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Thermal stress and probability of failure analyses of functionally graded solid oxide fuel cells

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ABSTRACT

Thermal stresses and probability of failure of a functionally graded solid oxide fuel cell (SOFC) are investigated using graded finite elements. Two types of anode-supported SOFCs with different cathode materials are considered: NiO-YSZ/YSZ/LSM and NiO-YSZ/YSZ/GDC-LSCF. Thermal stresses are significantly reduced in a functionally graded SOFC as compared with a conventional layered SOFC when they are subject to spatially uniform and non-uniform temperature loads. Stress discontinuities are observed across the interfaces between the electrodes and the electrolyte for the layered SOFC due to material discontinuity. The total probability of failure is also computed using the Weibull analysis. For the regions of graded electrodes, we considered the gradation of mechanical properties (such as Young's modulus, the Poisson's ratio, the thermal expansion coefficient) and Weibull parameters (such as the characteristic strength and the Weibull modulus). A functionally graded SOFC showed the least probability of failure based on the continuum mechanics approach used herein.

1. Introduction

A solid oxide fuel cell (SOFC) is an electrochemical device, which converts the chemical energy of hydrocarbon fuels into electrical power at elevated temperatures [1,2]. It has recently received increasing attention due to its high power density, fuel flexibility, and strong potential for generating electricity and heat for industry and auxiliary power in vehicles. In addition to high-temperature (HT) SOFCs, intermediate-temperature (IT) SOFCs have also gained considerable attraction. A reduced operating temperature allows low cost metallic interconnects [3], helps avoid material compatibility challenges pervasive at high temperatures [4], reduces sealing and thermal degradation problems [5], and eventually accelerates the commercialization of SOFC technology. The mechanical strength of SOFC components is one of the key issues for determining their performance and reliability under transient and steady-state thermal loading. Stresses in SOFC components can arise from manufacturing process (e.g. residual stresses); mismatch in thermal expansion coefficients (TEC) of cell components; spatial or temporal temperature variations; oxygen activity gradients; redox cycling, and external mechanical loading. The magnitude of stresses depend on material properties, operating conditions and geometry of the cell design [6]. Stresses caused by thermal gradients and TEC mismatch tend to increase with increasing in-plane dimensions. Further, SOFC stacks are usually clamped during operation in order to secure proper alignment and good contact between the cell components. This, together with the seals required around the edges of planar cells to separate the fuel and air compartments, can cause higher mechanical stresses transmitted to brittle elements in the stacks.

Selimovic et al. [6] studied steady state and transient thermal stresses caused by spatial and temporal temperature gradients and TEC mismatch. Nakajo et al. [7] studied mechanical issues in a standard SOFC repeat unit with an anode-supported cell during assembly, heat-up, current–voltage (IV) characterization, dynamic operation, load shutdown and cool-down phases using a thermo-electrochemical model. They also calculated the probability of failure of the cells using the Weibull method [8]. Laurencin et al. [9] developed a numerical tool to study the risk of cell failure due to residual stresses arising after the manufacturing process, at both operating temperature and after anode re-oxidation, and also due to the presence of material singularity like crack. Lin et al. [10] performed finite element analysis to predict thermal stress distribution in a planar SOFC stack at various stages using a temperature field obtained from an integrated thermo-electrochemical model [11]. Khaleel et al. [12] developed an electrochemisty module to supplement the capability of commercial finite element analysis package MARC to model SOFCs. Williford and Singh [13] developed a two-layered porous high performance cathode design as a means of exploring new microstructure and material options for SOFCs.

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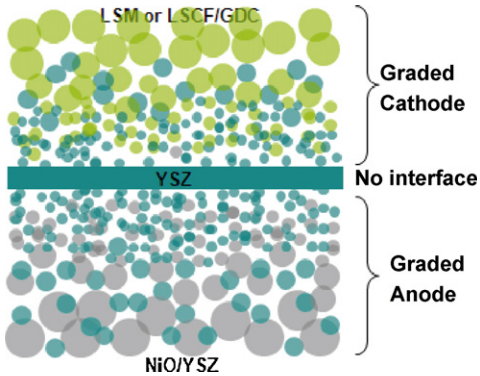

Fig. 1. Schematic of a unit cell SOFC with graded electrodes.

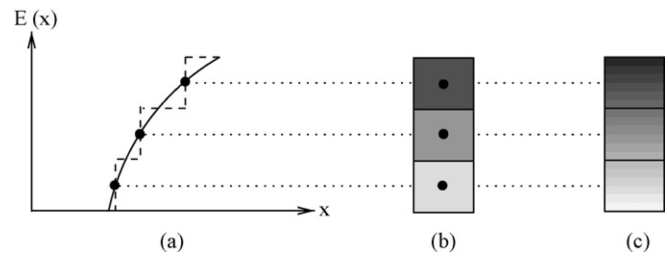

Fig. 2. Homogeneous vs. graded finite elements. (a) Property variation along the x-axis; (b) homogeneous elements; (c) graded elements. Note that the property of the homogeneous element corresponds to the property at its centroid [26].

