



Theoretical studies on the electrochemical and mechanical properties and microstructure optimization of micro-tubular solid oxide fuel cells

Jiayu Li^a, Wei Kong^a, Zijing Lin^{a,b,*}

^aHefei National Laboratory for Physical Sciences at the Microscale and Department of Physics, University of Science and Technology of China, Hefei 230026, China

^bKey Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, China

H I G H L I G H T S

- ▶ A thermal fluid electrochemistry model and a thermal mechanical model are presented.
- ▶ Current collection method significantly affects the output of mtSOFC.
- ▶ Effects of Ni content on electrochemical and mechanical performance are critically examined.
- ▶ Area current outputs of planar and micro-tubular SOFCs are found to be comparable.

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A comprehensive thermal fluid electrochemistry model for the analysis of the electrochemical performance and a thermal mechanical model for the analysis of the mechanical behavior of micro-tubular solid oxide fuel cell (mtSOFC) are presented. Material properties for the models are determined by the available theory and experiment and linked to the compositions and microstructures of the materials. Good agreement between the theoretical and experimental I – V relations is obtained. The mode is used to examine the effects of various parameters on the electrochemical and mechanical performance of mtSOFC. Collecting current from both sides of the anode is found to significantly increase the cell output. Increasing the Ni content or reducing the Ni particle size is generally helpful for improving the electrochemical performance, but the increased Ni content reduces the mechanical stability. The suitable Ni content is thus obtained. The LSM content is inconsequential to the mechanical stability and should be determined by achieving high electrochemical performance. Properly designed mtSOFCs are shown to provide high current outputs. Therefore, mtSOFC is a promising technology with both the benefits of planar SOFC for high current density and tubular SOFC for thermal cycling endurance.

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1. Introduction

Solid oxide fuel cells (SOFCs) are attractive power production devices due to their high energy efficiency and fuel flexibility as well as low pollutant emission [1]. Micro-tubular SOFC (mtSOFC) with tubular diameter under a few millimeters shows high performance on the thermal shock resistance, volumetric power density, fast startup and thermal cycling and has attracted increased attentions [2].

The basic principles governing the choices of SOFC materials have a lot in common for the tubular, planar and micro-tubular

designs. For example, the electrodes should have high conductivities for the charge transport, high catalytic activities for the required chemical and electrochemical reactions, adequate porosity for the gas diffusion, good chemical and mechanical compatibilities with the electrolyte and interconnect materials for the long-term operating stability [3]. Therefore, material compositions and microstructures suitable for tubular SOFCs (tSOFCs) and planar SOFCs (pSOFCs) are often the right choices for mtSOFCs. However, the mtSOFC design has its own distinct characteristics that should be examined to realize its full potential. There is a strong need for in-depth analysis of mtSOFC due to the fact that, as a relatively new design of SOFC, mtSOFC is less studied and understood and there is a large room for its improvement. As the experimental testing is expensive and time consuming, its ability to study the effects of different material parameters and operating conditions on the performance of mtSOFC is severely limited. Mathematical models

* Corresponding author. Hefei National Laboratory for Physical Sciences at the Microscale and Department of Physics, University of Science and Technology of China, Hefei 230026, China. Tel.: +86 551 3606345; fax: +86 551 3606348.

E-mail address: zjlin@ustc.edu.cn (Z. Lin).

incorporating the known physics and behaviors of mtSOFC materials to predict their performance are important tools for the understanding and technological improvement of mtSOFCs.

Numerous mathematical models have been built to study the effect of microstructure on the electrochemical performance [4–12]. De Caluwe et al. [10] developed a one-dimensional button-cell model to examine the influence of anode microstructure on the electrochemical performance. Joan et al. performed numerical analyses on the optimization of cathode microstructures for anode-supported pSOFCs [11]. Several thermal stress models with varying degrees of sophistication [13–24] are also proposed to study the mechanical properties of SOFCs. Yakabe et al. [17–19] evaluated the residual thermal stresses in the electrolyte of anode-supported pSOFCs by a combined experimental and numerical analysis. Selimovic et al. [20] studied the thermal stress of pSOFC in both the steady and transient states. Weil et al. [21] performed a finite element analysis on the magnitudes of thermally induced stress, strain and part deflection in the cell, seal and window frame components under uniform heating and cooling conditions. Nakajo et al. [22,23] used thermo-electrochemical models to study the mechanical issues and the current–voltage (I – V) characterization of pSOFC stacks during assembly, heat-up, dynamic operation, load shutdown and cool-down phases. Recently, Serincan et al. developed a multi-physics model to investigate the effects of different factors on the thermal stresses in a mtSOFC with the thermal expansion coefficients of materials treated as constants [25].

Though there is no shortage of research on the numerical modeling of SOFCs, the theoretical effort focusing on the effects of electrode composition and microstructure on both the electrochemical performance and mechanical property of mtSOFC is relatively rare in the open literature. However, such research effort is quite important for the understanding and development of mtSOFC. For example, a typical mtSOFC consists of a composite anode support, a thin electrolyte layer and a thin composite cathode layer. The composite electrode is a mixture of electron conducting material, such as Ni for the anode or La(Sr)MnO₃ (LSM) for the cathode, and the electrolyte-material, such as yttria-stabilized zirconia (YSZ) [3]. An Ni content close to 40 vol.% in the Ni–YSZ cermet may easily produce an area power density that is higher than its tSOFC counterpart, but substantially lower than that of the pSOFC design [3,26]. Increasing the Ni content to about 50% may significantly increase the power density [3], but the increased Ni content induces mechanical flaw [27]. Therefore, both the electrochemical and mechanical properties and their interplay should be taken into account in order to properly balance their different needs and improve the mtSOFC technology for practical applications.

