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Modeling of an anode supported solid oxide fuel cell focusing on thermal stresses

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ABSTRACT

A mechanical failure of a single component is sufficient to cause a solid oxide fuel cell (SOFC) breakdown. As an unfavorable issue for interfering the stable operation of SOFCs, thermal stress stemming from temperature gradient and mechanical mismatch can result in crack damage. Therefore, it is strongly significant to clarify the relationship of mechanical properties of the cell materials with distribution of the stress by taking into account the electrochemical reactions. A complete three-dimensional model for a planar anode-supported SOFC has been proposed and established in this study, which includes governing equations for momentum, gas-phase species, heat, electron and ion transport. The thermal gradients caused by the electrochemical reactions and heat transport processes of the counterflow leading to a maximum thermal stress is slightly larger than that is induced by the coflow. The influence of mechanical mismatch is analyzed and the results indicate that the strength of stress at two sides of a cell tends to be enlarged under fixed constraint conditions. Furthermore, the functional buffer layers can affect the stress between different components and inhibit the extent of degradation. This investigation is expected to offer a path to improve the matches of SOFC components and optimize the stack design.

Introduction

Fuel cells are believed to contribute to a significant fraction of the future power generation because of its high efficiency and low emissions of pollutants [1,2]. Among various types of fuel cells, the high temperature solid oxide fuel cell (HTSOFC) has many extendable advantages compared to other conversion devices due to its solid-state structure, fuel flexibility and non-necessity of precious metal catalysts [3,4]. The intermediate temperature solid oxide fuel cell (ITSOFC) has also gained considerable attentions for the alleviation of degradation arising from high temperature instability, reduced sealing problems and lower cost of components, beneficial to accelerate the commercialization of SOFC technology [5,6]. The typical operating temperature of a compact and planar ITSOFC is 600–800 °C, which minimizes the polarization losses and increases the tolerance to poisoning of fuel impurity [7,8]. However, severe thermal stress is still a concern to affect the lifetime of a single cell.

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A major challenge for SOFCs lies in balancing the thermal stresses from an inevitable thermal field causing the material to creep, rupture and crack at a typical SOFC operating condition. The mechanical failure of one cell is adequate to lead to malfunction of a stack. The rupture and cracks often occur to the planar solid oxide fuel cell (PSOFC) elements due to the mechanical mismatch and the fragile nature of ceramic [9]. Understanding the distribution of thermal stresses, induced in part by the stresses within the different components, is crucial to interpret the mechanism of mechanical failures and significant to the structural design of fuel cells, helpful for broadening the field of potential applications [10].

Thermal stresses within SOFCs have attracted increasing attentions in recent years. Half-cells (i.e., without the cathode side) were tested in situ to evaluate the limit of maximum anode stress, by assessing the necessary load to achieve a best contact on the electrode side of the cell using a pressure sensitive foil [11]. The biaxial flexure was used to obtain the residual stresses by observing the bending after removal of one electrode [12] and residual stresses in an anode-supported planar SOFC were also measured by X-ray diffraction to confirm the global and local macroscopic stress trend of the electrolyte [13]. Meanwhile, Malzbender et al. conducted ring-on-ring bending tests in an Instron 1362 machine (the European standard) [14]. However, experimental measurements of stresses are impossible to be realized at a real SOFC operating conditions owing to a high operational temperature. Since the thermal stress is closely related to electrochemical reactions like reforming inside a fuel cell, it is thus promising to establish a model by including endothermic and exothermic reactions etc. [15].

Numerical studies have become more and more important for fuel cell development and research in optimizing the design and operation parameters [16–19]. A 3D model was implemented to study the influence of foil thickness on residual stress in the bonded compliant seal design of planar solid oxide fuel cell and the results showed that the peak residual increased with the foil thickness increase [20]. Models have been developed to investigate the thermal stress within SOFCs based on delamination and transgranular fracture. Selimovic et al. developed the steady-state and transient thermal stress for a cross flow planar SOFC simulated using an in-house code by coupling the electrochemical, thermal and structural modeling [21]. Fluent and Abaqus were combined to study the thermal stress distribution and temperature profile, indicating anode is subjected to large tensile stresses and electrolyte is subjected to large compressive stresses [22].

The high thermal gradients, caused by the uneven distribution of heat sources and the heat transport process, tend to generate thermal stress, but it cannot result in a state of thermal shock compared to a spatially uniform thermal loading [23]. Hence, this research focuses on thermal stresses by comparing counterflow and coflow modes that can both cause thermal gradients with the same operating conditions, where we also take into account the exothermic electrochemical reactions occurring to the single cell.

Moreover, the effects of functional layers are included in this model. C. K. Lin et al. focused on the stack structure where the cross-plane of different components in single cell was neglected. In most cases, the mass and heat transport, electrochemical reaction inside the single cell were also not taken into account [24,25]. Similarly, L. K. Chiang et al. did not concentrated on the bilayers in previous works [26,27]. Since the layers are bond to the other components, mismatch in thermal expansion of the materials can result in the formation of thermal stresses, which is reflected in the curvature of the cells. The active layer can be fabricated using freeze-drying tape-casting combined with infiltration, drop-coating or spraying process [28–30]. The use of an active layer reduced cell resistance and increased power density. A dense structure (means low porosity) for active layers with approximated thermo-elastic properties and guaranteed sufficient porosity or only partial coverage of the free surface should be thus applied in a thermomechanical model. A functional layer cannot only offer sites for electrochemical reactions, but it will reduce the mismatch of the different materials induced by a temperature gradient and then relax the thermal stress or the chemically derived stress within electrolytes.

This work aims to investigate the stress fields arising in a planar anode supported cell at a simulated operational conditions. In this model, interconnects are fixed and securely bonded to the electrodes. To model the fixing situation in a stack, different fixed constraints is compared, which can be deemed as a reference for a practical application. A spatial temperature distribution profile is studied by solving the governing equations for electron, ion, heat, gas-phase species and the momentum transport, coupled to kinetics regarding the electrochemical reactions. After elaboration, a high residual compressive stress is calculated for the thin electrolyte layer. A slight tensile stress is proposed in the anode, in the vicinity of the anode/electrolyte interface.

Mathematical model

Stress analysis of an SOFC was performed using the commercial software COMSOL Multiphysics (version 5.0). A half-cell model with bipolar channels operating with humidified hydrogen, carbon monoxide and methane as fuel. The sketch of the model geometry for counterflow, not to scale, can be seen in Fig. 2(b). Note that, the co-flow geometry is the same as counter-flow while the fuel flow direction is in contrast. It should be also noted that we have assumed some boundaries of this single cell model to be constrained, i.e., the geometric entity is fixed and the displacements are zero in all directions. If a prescribed displacement is not settled in any direction, it is the same as a free constraint. This constrained case can be treated as the load operation for a situation where the single cell is fixed among stack equipment. Under the constraints of the interfaces, thermal stresses are generated to keep the size and interface continuous.

Electrochemical model

The reactions inside the SOFC are shown in Eqs.(1)–(5). Carbon monoxide is oxidized in the electrochemical reaction (Eq. (3)), but reacts faster with water in the water–gas shift reaction (WGSR) [31], as seen in Eq. (5) and Methane steam reforming (MSR) [32], as shown in Eq. (4).