Modeling of gas transport with electrochemical reaction in nickel-yttria-stabilized zirconia anode during thermal cycling by Lattice Boltzmann method

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Abstract:

This work reports an investigation of the impact of microstructure on the performance of solid oxide fuel cells (SOFC) composed of nickel yttria-stabilized zirconia (Ni YSZ). X-ray nano computed tomography (nano-CT) was used to obtain three-dimensional (3D) models of Ni-YSZ composite anode samples subjected to different thermal cycles. Key parameters, such as triple phase boundary (TPB) density, were calculated using 3D reconstructions. The electrochemical reaction occurring at active-TPB was modeled by the Lattice Boltzmann Method for simulation of multi-

component mass transfer in porous anodes. The effect of different electrode geometries on the mass transfer and the electrochemical reaction in anodes was studied by TPB distributions measured by nano CT for samples subjected to different thermal cycles. The concentration polarization and the activation polarization were estimated respectively. The results demonstrate that a combined approach involving nano-CT experiments in conjunction with simulations of gas transport and electrochemical reactions using the Lattice Boltzmann method can be used to better understand the relationship between electrode microstructure and performance of nickel yttria-stabilized zirconia anodes.

Keywords: solid oxide fuel cell; thermal cycling; active TPB; Lattice Boltzmann Method

1. Introduction

Solid oxide fuel cells (SOFCs) are all-solid state energy conversion devices that convert chemical energy to electricity. Because they do not operate by combustion and are therefore not subject to limitations of the Carnot cycle, SOFCs have the advantages of high energy conversion efficiency, low emission of pollutants, capability to produce both heat and power, less noise and high reliability, causing them to attract notable attention in recent years [1, 2]. SOFCs mainly consist of three parts: an anode, a cathode, and an electrolyte. During the cathodic reduction reaction, oxygen gas is converted into oxygen ions which are conducted to the anode through the electrolyte YSZ. On the other hand, the fuel gas hydrogen reacts with oxygen ions to form water, producing

extra electrons which are conducted through Ni to the external circuit. Therefore, the electrochemical reaction occurs only at the three-phase boundary (TPB), where the ion conductor YSZ, electron conductor Ni, and gas channel pores are in contact.

Connectivity of the three phases is an important factor to guarantee the transport of reactants and products. Additionally, there is a strong positive correlation between the performance of the SOFC and the density of active-TPB, which implies that the three phases must be connected [3]. However, because SOFCs operate at a high temperature (between 950 and 1300 K), the agglomeration of Ni particles occurs and the average Ni particle size increases with thermal cycling; which in turn is associated with a reduction in the Ni-phase connectivity and the three phase boundary length [4, 5].

In order to optimize anode structure design and to improve the performance of SOFCs, a variety of high-resolution imaging techniques are applied to obtain the microstructure of the porous electrodes. Previously, focused ion beam scanning electron microscopy (FIB-SEM) has been used to study changes in Ni-YSZ anode structure [6, 7]. Subsequently, due to the strong penetrating ability of X-rays, which can detect internal structure, and the development of the Computer Tomography (CT) technique, nano-CT was applied to nondestructively obtain the fine three dimensional (3D) structure of porous electrodes [8, 9]. By this technique, microstructural characteristics such as volume fraction, connectivity of each phase, active TPB density, tortuosity, etc. can be calculated based on 3D reconstructions. However, determination of the parameters does not give the whole story. These data can be used in other suitable

methods for further investigations in order to predict the performance of SOFCs.

Numerical simulation is thought to be an important approach to predict the performance of SOFCs. For instance, computational fluid dynamics (CFD) models have been used to simulate heat, mass, momentum and charge transport, as well as kinetics, by considering internal reformations and electrochemical reactions at the macro-scale [10]. However this model is not suitable to be used at sub-micron length scales because of non-continuum effects, complex geometries, multiple length scales, and heterogeneous reactions at the pore scale [11]. The Lattice Boltzmann method (LBM) is a promising alternative CFD method that is well-suited to capture the details of transport processes at the micro-scale [12, 13]. Detailed geometric information is required to carry out simulations using LBM. Several earlier studies have adopted a random statistical method to create the model-connected physical parameters [14-16]. Recently, due to the development of the a forementioned advanced 3D imaging techniques, real microstructure of an SOFC electrode sample can be reconstructed by nano-CT or FIB-SEM and can be used as the geometry input for the LBM model [17-19]. In our previous research, LBM was used to simulate gas transport in the 3D microstructure of Ni-YSZ anodes, obtained by nano-CT [20]. Concentration polarization, gas distribution, exhaustion of reactants, etc. were calculated on the basis of the diffusion results. In this paper, a new and more advanced model has been developed for simulating electrochemical reactions and mass transfer at the TPB. This means that detailed anode geometry, actual active TPB distribution, and simplified electrochemical reactions are taken into consideration during simulation. Thus the

simulated results should be more accurate and closer to the real state of anode.

