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Numerical study on thermal stresses of a planar solid oxide fuel cell

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ABSTRACT

A three-dimensional (3D) finite element model consists of positive electrode–electrolyte–negative electrode (PEN) and metallic interconnect (MIC) assembly is constructed by using commercial finite element software Abaqus. With the simulated temperature profile in the planar solid oxide fuel cell (SOFC), the finite element method is employed to calculate the thermal stress distribution in a planar SOFC. The effects of temperature profile, electrodes and electrolyte thickness, and coefficients of thermal expansion (CTEs) mismatch between components are characterized. The value and distribution of thermal stress are the functions of the applied materials CTEs, applied temperature profiles and thickness of anode and electrolyte. The calculated results can be applied as the guide for SOFC materials selection and SOFC structure design. The anode is subjected to large tensile stresses and the electrolyte is subjected to large compressive stresses during the first cooling from the sintering temperature. The chemical reduction of NiO to Ni in the porous anode lowers the absolute stress level in the PEN structure by 20%. The large tensile stresses in the anode and the large compressive stresses in the electrolyte relax partly when the SOFC operates at high temperature. Cracks could probably appear in the anode structure when the PEN structure is cooling to room temperature after the sintering.

1. Introduction

Fuel cells are the most efficient devices for the electrochemical conversion of chemical energy of hydrogen into electricity, and have been gaining increasing attention in recent years for environmentally friendly with little or no toxic emission and efficient distributed power generation. In the existing fuel cells, the solid oxide fuel cell (SOFC) with monolithic, planar and tubular geometries, as a high temperature fuel cell, makes a good performance in power generation and continues to show great promise as a future power source. In SOFC stack designs, the planar type design has received much attention recently, because it is simpler to fabricate and easier to be made into various shapes than the other type designs. Besides, the planar type SOFC offers higher power density relative to the tubular type SOFC due to the low electrical resistance as a result of the shorter current paths. A typical operating temperature of a solid oxide fuel cell is 600 °C–1000 °C, which leads to severe thermal stresses and warpage on the positive electrode–electrolyte–negative electrode (PEN) structures of SOFCs caused by the mismatch of the coefficients of thermal expansion (CTEs) of various layers in the PEN structures of SOFCs due to the temperature changes during the PEN manufacturing process and thermal cycling. And these may lead to cracks and destroy the SOFC structure.

Numerical studies were conducted by many investigators on electric performance of SOFC using simplified electrochemical models [1–3], e.g. the Tafel equation, which is linear of Butler-Volmer equation, is widely used for activation polarization calculation. For the model of concentration polarization, the Knudsen diffusion was neglected for gas diffusion through the porous electrodes [2,3]. Ferguson et al. [4] presented a numerical model with solving both flow equations and potential equation for various geometries of SOFCs. The thermo-fluid analysis of a planar SOFC was performed using the computational fluid dynamics tool `STAR-CD' by Yakabe et al. [5]. Since SOFCs operate at high temperature and the cell scale is tiny, experimental studies on the thermal stresses is difficult. The X-ray computer tomography was used to permit an assessment of the maximum defect size by Malzbender et al. [6]. The residual stress in the electrodes was estimated by curvature measurement by Selcuk et al. [7]. The X-ray diffraction method was used to measure the residual stresses in the electrolyte of the anode-supported cell by Yakabe et al. [8] and Fischer et al. [9]. Most advanced researches of thermal stresses of SOFC were made

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by establishing computer models and numerical simulations. Numerical studies for SOFC thermal stresses were conducted by different investigators. A two-dimensional model, based on the finite volume method, was developed in FORTRAN for simulation of a planar electrolyte supported SOFC by Selimovic et al. [10]. A 2-D mathematical model was developed to estimate the thermal stresses and to predict the lifetime of the cell [11] and the Weibull theory was used to predict the risk of cell degradation based on the 2-D calculation of stress field [12]. A stack modeling framework that combines thermo-electrochemical models, including degradation and a contact finite-element thermo-mechanical model based on an anode-supported SOFC was used to study the mechanical reliability and durability of SOFC stacks by Nakajo et al. [13,14]. The ANSYS software was used to carry out three-dimensional (3D) finite element analyses of SOFC bonded compliant seal designs by Weil et al. [15] and Jiang et al. [16].

