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Evolution of thermal stress and failure probability during reduction and re-oxidation of solid oxide fuel cell

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HIGHLIGHTS

- The stress and failure probability are studied during reduction and re-oxidation.
- The first paper to study the effect by using a three dimensional model.
- The stress varies mainly due to the change of volume rather than porosity.
- The re-oxidation significantly increases the stress and failure probability.
- The volumetric contraction during the reduction helps to decrease the stress.

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ABSTRACT

The reduction and re-oxidation of anode have significant effects on the integrity of the solid oxide fuel cell (SOFC) sealed by the glass-ceramic (GC). The mechanical failure is mainly controlled by the stress distribution. Therefore, a three dimensional model of SOFC is established to investigate the stress evolution during the reduction and re-oxidation by finite element method (FEM) in this paper, and the failure probability is calculated using the Weibull method. The results demonstrate that the reduction of anode can decrease the thermal stresses and reduce the failure probability due to the volumetric contraction and porosity increasing. The re-oxidation can result in a remarkable increase of the thermal stresses, and the failure probabilities of anode, cathode, electrolyte and GC all increase to 1, which is mainly due to the large linear strain rather than the porosity decreasing. The cathode and electrolyte fail as soon as the linear strains are about 0.03% and 0.07%. Therefore, the re-oxidation should be controlled to ensure the integrity, and a lower re-oxidation temperature can decrease the stress and failure probability.

1. Introduction

Solid oxide fuel cells (SOFC) are efficient devices for the conversion of chemical energy into electricity, which have received sustained attention in recent years [1]. However, since the operating condition is harsh, the durability and structural integrity at high temperature are the main challenges for their commercialization [2].

For high efficiency, high operating temperature is adopted for the anode-supported SOFC. In this case, severe thermal stresses could arise due to the mismatch of mechanical properties of materials, temperature gradients and reduction-re-oxidation reactions [3–5]. Such thermal stresses can lead to performance degradation and mechanical failure of SOFC [6–9]. The thermal stresses induced by the coefficient of thermal expansion (CTE) mismatch and temperature gradient have been widely studied [10–14]. Another important factor affects the fracture is the reduction/re-oxidation. Malzbender et al. [15] observed that cracks predominantly located along and near the glass-ceramic sealant during the reduction/re-oxidation, and the cracks were larger in the anode substrate, but could also be detected in the electrolyte. The redox cycling causes remarkable thermal stresses, leading to severe damage and even complete loss of integrity [16,17].

Nickel doped-yttria stabilized zirconia (Ni-YSZ) is widely used as the material of anode in SOFC due to its high activity, high electrical conductivity and relatively low cost, but the presence of Ni can result in undesirable chemically induced strain when the anode is re-oxidized [18,19]. After fabrication, Ni-based anode cermet is in oxidized state.