This work describes a detailed multi-physics model for the numerical simulation of mtSOFCs. The physical properties of composite materials are determined by the available theories and experimental data. The model is used to examine the electrochemical and mechanical performances of mtOFCs with the representative Ni/YSZ/LSM material set. Effects of the material microstructures such as Ni and LSM contents and their particle sizes on the electrochemical performance and thermal mechanical behavior of mtSOFC are systematically examined. The desirable material compositions and microstructures are thus deduced.

2. Theoretical method

There are two main components in our mathematical model: a thermal fluid electrochemistry model for the analysis of the electrochemical performances and a thermal mechanical model for the analysis of the mechanical behaviors of mtSOFCs. The microstructure based multi-physics electrochemistry model and the structural mechanics model are solved sequentially. The thermal

stress distributions in mtSOFC are evaluated with the temperature fields obtained from the thermal fluid electrochemistry model. The thermal stress distributions and mechanical properties are used by the structural mechanics model to calculate the probability of mechanical failure of the mtSOFC materials. The electrochemistry model and the structural mechanics model may be assembled from various literatures [7,14,28–31]. The precise details of the models used in this work are described in the following.

2.1. Electrochemistry model

The multi-physics electrochemistry model involves coupled electrochemistry, thermal, fluid and electrical transport equations with microstructure-based properties. The basic model parameters for the electrochemical, electrical and thermal properties are determined by the experimental data [32]. The effects of the electrode composition and microstructure on the material properties are considered by the microstructure based effective property theory [33]. Effects of the electrode composition on the electrochemical performance of mtSOFC may then be revealed.

The overall performance of SOFC depends on the operating cell voltage and the output current. The cell operating voltage, V_{cell} , is lower than the open circuit potential (Nernst potential) due to various polarizations such as activation polarization, ohmic polarization and concentration polarization, and may be formally expressed as [30]:

$$V_{\text{cell}} = E_0 - \eta_{\text{ohm}} - \eta_{\text{con}} - \eta_{\text{act}} \quad (1)$$

where η_{act} is the activation overpotential for the electrochemical reactions, η_{con} is the concentration polarization due to the resistance for the gas transport in porous electrodes, η_{ohm} is the ohmic overpotential and E_0 is the open circuit potential. The open circuit potential of the fuel and oxidant used may be calculated as:

$$E_0 = -\frac{\Delta G^0}{2F} + \frac{RT}{2F} \ln \frac{p_{\text{H}_2}^0 (p_{\text{O}_2}^0)^{0.5}}{p_{\text{H}_2\text{O}}^0} \quad (2)$$

where ΔG^0 is the free energy change of the reaction $\text{H}_2 + 0.5\text{O}_2 \rightleftharpoons \text{H}_2\text{O}$ at the working temperature and when the partial pressures of all the reacting gas species are 1 atm [34].

The concentration polarization (η_{con}) is the sum of the concentration polarizations of anode, $\eta_{\text{con}}^{\text{a}}$, and cathode, $\eta_{\text{con}}^{\text{c}}$. They may be calculated as:

$$\eta_{\text{con}}^{\text{a}} = \frac{RT}{2F} \ln \left(\frac{p_{\text{H}_2}^0 p_{\text{H}_2\text{O}}}{p_{\text{H}_2} p_{\text{H}_2\text{O}}^0} \right) \quad (3)$$

$$\eta_{\text{con}}^{\text{c}} = \frac{RT}{2F} \ln \left(\frac{p_{\text{O}_2}^0}{p_{\text{O}_2}} \right)^{0.5} \quad (4)$$

where p_{H_2} ($p_{\text{H}_2\text{O}}$) and $p_{\text{H}_2}^0$ ($p_{\text{H}_2\text{O}}^0$) denote the partial pressure of H₂ (H₂O) at the anode three phase boundary (TPB) and the anode-fuel channel interface, respectively. p_{O_2} and $p_{\text{O}_2}^0$ are respectively the partial pressure of O₂ at the cathode TPB and the cathode–air channel interface.

The ohmic overpotential includes the electronic and ionic ohmic overpotentials of the anode, cathode and electrolyte and the contact overpotential due to contact ohmic resistance at the interface of different cell components, which may be written as:

$$\eta_{\text{ohm}} = \eta_{\text{ohm}}^{\text{a,e}} + \eta_{\text{ohm}}^{\text{a,i}} + \eta_{\text{ohm}}^{\text{c,e}} + \eta_{\text{ohm}}^{\text{c,i}} + \eta_{\text{ohm}}^{\text{ele,i}} + \eta_{\text{ASR}} \quad (5)$$

Here $\eta_{\text{ohm}}^{\text{a,e}}$ and $\eta_{\text{ohm}}^{\text{c,e}}$ are the electronic ohmic overpotentials of the anode and the cathode, respectively. $\eta_{\text{ohm}}^{\text{a,i}}$, $\eta_{\text{ohm}}^{\text{c,i}}$ and $\eta_{\text{ohm}}^{\text{ele,i}}$ are

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