For a traditional layered SOFC with Strontium-doped Lanthanum Manganite (LSM) as the cathode and Yttria Stabilized Zirconia (YSZ) as the electrolyte, the performance is often limited by the oxygen reduction processes at the cathode [14–16]. In order to improve the SOFC performance, material composition and microstructural skeleton must be optimized to provide a higher density of active sites such as triple phase boundaries. Towards this end, several composite electrodes such as YSZ-LSM, LSM-GDC (e.g. $Ce_{0.8}Gd_{0.2}O_2$, Gadolinium Doped Ceria), and GDC-LSCF (e.g. (La,Sr)(Co,Fe)O_3, Lanthanum Strontium Cobalt Ferrite) have been developed to improve electrode reactions and increase triple phase boundaries [17]. Grading both the anode and the cathode electrodes will enhance interlocking between the electrodes and the electrolyte and may improve electrochemical performance. Fig. 1 shows schematic of a SOFC with graded electrodes utilizing the concept of a functionally graded material (FGM). Graded regions in both electrode sides are realized by varying its composition, microstructure and porosity. As the composition changes, so do the effective material properties, thereby avoiding sharp material discontinuities which may otherwise result in delamination during thermal cycling [17]. Zha et al. [18] showed that graded cathodes fabricated using a sol–gel/slurry coating process led to relatively low polarization resistance at intermediate temperatures. Ni et al. [19] found that grading both porosity and particle size in the electrodes are effective to enhancing SOFC performance. Holtappels and Bagger [20] showed that five and nine layer cathodes have better electrochemical performance than a conventional two layer cathode mainly because of gradation of the composition and microstructure. From a mechanical viewpoint, the use of FG electrodes would greatly improve bonding strength and compatibility between electrodes and electrolyte, reduce the magnitude of residual and thermal stresses, and may reduce the crack driving force [21–23].

During the operation of the solid oxide fuel cell, rapid start-up and shut-down may be necessary in portable and transportable applications which may lead to rapid temperature changes. Rapid temperature change leads to significant temperature differences between the surface and the mean body leading to a state of thermal shock. A thermal shock introduces stress in a material due to temperature differences between the surface and the interior, or between different regions of the body [24]. When a body is subjected to an external disturbance thermally by sudden contact or very rapid body heating, the dynamic effect then depends on the ratio of two significant times: the thermal time (t_T) over which significant change in the external disturbance takes place i.e. the time measuring the rapidity of temperature rise in the body, and the mechanical time (t_M) characterizing the wave propagation across the body. Inertia plays a significant role in thermoelasticity if the thermal time is of the same order as that of the mechanical time [25]. The transient nature of the temperature field in SOFC is partly due to the electrochemical reactions occurring in it. Although the temperature field in the SOFC is dynamic in nature when it goes through heat-up, steady state and shut-down phases, we can see that inertia does not play a significant role in the transient thermal stress analysis in the viewpoint of its temporal variation. As compared to high thermal gradients, a spatially uniform thermal loading can also create a state of thermal shock [25] in a body but the thermal time (t_T) has to be of the same order as that of the mechanical time (t_M). For the model considered in this paper, the mechanical time (=L/c, where L is the largest distance from the point where the external disturbance (thermal shock) occurs and c is the velocity of wave propagation) is of the order of few microseconds or lesser. This specific thermal shock problem is not quite relevant to SOFC applications.

The objective of this paper is to perform thermal stress and probability of failure analyses of functionally graded SOFC under spatially uniform and non-uniform temperature loads. We have not considered inertia effects and residual stresses the latter of which are specific to various steps of manufacturing processes and cell dimensions and configurations. All of the materials are assumed to behave as linear elastic and isotropic. Although SOFC electrodes are porous in reality, we modeled them as contiua with effective thermo-mechanical properties. We analyzed three-dimensional (3D) SOFCs consisting of NiO-YSZ/YSZ/LSM (LSM, $La_{0.8}Sr_{0.2}MnO_3$) and NiO-YSZ/YSZ/GDC-LSCF (GDC, $Ce_{0.8}Gd_{0.2}O_2$; LSCF, $La_{0.58}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta}$). We also studied a semi-functionally graded HT-SOFC which has functional layers placed between the electrodes and the electrolyte. The total probability of failure of the SOFC cell layers are computed using the Weibull analysis [8].

This paper is organized as follows. Section 2 presents 3D graded finite element formulation. Section 3 presents thermal stress analysis of layered, semi-FG, and FG SOFCs under spatially uniform and non-uniform thermal loads. Section 4 presents the probability of failure analysis of the SOFC using the Weibull analysis. Section 5 addresses conclusion and potential extension of the current work.

2. Three-dimensional graded finite elements

In this study, we used the displacement-based finite element method and graded finite elements [26] to model spatial material gradation using the direct Gaussian integration formulation. Fig. 2 shows graded finite elements compared with the conventional homogeneous finite elements. By means of the principle of virtual work, the element stiffness matrix ($\mathbf{k}^e$) and the equivalent nodal force vector ($\mathbf{f}^{ext}$) (under an initial strain (ε_0)) of a finite element are formulated as:

$$\mathbf{k}^e = \int_{\Omega} \mathbf{B}^T \mathbf{D}(\mathbf{x}) \mathbf{B} d\Omega, \quad \mathbf{f}^{ext} = \int_{\Omega} \mathbf{B}^T \mathbf{D}(\mathbf{x}) \, \varepsilon_0 \, d\Omega \tag{1}$$