2. Mathematical Model and nano-CT experiments

2.1. Theory of the cell

Generally, in the operating state, ohmic loss and concentration polarization are the predominant contributors to loss of SOFC voltage. In this work, Ni-YSZ was used as a composite anode because Ni-based cermet has low resistance, and YSZ provides good mechanical support, which blocks the agglomeration of Ni particles [21]. Concentration polarization is only related to concentrations of reactants and products associated with electrochemical reactions occurring at the functional layer. When the functional layer is very thin and has a length of about ten microns, its structure has a significant influence on concentration polarization and the performance of the SOFC. The overall reaction in an SOFC is the oxidation of H_2 to form H_2O , namely,

In the ideal state, the cell reaction can be described by the Nernst equation. The potential between the anode and cathode is related to the net free energy [22, 23].

$$E = -g / 2F \quad (2)$$

$$E = -\frac{G^0}{2F} - \frac{RT}{2F} \ln \left(\frac{p_{H_2O}^a}{p_{H_2}^a p_{O_2}^{c/2}} \right) = E^0 + \frac{RT}{4F} \ln \left(\frac{p_{O_2}^c p_{H_2}^{a/2}}{p_{H_2O}^a} \right) \quad (3)$$

2.2. Method

The LBM model has been widely used to simulate gas diffusion in multi-component systems. It adopts a discrete particle velocity distribution function (PDF) $f_i^\alpha(\vec{x}, t)$ as the main variable [24]. The particle velocity distribution function, $f_i^\alpha(\vec{x}, t)$, is defined as the number of molecules of species α moving in the direction

i with the velocity e_i^α at the lattice point $\vec{x}$ and at time t .

In this paper, the D3Q19 velocity model for 3D simulation has been adopted to simulate ternary gas transport and reactions in the Ni-YSZ anode function layer. There are 19 discrete velocity directions e_i^α at each lattice point. All 19 discrete velocity directions start from the center of the lattice and can be divided into three types, where direction $i = 0$ remains the original position: directions $i = 1, 2, \dots, 6$ point to the six face centers of the lattice and the rest twelve directions $i = 7, 8, \dots, 18$ point to the twelve edge centers.

The LBM consists of three elements: discrete velocity, lattice, and the lattice Boltzmann equation. Briefly, the lattice Boltzmann equation contains two parts: streaming and collision, as shown in Eq. (4). Streaming describes the movement of particles and collision describes the interactions between particles of the same or different species, as shown in Eq. (5) and (6), respectively [25]. At the streaming step, the bilinear interpolation method is used to describe that species with higher molecular weights have lower travelling speed, where the temperature and average kinetic energy of all species are assumed to be constant [26]. By simulating streaming and collision processes across a limited number of particles, the intrinsic particle interactions evince a microcosm behavior applicable to the greater mass.

$$f_i^\alpha(\vec{x} + \delta e_i^\alpha, t + \delta) = f_i^\alpha(\vec{x}, t) + \Omega_i^\alpha(\vec{x}, t) \quad (4)$$

$$f_i^{\alpha,(\text{eq})} = \omega_i n_\alpha \left[1 + \frac{e_i^\alpha \cdot u}{c_{s,i}^2} + \frac{(e_i^\alpha \cdot u)^2}{2c_{s,i}^4} - \frac{u \cdot u}{2c_{s,i}^2} \right] \quad (5)$$

$$\Omega_i^\alpha(\vec{x}, t) = \frac{f_i^\alpha(\vec{x}, t) - f_i^{\alpha,(\text{eq})}(\vec{x}, t)}{\tau_i} \quad (6)$$