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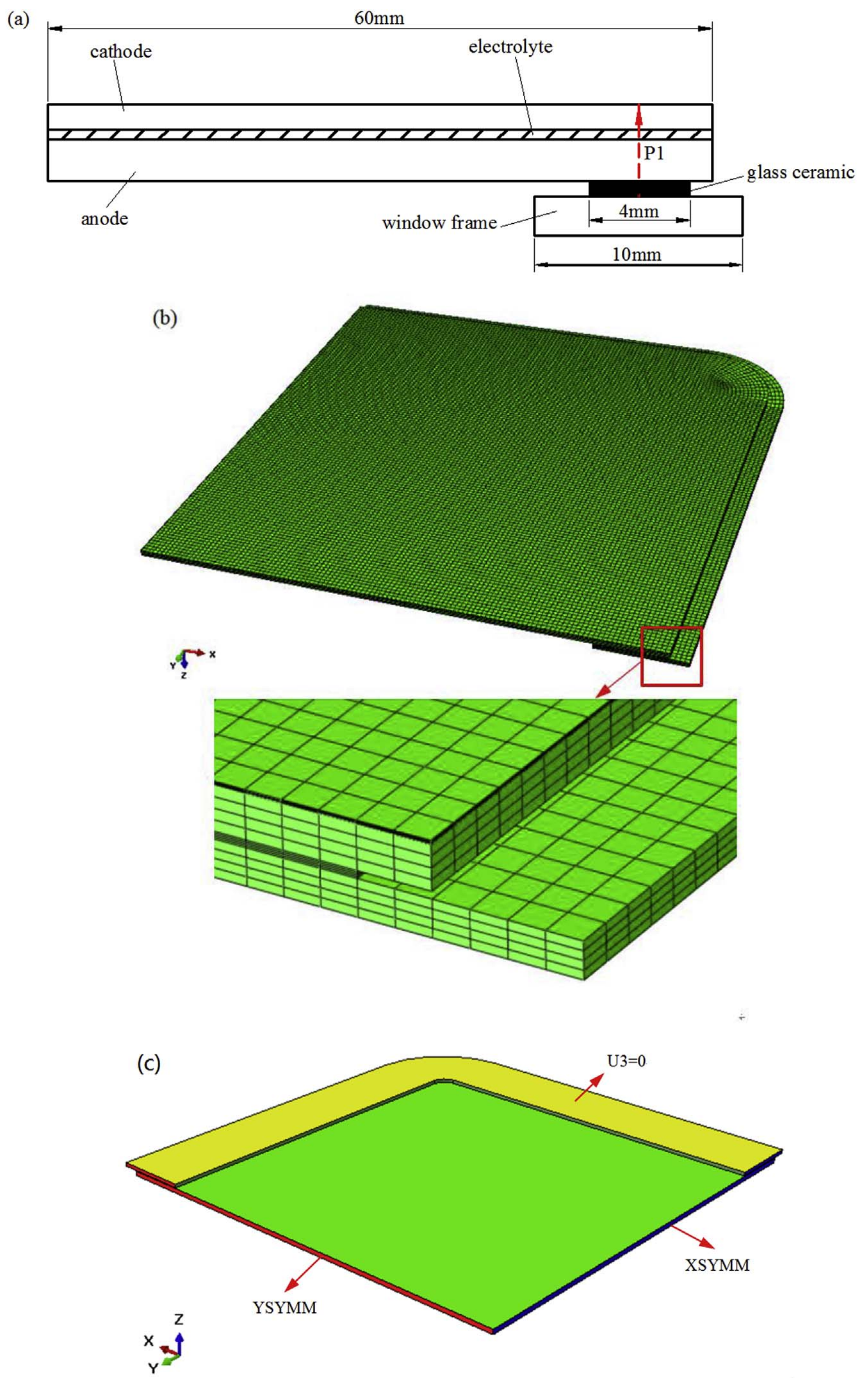

Fig. 1. Sketching (a), finite element meshing (b) and boundary conditions (c) of the planar SOFC.

During operation, nickel-oxide (NiO) changes into Ni when the anode is supplied with fuel H_2. As a result, the porosity of anode is increased since the volume of Ni is smaller than that of NiO [20]. Both the contraction and negligible dimensional change of anode were detected due to the different as-sintered porosity of anode [21]. Once the fuel supply is interrupted at high temperature, or the fuel supply becomes insufficient, oxidation of anode will occur [22]. With nickel oxidizing and the solid volume expansion, the porosity decreases and the elastic modulus increases [23]. The change of porosity has a great influence on the mechanical properties of NiO-YSZ. Linear, exponential and non-linear correlations have been proposed to express the dependence of Young's and Shear modulus on the volume fraction of porosity [24]. Biswas et al. [25] found that the hardness and elastic modulus of the Ni-based anode are severely decreased when the porosity increased from 12% to 36.68%. Luo et al. [26] found that the increase of porosity can decrease the thermal stress and thus reduce the failure probability. The volume expansion of the anode due to nickel oxidation yields stresses that are proportional to the expansion in different layers [26]. Sarantaridis and Atkinson [27] developed a mechanical model of the stress and damage caused by expansion upon oxidation based on the release of stored elastic energy under plane strain conditions. The electrolyte would crack if the linear strain of anode exceed 0.1–0.2%, and Laurencin et al. [28] found that the cathode and electrolyte fracture when the anodic strain exceeds 0.09% and 0.15%, respectively. Toros [29] found that the re-oxidation and the stresses generated within the anode relies on the temperature of re-oxidation. The stresses in anode generated by re-oxidation are significantly higher than the fracture strength of the materials, leading to the fracture of anode and failure of SOFC.

Although the effects of re-oxidation on failure have been studied by J. Malzbender [15] and D. Sarantaridis [23], the stress evolution in the