the performance at high temperature of 1273 K.

Introduction

Solid oxide fuel cell (SOFC) power generation promises high energy efficiency while producing low emissions [1–4]. However, further commercialization of SOFCs is hampered by high operating temperatures (over 1000 K) [5–7], which limits the selection of materials. Moreover, severe thermal stress due to the high operating temperatures can cause serious structural failure (e.g., cracking and delamination) [8,9]. For example, a model for crack nucleation in SOFCs under thermal cycling was previously developed and validated by Liu et al. [6]. Additionally, Liu et al. [9] investigated the detrimental effect of degradation of the anode microstructure on overall cell performance during thermal cycling. Due to the adverse effects of high operating temperature, much attention has been focused on lowering SOFC operating temperature [10–12]. However, decreasing the operating temperature can significantly reduce SOFCs efficiency as well as the power output [13]. Thus, anode-supported SOFCs were developed as one of attempts to lower the operating temperature while maintaining overall cell performance [3,14]. Investigation on anode-supported SOFC shows electrode microstructure plays a vital role in determining SOFC electrochemical behavior [5,15–17]. The

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triple phase boundary (TPB) is widely considered to be one of the key microstructural features responsible for determining the electrochemical behavior of SOFCs [5,17,18]. As shown in Fig. 1, the TPB is the contact area among the three phases (i.e., the ion conducting phase, electron conducting phase, and gas phase) necessary for electrochemical reactions in the electrodes [19,20]. Power output of a SOFC is directly dependent on TPB area within the electrodes [9,17,21]. Many studies, including but not limited to [22,23], show that optimizing the TPB area of the electrode is an important factor in achieving maximum power output. A precise structural characterization of TPB area is therefore crucial to correlate the electrochemical performances with its microstructure [17]. Experimental studies use high quality sample preparation and high resolution techniques such as Focus Ion Beam (FIB) [24,25] and Atomic Force Microscopy (AFM) [26–31] techniques to explore TPB microstructure. The FIB-SEM (Scanning Electron Microscopy) technique is used for three dimensional (3D) reconstruction of TPB microstructure. Wilson et al. [32] determined key microstructural parameters of TPB such as phase volume fractions, tortuosity, etc. of LSM-YSZ composite cathode using the FIB-SEM techniques. Symmetric LSM-YSZ-LSM cells were also investigated using the aforementioned techniques [33]. Size, shape, and topology of granular cermet were analyzed by Holzer et al. [34] using FIB-SEM techniques. AFM method is used to approximate electrochemical functionality [35]. Local irreversible electrochemical processes in the electrochemically active surface is demonstrated by using scanning probe microscopy approach [35].

Those aforementioned experimental investigations provide insight into the SOFC microstructure and its performance, however, the numerical model is required for theoretical explanation of experimentally observed phenomena as well as evaluating SOFCs' performance enhancement. Previous research has explored functionally graded electrode to optimize the TPB area of an electrode. Costamagna et al. [36] developed a microscopic model of an electrode formed by nearly spherical electronic and ionic conducting particles (i.e., randomly packed sphere theory). This modeling approach had also been used in recent studies [37,38]. The results showed that volumetric composition and particle size strongly influence power output. Hussain et al. [39] investigated a 1-D anode supported cell with a thin layer of reaction zone in the vicinity of the electrode. Greene et al. [40] confirmed a functionally graded electrode can increase electrochemical activity and cell performance. Ni et al. [41] presented a model exploring linearly graded electrodes to improve the peak power density of SOFCs.

These aforementioned microstructure models investigated particle-size graded electrodes and how it can be beneficial to improve power output. In addition, controlling electrode porosity can further improve the performance of SOFCs with optimized TPB [42–44]. Experiments conducted by Holtappels et al. [45] showed porosity graded SOFC anodes can optimize gas transport to achieve high electrochemical activity at the anode-electrolyte interface. Joshi et al. [46] applied the lattice Boltzmann method to formulate a diffusion model. Liu et al. [3] developed an electrode-level model that focuses on the effects of particle-size- and porosity-graded anode on the performance of SOFCs. Despite previous efforts, much investigation is yet to be done on cell level modeling that considers particle-size- and porosity-grading in both anode and cathode. More attention should be focused on microstructural optimization from the standpoint of lowering operating temperature. In this work, we investigate offsetting adverse effects of lowering operating temperatures by tailoring the microstructures of SOFC electrodes considering the electrochemical behavior of both electrodes' based on grading range as well as grading profile. In detail, our previous developed electrode-level model [4] is extended to a full cell-level model, which incorporates the microstructures of both electrodes. The performance of functionally graded electrodes is numerically analyzed using the developed cell-level model. The cell-level model is applied to provide insight into reducing SOFC operating temperature via optimizing electrodes' microstructures.

Model development

In this paper, our previous models [3,4] are extended to a cell level model for SOFCs. Both macro-scale and micro-scale characteristics of SOFC electrodes are considered. The micro-model considers the microstructural features, such as particle size, pore diameter, particle coordination number, and TPB area. Effective resistivity and effective conductivity of SOFC electrode are treated by the micro-model based on aforementioned microstructural parameters. The macro modeling is mainly focused on three different types of voltage losses: activation loss, ohmic loss, and concentration loss. Additionally, macro-scale modeling focuses on investigating the effects of porosity change and different porosity/

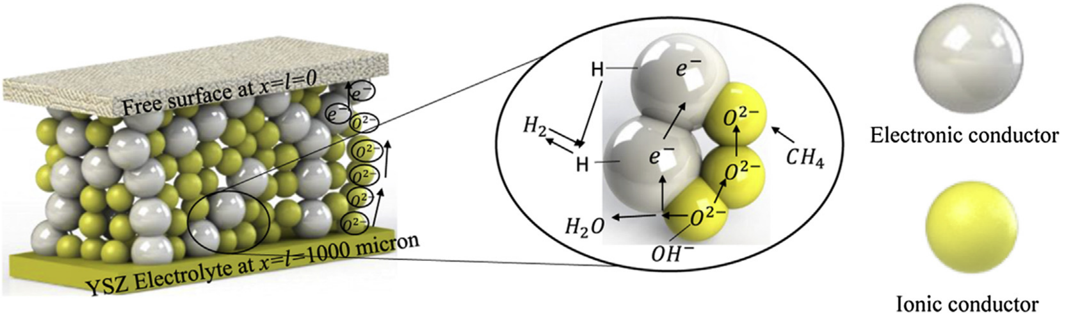

Fig. 1 – Schematic of TPB microstructure.