In Eq. (5), w_i is the weight factor along the direction i , c_s is the dimensionless speed of sound. The particle density or concentration n_α and velocity u_α can be obtained by Eq. (7) and Eq. (8):

$$n_\alpha = \sum_{i=0}^{18} f_i^\alpha \quad (7)$$

$$n_\alpha u_\alpha = \sum_{i=0}^{18} f_i^\alpha e_i^\alpha \quad (8)$$

Considering the electrochemical reaction in this study, the source term $F_i^\alpha(\vec{x}, t)$ is added to the equation, as shown in Eq. (9) and (10) [27-29]:

$$f_i^\alpha(\vec{x} + \delta e_i^\alpha, t + \delta) = f_i^\alpha(\vec{x}, t) + \Omega_i^\alpha(\vec{x}, t) + F_i^\alpha(\vec{x}, t) \quad (9)$$

$$F_i^\alpha(\vec{x}, t) = w_i \delta \sum_{r=1}^{N_r} \frac{\lambda_r \delta}{\bar{q}} R_r \quad (10)$$

where w_i is the weight factor along the direction i , δ is time step in the simulation, λ_r is the stoichiometric coefficient, R_r is the reaction rate in lattice units for the r -th reaction, N_r is the total number of reactions, and $\bar{q}$ is the number of velocity directions. The bounce-back rule is used as a boundary condition for the non-equilibrium portion [30].

In this study, a two-component synthetic reaction was used to model the reaction process [31], is given by Eq. (11):

where k_a is reaction coefficient and thought as a constan, C and R are the reactants, P is the product. Here, H_2 and O^{2-} were considered to be directly reacting at the reaction sites with constant reaction rate.

Because electrochemical reactions only occur at the interface between triple

phases, the sites were set next to actual active TPB measured by nano-CT, in contrast to earlier studies in which the reaction sites were randomly placed. Figure 1 shows 3D renderings of the anode sample and distribution of reaction sites. As is shown in Figure 1(b), the sites colored in green are located at the solid-pore interface.

Figure 1. (a) 3D rendering of an anode sample with Ni shown in red, YSZ shown in yellow, pore shown in blue; (b) Corresponding 3D distribution of reaction sites (green) and pore (blue).

In this study, a mixture of gases consisting of H_2 , H_2O , and N_2 , was allowed to flow from $z=0$ to $z=L$. Normally, the concentration condition (0.47, 0.03, 0.5) was used at the inlet while a flux condition was used at the outlet [20, 32]. As is known, the reaction mechanism in the SOFC anode is comprised of several steps [33]. In this study, the objective was to study the effect of actual TPB length on distributions of gas transport and on the performance of the anode. Thus, in order to simplify the simulation, H_2 and O^{2-} were considered to be directly reacting at these sites and the electrochemical reaction coefficient was assumed to be constant [27, 31].

2.3 Nano-CT experiments

Synchrotron based nano-computed tomography experiments were carried out at

beamline 4W1A of the Beijing Synchrotron Radiation Facility (BSRF), China. The details of the experimental setup can be found in a previous publication [34]. Four Ni-YSZ anodes that were subjected to either 2, 4, 6 or 8 thermal cycles and a non-cycle anode were imaged at 8.4 keV (above the Ni edge). 181 projections were collected at 1 degree increments with a 15 μm field of view and a spatial resolution of 30 nm. Then the samples were reconstructed from 181 projected images via the software based on filtered back-projection algorithm from Carl Zeiss X-ray Microscopy Inc. The 3D rendering and segmentation were performed using the Amira software (FEI Visualization Science Group, Mérégnac, France).

3. Results and Discussion

Microstructures of Ni-YSZ anodes have been obtained and further studied based on the results of nano-CT imaging. In this study, the samples subjected to different thermal cycling times are used as inputs for the mathematical model.

3.1. Change in active TPB density during thermal cycling

A method for measuring active TPB length and density has been previously reported [35]. Table 1 shows the change of total TPB and active TPB density of Ni-YSZ anodes after varying numbers of thermal cycles (0, 2, 4, 6, 8 cycles). Generally, there is a negative correlation between the frequency of thermal cycling and TPB density. The no-cycle sample has a much higher total TPB density up to 5.1337×10^6 $\text{m} \cdot \text{cm}^{-3}$ and active TPB density up to 3.25×10^6 $\text{m} \cdot \text{cm}^{-3}$. As the number of thermal cycles is increased from 0 to 8 times, active TPB density decreases from 3.25×10^6 $\text{m} \cdot \text{cm}^{-3}$ for

the no-cycle sample, to $0.199 \times 10^6 \text{ m} \cdot \text{cm}^{-3}$ for the 8-cycle sample. Due to the high operating temperatures of SOFCs, small Ni particles in anodes agglomerate to form larger particles in the early stages, and after a certain number of thermal cycles, the microstructure reaches a steady state [4]. Therefore, samples subjected to more thermal cycles most likely have a higher volume fraction of large-sized Ni particles.