The purpose of the present work is to study the thermal stresses in the SOFC components using a three-dimensional (3D) model simulation. In order to derive the stresses, a 3D numerical model of SOFCs for various geometries with complete polarization is employed in this study including methane reforming and the water-gas shift. This model is coupled with the governing equations through the user defined function (UDF) interface provided by the commercial computational fluid dynamics (CFD) software, Fluent. Transport equations for mass, momentum, species, energy and electrical potential are solved using the software, Fluent. The electric characteristics of the conductive components and the profile characteristics of the temperature for the planar configured SOFC are studied. A 3D finite element thermal stresses model consists of PEN and interconnects assembly is constructed by using the commercial finite element analysis (FEA) software Abaqus based on the temperature profile in the planar SOFC calculated by the electrochemical model. The effects of temperature profile, electrodes and electrolyte thicknesses and CTE mismatches between components are characterized. The calculated results can be applied as the guide for the SOFC materials selection and the SOFC structure design to improve the SOFC structural performance and its reliability.

2. Mathematical model

2.1. Model geometry

A fuel cell stack modeling exercise was conducted by International Energy Agency (IEA) involving seven European countries and Japan in 1995. Two cases of SOFC stack operation were simulated: (1) one cell stack operating with humidified hydrogen fuel and air feed and (2) one cell stack operating with direct internal steam reforming of methane and air. These two cases were called “Benchmark Test 1” and “Benchmark Test 2” in the IEA database. In this work, a simplified single unit cell model with bipolar channels is studied. Furthermore, since the geometry of the single unit is symmetric, only half of the one repeating unit is simulated. The configuration of a half unit cell is illustrated in Fig. 1. Both co-flow and counter-flow planar SOFC are modeled in this work. The geometrical parameters of a single cell for the calculation are given as follows: channel reaction area 3 mm × 100 mm, channel height 1 mm, underneath MIC reaction area 2.42 mm × 100 mm, MIC rib width 2.42 mm, electrolyte thickness 150 μm, anode thickness 50 μm, cathode thickness 50 μm, and bipolar plate thickness 2.5 mm. As shown the half unit cell in Fig. 1, the active area in the numerical computation contains a half channel reaction area and a half underneath MIC reaction area, which equals to2.71 mm × 100 mm. The permeability of the porous electrode is 1×10^{-8}/m and the porosity is 0.2.

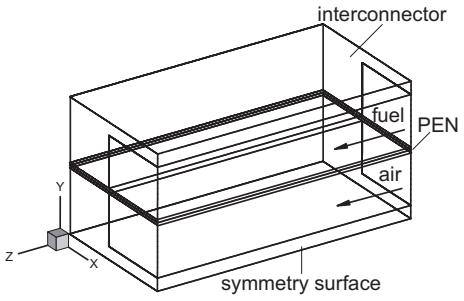

Fig. 1. The model geometry of the half single unit cell for the planar SOFC.

2.2. Electrochemical model

The electrochemical reactions taken into account in the SOFC are as follows:

$$\text{Anode side}: H_2 + O^{2-} \rightarrow H_2O + 2e^-$$

$$\text{Cathode side}: 1/2O^2 + 2e^- \rightarrow O^{2-}$$

$$\text{Overall reaction}: H_2 + O^{2-} \rightarrow H_2O + 2e^-$$

For the internal steam reforming of the SOFC, the reforming reaction and water-gas shift reaction are added within the anode:

$$\text{Methane steam reforming}: CH_4 + H_2O \rightarrow CO + 3H_2$$

$$\text{Water} - \text{gas shift}: H_2O + CO \rightarrow CO_2 + H_2$$

Electrochemical reactions were assumed to occur at the interfaces between electrodes and electrolyte. The shift reaction is fast enough and in this model we assume that the shift reaction is in chemical equilibrium in the anode.

As an energy conservation system, the voltage generated by the SOFC can be calculated by combining the energy conservation and entropy balance of the electrochemical reaction for the SOFC [17]. A complete polarization model is employed in this paper [18]. The voltage generated by SOFC is modeled as

$$E_v = -\frac{1}{z_e F}\left[\sum_i (\lambda_i g_i)_p - \sum_i (\lambda_i g_i)_r\right] - (\eta_{act} + \eta_{conc} + \eta_{ohm}) \tag{1}$$

where

$$g_i(T, p_i) = h_i(T) - Ts_i(T, p_i) = \int_{T_0}^{T} c_{pi}(T)\mathrm{d}T - T\int_{T_0}^{T} \frac{c_{pi}(T)}{T}\mathrm{d}T - RT\ln\frac{P_0}{p_i} \tag{2}$$

In the SOFC, the voltage losses include the activation polarization η_{act}, concentration polarization η_{conc} and ohmic polarization η_{ohm}.The activation polarization is the energy barrier existing between the electronic and the ionic conductors in the electrochemical reaction. The activation polarization occurs at both electrodes in all ranges of current density. It is calculated by the Butler–Volmer equation [26]. The transfer coefficient β is assumed to 0.5 in this work, the activation polarization can be calculated by