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Numerical study on the mechanical stress and mechanical failure of planar solid oxide fuel cell

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HIGHLIGHTS

- A solid mechanics model combined with fully coupled flow-heat-mass-current transport.
- Simulations based on and validated by the newest experimental data.
- Effects of Ni content and oxidation state on stress and failure probability revealed.
- Importance of reducing temperature gradient for the increased lifetime illustrated.

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ABSTRACT

Damage by mismatch of thermal expansion coefficients and temperature gradient is a major factor limiting the long-term stability of solid oxide fuel cell (SOFC). Numerical simulations are performed to provide in-depth information about the mechanical stress, mechanical failure probability and creep strain rate of planar SOFC. The dependences of the mechanical performance of SOFC on the Ni content and its oxidation state as well as the temperature (T) are revealed. Based on a realistic T-profile obtained by multi-physics simulation of a SOFC stack model, it is shown that the maximum creep strain rate of the operating stack is 40% higher than that of an isothermal stack with the same average T. A T-distribution deduced from a multi-physics fully coupled model is essential for a reliable prediction of the creep rate and the corresponding lifetime of an operating stack.

1. Introduction

Solid oxide fuel cell (SOFC) is an attractive electricity generation device due to their advantages of high electrical energy conversion efficiency [1], low environmental pollution [2] and fuel flexibility [3]. The planar design of SOFC is widely studied for its high power density [4]. However, the planar design is also prone to thermal stress induced mechanical failure, hindering its commercialization [5].

A typical anode-supported planar SOFC consists of a thick porous composite anode, a thin dense electrolyte, a thin porous composite cathode as well as bipolar interconnect and sealant materials [6]. The mismatch of thermal expansion coefficients (TECs) of these materials necessarily induces thermal stress that can cause mechanical failure. Moreover, creep strain is inevitable during the long-term operation of SOFC, limiting its service lifespan. To be commercially viable, it is critically important to choose material, structural and operating parameters that avoid high mechanical stress, reducing the possibility of mechanical failure and extending the operation lifetime. This requires an exploration of a huge parametric space to identify the desirable combinations. As experiments are expensive and time consuming, they are unsuitable for exploring the parametric space. Besides, it is difficult to conduct mechanical measurements during the high temperature operations of SOFCs. Consequently, mathematical simulations [7] incorporating the known physics and material parameters to predict the thermal stress and mechanical failure probability are invaluable for the understanding and development of the SOFC technology [8].

A number of mechanical stress analyses of SOFCs with varying degrees of complexity have been reported in the literature. Some studied the residual stresses within the cathode-electrolyte-anode, or positive-electrolyte-negative (PEN), assembly at the room temperature [9], or the thermal stress at the operating temperature under an isothermal condition [10,11]. Others performed the thermal stress analysis with the temperature profiles obtained through employing some coupled thermo-electrochemical models of SOFCs [12]. Generally, these studies

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considered only a given set of material property parameters. A systematic study on the dependence of the thermal stress distribution on the electrode compositions such as the Ni content and the effect of anode porosity is still lacking. Moreover, the existing results are often obtained by assigning the sintering temperature as the stress free temperature [13]. Considering the recent results that the stress free temperature should be the reducing temperature [14], the mechanical analysis should be revisited.

Creep strain rate calculations have been used for the prediction of the mechanical failure time of SOFCs [15,16]. The creep strain rate depends on the thermal stress and mechanical properties of the materials [17,18]. Consequently, the existing study on the creep strain rate analysis suffers from the same limitations of the existing thermal stress analysis, i.e., based on an incorrect assumption about the stress free temperature and with no consideration about the variation of the material compositions. The former means that the result may be misleading. The latter means that the result, even if approximately correct, is not informative for the design optimization of the composite electrode materials. Besides, the study of the creep strain rate of SOFCs under operating conditions is rather rare and more studies are required.

This paper reports an in-depth analysis of the mechanical performance of planar SOFCs consisting of the typical material set of Ni-YSZ anode, YSZ electrolyte and LSM-YSZ cathode. The most recent experimental data are incorporated in the mechanical model and the simulation results are compared with experiments where available. The effects of anode Ni content, Ni oxidation-reduction state and operating temperature on the mechanical stress, failure probability and creep strain rate of SOFC are examined systematically. In addition, the creep strain behavior of operating SOFC stack is investigated with a realistic temperature profile deduced from a multi-physics fully coupled stack model. The approach of combining a coupled flow, heat, mass and current transport with a solid mechanics model is an important step towards fully understanding the mechanical failures of operational SOFC stacks.

