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Microscopic Image-Based Finite Element Analysis of Porous Composite Cathode Microstructures

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Abstract

We reconstruct three-dimensional (3D) microstructures of porous ceramic composite cathodes of solid oxide fuel cells (SOFCs) using a series of two-dimensional (2D) images. We then discretize the reconstructed 3D models into 8-node brick elements, and analyze the models and performed stress and probability of failure analyses using a general-purpose commercial finite element (FE) software package. We numerically investigate the effects of volume fractions and temperature-dependent material properties on the thermo-mechanical stress behavior of cathode microstructures.

Keywords: Microstructure reconstruction, Ceramic composites, Composite electrodes, Homogenization techniques

Introduction

A solid oxide fuel cell (SOFC) is an electrochemical power source that converts the chemical energy of fuels into electrical energy [1]. SOFCs have received attention from researchers due to their ability to deliver clean energy at high efficiencies [1]. An SOFC consists of anode, cathode, electrolyte, and interconnect wires [1]. The electrolyte is a solid oxide such as yttria-stabilized zirconia (YSZ). The porous anode is a ceramic-metal composite ('cermet') of nickel and zirconia (Ni-YSZ). The porous cathode is a composite of ceramic materials such as strontium-doped lanthanum manganite and yttria-stabilized zirconia (LSM-YSZ) [1]. Typical SOFC operating temperatures lie in the range of 600 – 1000 ^{0}C [1]. Such high operating temperatures lead to durability and mechanical integrity issues during thermal cycling of SOFCs [1]. Thermal stresses may arise due to mismatch of coefficients of thermal expansion (CTEs) between various components, while stress concentration effects may arise due to the porous microstructure of the electrodes. Thus, in order to increase the durability of SOFCs, it is very important to investigate methods of mitigating the adverse effects of thermal stress. One plausible concept for reducing the undesirable effects of CTE mismatch between SOFC components involves gradual variation of phase volume fractions to eliminate sharp boundaries between components. In this paper, we use image-based finite element analysis to investigate the effects of varying phase volume fractions on the mechanics of cathode microstructures under thermal stress.

Finite Element Analysis of Cathode Microstructures

Three-dimensional (3D) FE microstructure models are reconstructed from two-dimensional (2D) SEM images of a cathode microstructure, which are obtained from Dr. Scott Barnett's group [2]. These images are of the real cathode microstructure

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having 50:50 LSM:YSZ composition (see Figure 1(a)). We developed heuristic algorithms to transform the original 2D images of the 50:50 LSM:YSZ cathode into images corresponding to a derived, 30:70 LSM:YSZ cathode. We first identified the pixels neighboring the interfaces between LSM (white), YSZ (gray), and pore (black) phases in the original cathode images. We then modified the values of these pixels using heuristic rules derived through trial-and-error procedures, to increase the number of YSZ (gray) pixels and decrease the number of LSM (white) pixels, until the correct volume fractions of each phase were obtained in the derived 30:70 cathode model (see Figure 1(b)).

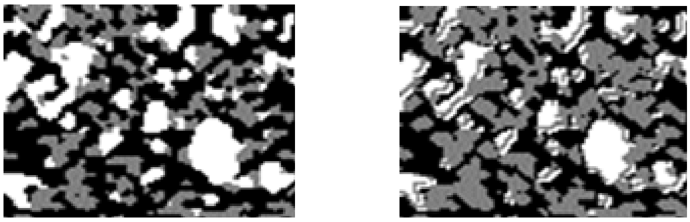

Figure 1(a) 2D SEM image of 50:50 cathode (left) [2]; (b) Derived image of 30:70 cathode (right)

Finite element analyses of the cathode microstructure models are carried out to investigate thermal stresses induced by steady-state temperature change from room temperature (20^{o}C) to operating temperature (820^{o}C), i.e. $\Delta T = 800^{o}C$. Table 1 lists the material properties used. The variation of the CTE of YSZ with temperature [3] and the variation of the Young's modulus of LSM and YSZ with temperature [4] are considered. The CTE of LSM is assumed constant over the temperature range. The details of the material properties used can be found in [5].

