Topology Optimization of a Composite Cathode in a Solid Oxide Fuel Cell

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Introduction

A solid oxide fuel cell (SOFC) is an electro-chemical device that generates electric energy and heat directly from chemical energy [1]. The working principle of a SOFC is illustrated in Fig. 1.

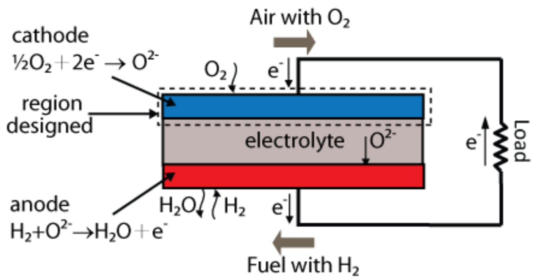

Fig. 1. Schematic arrangement of a SOFC

One path to improve the performance of a SOFC is to minimize the cathode resistance [2]. Recently, experiments with composite cathodes have shown low resistances results [3] and detailed models of cathode microstructures have been used in optimizing their performance [4,5]. In this work a two-material composite cathode is considered, and the cathode resistance is minimized by designing the cathode microstructure using topology optimization method. The composite cathode consists of an ionic-conducting scaffold and a coating of electrocatalytic particles applied on the surface of the scaffold.

A simplified 2-D model with design dependent boundaries is used in the analysis model of the cathode. Similar optimization problems have been discussed before using topology optimization in [6,7,8]. In the following, a solid isotropic material with penalization (SIMP) [9] based topology optimization model is proposed. An example is used for illustration.

Topology Optimization Problem

In a manner proposed by Tanner et al [10] and Nicholas and Barnett [11], the electrical potential distribution in the ionic-conducting scaffold, illustrated in Fig. 2(a), is governed by Laplace's equation

$$\nabla \cdot (k_0 \nabla \phi) = 0 \quad \text{in} \quad \omega$$

where k_0 is the conductivity in the ionic conductor.

The effect of the electrocatalytic coating can be written as a Robin boundary condition on the scaffold surface

$$k_0 \nabla \phi \cdot \vec{n} = h_0 (\phi_\infty - \phi) \quad \text{on} \quad \Gamma_\omega$$

where h_0 is a property related to the surface resistance of the coating.

By assuming a horizontal periodicity with an (irreducible) unit cell, the analysis model can be extended to a rectangular design domain Ω, as illustrated in Fig. 2(b). A constant electrical potential $\phi = 0$ is applied on Γ_0. A density based topology optimization model can be set up after discretizing the design domain using rectangular elements, and representing the element material properties as a function of element density ρ_e.

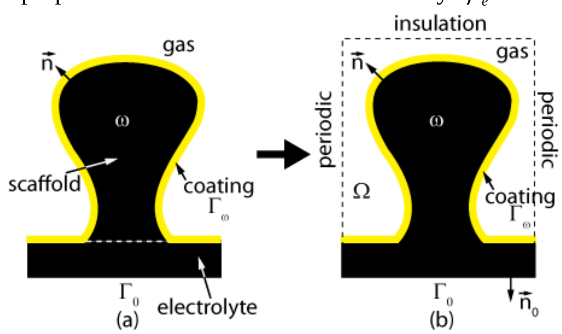

Fig.2. Sketch of (a) the geometrical configuration of the analysis model and (b) the periodic design domain

The objective is to maximize the current through the cathode, which is equivalent to minimizing resistance. One trivial way of decreasing the cathode resistance is to increase the amount of material *W* and perimeter *P* of the scaffold. To show the effect of designing the shape alone, *W* and *P* are constrained. Then the topology optimization problem becomes

Find the element density vector ρ that

$$\text{Maximizes} \quad f(\phi,\rho) = \int_{\Gamma_0} -k_0 \nabla\phi \cdot \vec{n}_0 dl$$

$$\text{Subject to}$$
$$W \le W_R$$
$$P \le P_R$$
$$0 \le \rho_e \le 1, \quad e = 1,2,\cdots,N$$

Example with varying P_R

In this example the unit cell is 40×60 (elements). Material properties are such that $\ell h_0/k_0 = 25$, where $\ell = 1$ is the length and height of one element. Figure 3 illustrate the design for P_R equal to 180ℓ and 360ℓ, with $W_R = 0.25 * W_\Omega$, where W_Ω is the total area of the region Ω.

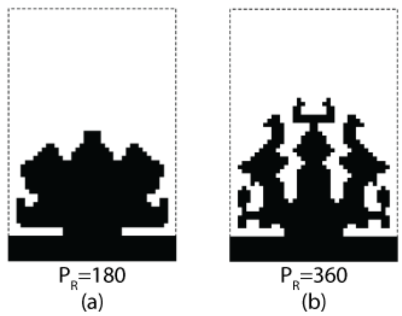

Fig.3. Optimized design for (a) $P_R = 180\ell$ and (b) $P_R = 360\ell$

The resistances R_P for Fig. 3(a) and (b) are 113 and 74. Compared with the reference values 194 and 213 which are calculated from the single column design in [9], the optimized designs have improvements of 42% and 65%. Although the perimeter of (b) is twice the perimeter of (a), R_P of (b) decreases less than a half of R_P of (a). This is because by increasing the current, the scaffold resistance begin to dominate in the cathode resistance.

Conclusion

A simplified topology optimization model is presented to improve the performance of SOFC by optimizing the microstructure of the cathode. Compared with a single column microstructure, the improvements of more than 40% can be achieved. The effect of changing material properties and constraints will be discussed in the full paper.

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