3.2. Gas diffusion with electrochemical reactions

Our previous research focused on the impact of microstructural changes on gas diffusion, and the anode/electrolyte interfaces were treated as being electrochemically active in order to replace the actual distribution of the active TPB. Electrochemical reactions occurring at reaction sites were not considered [20]. Although this approach can demonstrate how microstructural changes influence gas diffusion and concentration polarizations at the TPB sites, it is of greater interest to study the electrochemical reactions occurring at the active sites (active-TPB) during mass transport. In this study, the electrochemical reaction ($\text{H}_2 + \text{O}^{2-} = \text{H}_2\text{O} + 2\text{e}^-$) occurring at active-TPB has been simulated based on the 3D distribution of the active-TPB calculated from 3D reconstruction. In other words, both the electrochemical reaction and gas transport processes were considered when simulating the impact of microstructural evolution of Ni-YSZ subjected to thermal cycles, on mass transfer in anodes. Figure 2(a) is a 3D rendering of the distribution of the H_2O mole fraction in a no-cycle Ni-YSZ anode sample at operating temperature of 1073 K and operating potential of 0.75 V, when the electrochemical reaction were included in the simulation. Figure 2(b) shows a vertical section of the results without the electrochemical reactions. It can be observed that H_2O

mole fraction has an even distribution that varies in a small range from 0.315 to 0.335.

Without reactions, the factors affecting gas distribution, such as pore connectivity, are only associated with the microstructure of the anode.

Figure 2. (a) Distribution of H₂O mole fraction in a no-cycle Ni-YSZ anode sample at operating temperature of 1073 K and operating potential of 0.75 V and schematic section direction; (b) distribution of H₂O mole fraction for pure diffusion; (c) corresponding distribution of active sites (red) in the section; (d) distribution of H₂O mole fraction with reaction included.

It is known that because the electrochemical reactions only occur at the active TPB sites, the densities and distributions of the active TPB sites in anodes have a great impact on electrochemical reactions and further affect the performance of SOFCs. As mentioned above, actual TPB distribution was adopted in the mathematical model used

in this study. Figure 2(c) shows the 2D distribution of active sites corresponding to the slice shown in Figure 2(b), while Figure 2(d) shows gas transport results for a no-cycle sample with electrochemical reactions. A comparison of Figures 2(b) and (d) shows a clear difference in the distributions of H_2O mole fractions in these two slices. When the electrochemical reaction occurring in the TPB sites is considered in the simulation, the distribution of H_2O mole fractions fluctuates in the range from 0.325 to 0.380. This range is considerably larger than that obtained without considering the electrochemical reaction. Furthermore, from Figures 2(c) and 2(d), it can be observed that the distribution of reactant and product mole fractions agrees well with the distribution of the active TPB sites. Locations which have more active-TPB sites have higher mole fractions of H_2O . This is because H_2O is produced at the active TPB sites and the accumulation of H_2O is related to the electrochemical reaction [32]. Thus, these results demonstrate the relationship between the active TPB densities and the electrochemical reaction. The consumption of fuel gas and accumulation of reactant at TPB sites impedes the following electrochemical reaction and gas transport and is a known cause of concentration polarization.

3.3. Gas diffusion in Ni-YSZ anodes after different numbers of thermal cycles

Figure 3. (a) Distribution of H₂ mole fraction in a no-cycle sample (b) subjected to 8 times thermal cycle at operating temperature of 1073 K and operating potential of 0.75 V; (c) average H₂ mole fractions vary with anode thickness for anodes after 0, 2, 4, 6, 8 thermal cycles.

As discussed above, thermal cycling affects the microstructure parameters of the anode, such as the density of active TPB. The density of active TPB regions reaches a steady state as the number of thermal cycles increases. After 8 or more times of thermal, the density is approximately $0.199 \times 10^6 \text{ m} \cdot \text{cm}^{-3}$, which is close to the normal range [36]. Here, the reaction rate at reaction sites is assumed to be $1.06 \text{ kmol} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$ [27]. Figure 3 shows distributions of H₂ mole fractions in samples subjected to different numbers of thermal cycles at operating temperature of 1073 K and operating potential of 0.75 V. Because an anode sample with more thermal cycles has a lower active TPB density, the

distributions of H_2 mole fractions in different anodes are different. From Figure 3, it can be observed that the H_2 mole fraction in the whole anode after 0 thermal cycles is lower than that of the anode after eight thermal cycles. This means that exhaustion of H_2 decreases as the number of cycles increases from 0 to 8, which is consistent with the densities of active TPB sites. The one exception was the sample after 4 cycles, which had a higher active TPB density while also having largest H_2 mole fraction. This was believed to be an outlier. The reason may be extremely heterogeneous distribution of the active sites and pore phase in this anode, which has an influence on H_2 diffusion.