2. Computational method

A standard structural mechanics model with a set of properly chosen material properties is used to determine the mechanical stress distributions of SOFCs. The obtained stress distributions are then used to compute the mechanical failure probabilities and creep strain rates of the SOFC components.

2.1. Structural mechanics model

According to the theory of elasticity [19], the stress-strain relationship can be expressed as,

$$\sigma = D\varepsilon_{el} + \sigma_0, \tag{1}$$

where σ is the stress tensor, D is the elasticity matrix, ε_{el} is the elastic strain tensor. σ_0 is the initial stress tensor.

The total strain, ε, generally consists of four components,

$$\varepsilon = \varepsilon_{el} + \varepsilon_{th} + \varepsilon_c + \varepsilon_0, \tag{2}$$

where ε_{th} is the thermal strain, ε_c is the creep strain and ε_0 is the initial strain.

D for an isotropic material is defined as [20]:

$$\mathrm{D}= \frac{\mathrm{E}}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix} \tag{3}$$

where E is the Young's modulus and υ is the Poisson's ratio of the material defined by:

$$\upsilon = \frac{E}{2G} - 1, \tag{4}$$

where G is the shear modulus of the material.

The thermal strain can be computed with,

$$\varepsilon_{th} = \alpha(T - T_f) \tag{5}$$

where α is the temperature dependent thermal expansion coefficient (TEC), T is the temperature and T_f denotes the stress free temperature.

The three-dimensional (3D) structural mechanics model is solved with the following boundary conditions: (1) Bonding-contacts for the anode-electrolyte-cathode assemble, (2) tight-contact and no separation between PEN and interconnect. Besides, it is assumed that there is no constraint or force applied on the outer surface of the cell/stack. The assumption is reasonable as the load on a stack is typically of the order of 1 MPa or less [21] and inconsequential to the results obtained in this study. The whole computational domain is set to be free deformation. The 3D structural mechanics model, together with the above boundary conditions, was solved by the finite element commercial software ANSYS® [22].

2.2. Effective material property model

Mechanical property parameters of the SOFC components are required to solve the structural mechanics model. The anode and cathode are porous composite materials. The effective properties of the porous composite anode and cathode materials are determined in two steps.

First, the mechanical parameters of dense composite material are calculated using the composite sphere method (CSM) [23]. CSM treats the composite material as a spherical matrix of one phase and the spherical impurities of the other phase that are concentrically placed in the matrix. The bulk and shear moduli of the dense composite material are computed as,

$$K_{dense} = K_2 + \frac{V_1}{1/(K_1 - K_2) + 3V_2/(3K_2 + 4G_2)} \tag{6}$$

$$G_{dense} = G_2 + \frac{V_1}{1/(G_1 - G_2) + 6V_2/(3K_2 + 2G_2)/[5G_2(3K_2 + 4G_2)]} \tag{7}$$

where K_{dense} and G_{dense} corresponds respectively to the bulk and shear modulus of the dense composite material (K= $E/3(1-2\nu)$). V_i is the volume fraction of the matrix ($i = 1$) or the impurity ($i = 2$) phase in the composite material. The results of Eqs. (6) and (7) depend on which material phase is assumed to be the matrix or the impurity, but the higher values are the recommended ones [23].

Second, the effects of porosity on the mechanical properties are determined by the method of Ramakrishnan and Arunachalam [24]. In this method, the effective Young's modulus, shear modulus and Poisson's ratio for the porous composite medium are calculated as,

$$E_{porous} = E_{dense} \frac{(1-\varphi)^2}{1 + (2 - 3\nu_{dense})\varphi} \tag{8}$$

$$G_{porous} = G_{dense} \frac{(1-\varphi)^2}{1 + (11 - 19\nu_{dense})/(4 + 4\nu_{dense})\varphi} \tag{9}$$

$$\nu_{porous} = \frac{1}{4} \frac{4\nu_{dense} + 3\varphi - 7\nu_{dense}\varphi}{1 + 2\varphi - 3\nu_{dense}\varphi} \tag{10}$$

where φ is the porosity of the medium. The subscripts "porous" and "dense" are used to denote quantities for porous and dense materials, respectively.

The effective TEC of the composite material is calculated as [25],

$$\alpha = \sum_i \left[\alpha_i V_i + 4 \frac{G_m}{K_m} \frac{K_m - K_i}{4G_m + 3K_i} (\alpha_m - \alpha_i) V_i \right] \tag{11}$$

Notice that the effect of porosity on α is negligible [26].