Table 1 Room temperature material properties used in FE analyses of cathode [6]

Material	Young's modulus (GPa)	Poisson's ratio	CTE ($10^{-6}\ {}^{0}C^{-1}$)
YSZ	205	0.30	10.40
LSM	40	0.25	11.40

The 3-D FE models of the cathode have approximately 260,000 elements and 400,000 nodes. Von Mises stress (in Pa) contour plots for the 50:50 wt. % LSM:YSZ cathode are shown in Figure 2. Figure 2 also shows the physical dimensions of the 3-D reconstructed finite element model of the 50:50 LSM:YSZ cathode microstructure. Figure 2 shows that as ΔT increases from 500^{0}C to 800^{0}C, the stresses in the cathode increase, as expected. Thermal stress is proportional to CTE and ΔT, and the CTE of YSZ increases with temperature [5]. Also, the stresses are greater near the pores due to stress concentration.

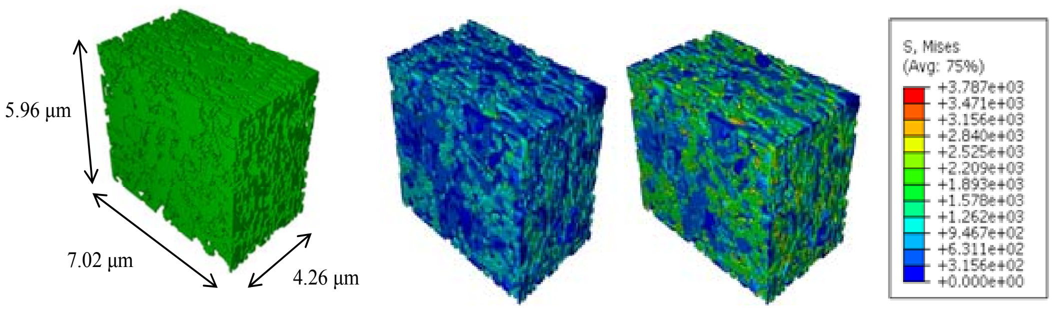

Figure 2 Von Mises stress (in Pa) for 50:50 LSM:YSZ cathode: $\Delta T = 500^{0}C$ (middle) and 800^{0}C (right)

Ceramic materials exhibit brittle behavior under tensile stress. Also, unlike metals, they show wide variability in tensile strength values and follow a statistical strength distribution. Thus, the Weibull method of analysis [7] is used to calculate the

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probability of failure of the SOFC cathode. According to the Weibull method, the survival probability of a particular component *j* under the action of a tensile stress σ is given by [7]:

$$P_s^j(\sigma, V_j) = \exp\left(- \int_{V_j} \left(\frac{\sigma}{\sigma_0} \right)^m \frac{dV_j}{V_0} \right) \qquad (1)$$

where j = cathode, V_j is the volume of component j, V_0 is a characteristic specimen volume for the material of component j, σ_0 is the characteristic strength of the material of component j, and m is the Weibull modulus. The characteristic strength σ_0 is also the scale parameter for the distribution, while the Weibull modulus m is the shape parameter. The reference volume V_0 is related to the characteristic strength σ_0. The Weibull parameters used for the ceramic materials are shown in Table 2 [7]. Using FEA, we obtained centroidal principal stresses in each finite element. We used tensile principal stress values to estimate the probability of survival (P_s) of the LSM and YSZ phases of the cathode. The probability of failure (P_f) of each phase is calculated as $P_f = 1 - P_s$.

Table 2 Weibull parameters for cathode ceramic materials at room temperature [7]

Material	Weibull modulus, m	Characteristic strength, σ_0 (MPa)	Reference volume, V_0 (mm^3)
LSM	7.0	52.0	1.21
YSZ	7.0	446.0	0.35

Figure 3 shows the P_f values for the two cathode models. The probability of failure of the cathode increases with increasing ΔT values (and hence increasing stresses), for both temperature-independent and temperature-dependent material properties. For temperature-independent material properties, the 30:70 LSM:YSZ cathode model exhibits lower P_f values than the 50:50 LSM:YSZ model over the entire temperature range. This may be due to greater stress concentration in the 50:50 LSM:YSZ cathode model, given its higher pore volume fraction (48.95%) compared with the 30:70 LSM:YSZ cathode model (43.93%).