Figure 4. (a) Distribution of H_2O mole fraction in a no-cycle sample (b) subjected to 8 times thermal cycle at operating temperature of 1073 K and operating potential of 0.75 V; (c) average H_2O mole fractions vary with anode thickness for anodes after 0, 2, 4, 6, 8 thermal cycles

Figure 4 shows the distributions of H_2O mole fractions in anodes subjected to

different thermal cycles at operating temperature of 1073 K and operating potential of 0.75 V. The H₂O was produced at the active-TPB sites and later diffused from the output side to the input side. Figures 4(a) and (b) show the 3D distributions of H₂O mole fractions in the anodes with 0 thermal cycle and with 8 thermal cycles. The difference in distributions of H₂O mole fractions in those two anodes can be observed directly. In order to quantitatively estimate the difference, the average H₂O mole fraction in each slice is calculated as shown in Figure 4(c), which indicates that the average H₂O mole fraction decreases as the number of thermal cycles increases. For example, the average H₂O mole fraction in the output side of the anode with 0 thermal cycles is approximately 0.421, while after 8 thermal cycles, the number decreases to 0.340. This result indicates that electrochemical reaction in the anode with 0 thermal cycles is stronger than in the anode with 8 thermal cycles, and more H₂O is being produced in the anode with 0 thermal cycles.

3.4 Effect of the mole fraction distributions of H₂ and H₂O on the concentration polarization

Based on the mole fraction distributions of H₂ and H₂O, the concentration polarization of the anodes was calculated using the Eq.(12) [24, 37]:

$$\eta_{conc} = -\frac{RT}{2F} \ln \left(\frac{p_{H_2, A/E} p_{H_2O, bulk}}{p_{H_2, bulk} p_{H_2O, A/E}} \right) \quad (12)$$

where $p_{i, A/E}$ represents the partial pressure of gas species i at the electrode electrolyte interface, $p_{i, bulk}$ represents the partial pressure of gas species i in whole anode, R is the universal gas constant (8.3145 J mol⁻¹K⁻¹), F the Faraday constant (9.6485 × 10⁴ C mol⁻¹), T the temperature.

Table 2 shows the concentration polarization of the anodes operating at 1073K. It can be found that the concentration polarization is 169.5 mV for non-cycled sample and decreases to 145.2 mV for 8-cycles sample, which is caused by the H_2 and H_2O molar fraction variation in no-cycle anode was larger than that of the other four samples. Previous study had demonstrated that smaller particle diameter can increase TPB length, while increase mass transport resistance [38]. In this study, no-cycle anode has the largest TPB length. This indicates that amount of small particle diameter (Ni) in no-cycle anode should be greater than that of the rest samples. As show in Figure 5, the volume fraction of small Ni particle diameter ($<0.5\mu m$) in no-cycle anode is largest among three samples. Moreover, the biggest Ni particle diameter in no-cycle anode is about $2.5\mu m$. This is consistent with our result which no-cycle anode has largest TPB density.

Figure 5. The distribution of volume fraction of Ni phase with different diameter size.

3.5 Effect of TPB length on the activation polarization of the anodes

Previous studies suggest that current density is related to the exhaustion of fuels [39]. An anode with a higher density of active TPB exhausts more H_2 and produces

more H₂O during tests, enabling it to provide a relatively higher current density. In order to understand the impact of gas transport and TPB length on the performance of an anode, the activation polarization η_{act} had be calculated using Eq.(13) and (14) [37]:

$$\eta_{act} = \frac{RT}{F} \ln \left[\frac{J}{2J_0} + \sqrt{\left(\frac{J}{2J_0} \right)^2 + 1} \right] \quad (13)$$

$$J_0 = kL_{TPB} \times \left(\frac{P_{H_2}}{P_{ref}} \right) \left(\frac{P_{H_2O}}{P_{ref}} \right) \exp \left(-\frac{E_{act}}{RT} \right) \quad (14)$$

where J_0 is the exchange current density, J current density, k the coefficient for exchange current density (1.54×10^{-2} A), L_{TPB} the length of TPB and E_{act} activation energy for anode (1.0×10^5 J mol⁻¹ [37]).

Based on the obtained TPB length of anodes, the activation polarization of four samples had been given as shown in Figure 6. It can be found that with increase of current density, the activation polarization in each anode increases. Furthermore, the activation polarization increases with the decrease of TPB length. For example, when current density is 5000 Am⁻², the activation polarization is 44.5 mV for no-cycle anode and increases to 206.1 mV for 8-cycles. This implies that an anode with a higher density of active TPB has lower activation polarization and exhibit better performance. Density of active TPB can be used to characterize the performance of the SOFC.

Figure 6. The curves of the activation polarization in four anode samples varying with the current density.

3.6 The lattice number independent study and modeling validation

The lattice number independent study had been done to determine whether the simulated results is independent of sample size. Three different size structures ($35 \times 35 \times 35$, $60 \times 60 \times 60$, $80 \times 80 \times 80$) were selected from the no-cycle anode. Based on these structures, simulations of gas transport with electrochemical reaction were carried out. Then mole fractions of H_2 and H_2O along the thickness of structures were obtained as shown in Figure 7. It can be found that change trend of smallest structure ($35 \times 35 \times 35$) is different from that of the other three structures. This indicates that the simulated results of smallest structure is dependent of its size. When lattice number increase to 80, the change trend of H_2 and H_2O mole fractions is closed to that of no-cycle anode used in this study. Moreover, in our previous study, we shown that when the size of the reconstructed volume is more than $79 \times 79 \times 79$, this volume can be representative of the full electrode. Thus in this study the simulated results should be independent of sample size.

Figure 7. H₂ and H₂O mole fractions in different size anodes.

The LBM mass transfer model has previously been used for modeling mass transport [20]. The study had verified the implementation of LBM mass transfer model and proved that the present LBM is capable of simulating the multi-component mass transfer much more accurately in the porous electrodes of SOFC.

4. Conclusions

As reactions occurring at active TPB sites affect gas transport in anodes, density of active TPB plays an important role in the performance of the SOFC. In this paper, microstructure of Ni-YSZ anodes subjected to different thermal cycle times were obtained nondestructively based on nano-CT results. During thermal cycling, small-sized Ni particles agglomerate to form large-sized particles. This leads to a reduction in density of active TPB sites. Actual distributions of active TPB as well as reaction sites were included in the gas diffusion model. Compared with previous research, the results show that H₂ is exhausted and that H₂O is accumulated at reaction sites. This accumulation impedes the following electrochemical reaction and gas diffusion and causes a higher local concentration polarization. The calculated the concentration polarizations shown that Ni particle size and higher active TPB density had an impact

on the H₂ transport in anodes. Moreover, the anode with higher TPB length had lower activation polarization. These results demonstrate some reasons that why anode with a higher density of active TPB sites generally corresponds to better performance of the SOFC. In order to further understand the relationship between microstructural parameters or operation conditions and the performance of SOFC from micro to macro scale, further studies should be focused on developing and integrating multi-scale models to study mass transport with electrochemical reactions, electronic/ion transport, temperature distributions and the microstructure of electrodes for fuel cell designs.

Acknowledgments

This work was supported by grants from the Major State Basic Research Development Program of China (973 Program) (Nos.2012CB825804 and 2013CB933104), the Ph.D. Programs Foundation of the Ministry of Education of China (No. 2012340213002), and the National Science Foundation of China (Nos. 11275204, 11475175, 21427804, 11405175 and 11205189).

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Table 1

TPB density calculated from the anode samples subjected to thermal cycles

	No cycles	2 cycles	4 cycles	6 cycles	8 cycles
Active-TPB density ($\times 10^6 \text{ m}\cdot\text{cm}^{-3}$)	3.2578	2.2554	1.1424	0.3533	0.1994
Total TPB density ($\times 10^6 \text{ m}\cdot\text{cm}^{-3}$)	5.1337	2.9904	2.4605	0.4707	0.4983

Table 2

Simulated results from LBM modeling

	No cycle	2 cycles	4 cycles	6 cycles	8 cycles
H ₂ % at outlet	16.51	18.95	21.02	20.95	22.70
H ₂ O% at outlet	42.01	39.92	35.29	36.77	34.02
Concentration polarization (mV)	169.5	167.2	161.5	152.5	145.2