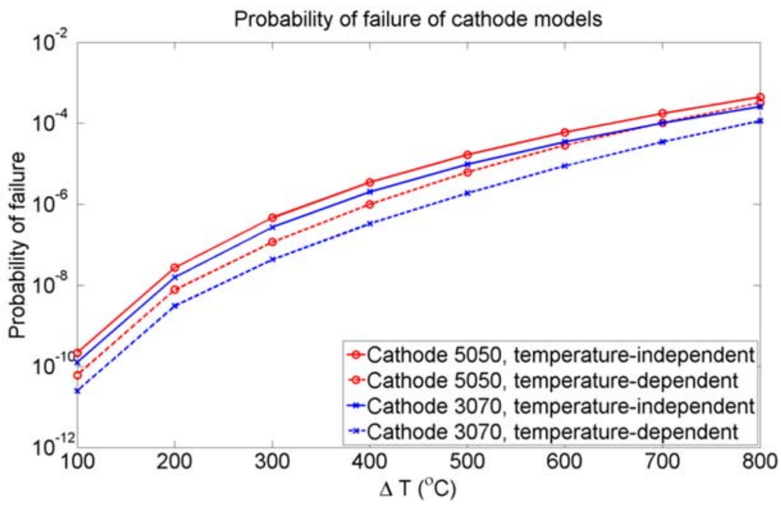

Figure 3 Probability of failure of cathode models

Figure 3 also shows that when temperature-dependent material properties are considered, the volume fraction of YSZ plays a significant role in determining the P_f values, since the Young's modulus of YSZ undergoes a large decrease with increasing temperature [5]. Thus, we may anticipate that lower stresses will be induced in the 30:70 model, since it has a higher volume

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fraction of YSZ than the 50:50 model. These results are confirmed in Figure 3, i.e. the 30:70 LSM:YSZ model shows lower P_f values than the 50:50 model, for temperature-dependent material properties. Figure 4 shows the statistical distribution of principal tensile stress values among the elements of the YSZ phase of the 50:50 and 30:70 LSM:YSZ cathode models, at 800°C, considering temperature-dependent properties. The ratio of maximum principal tensile stress (MPTS) to Weibull strength shown on the horizontal axis may be interpreted as a simplified failure measure for the YSZ elements, with ratios ≥ 1 indicating failure. The curves shown in Figure 4 are lines joining the tops of histogram bars centered on the corresponding values on the horizontal axis. We observe that both cathode models have relatively small fractions of YSZ elements with principal tensile stresses equaling or exceeding the Weibull strength of YSZ. Most of the elements in the YSZ phase have MPTS-to-Weibull strength ratios < 1. This fact explains the small magnitudes of P_f values – between 2.5 x 10^{-11} and 4.5 x 10^{-4} – calculated from the Weibull analysis. From the inset shown in Figure 4, we also observe that the 50:50 cathode model has a higher number of YSZ elements with stress ratios ≥ 1 than the 30:70 cathode model. This observation also supports our previous comment about the P_f values of the 50:50 and 30:70 LSM:YSZ cathode models.

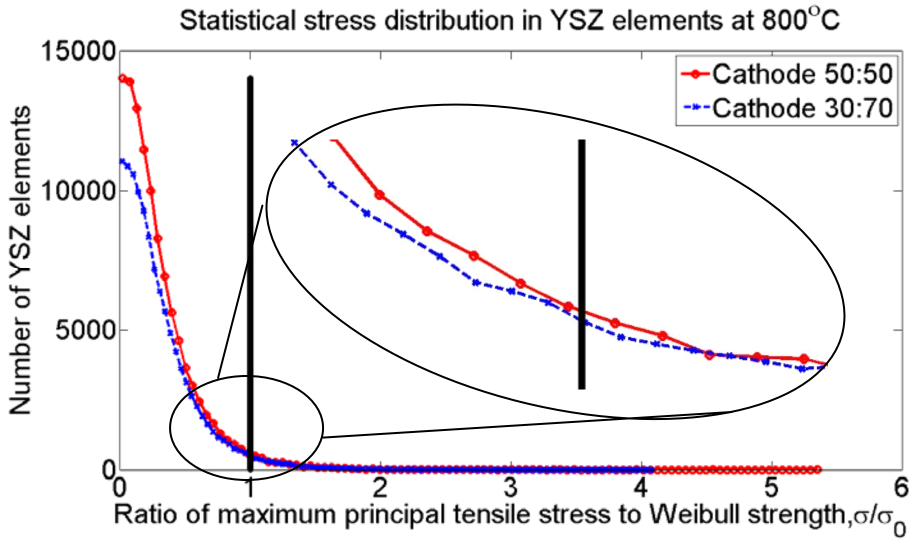

Figure 4 Statistical distributions of principal tensile stresses in 50:50 and 30:70 LSM:YSZ cathode models

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