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Modeling of solid oxide fuel cells with optimized interconnect designs

Shumao Zeng [a], Xiaoqiang Zhang [a], Jun Song Chen [a,b], Tingshuai Li [a,b,*], Martin Andersson [a,c]

[a] School of Materials and Energy, University of Electronic Science and Technology of China, 2006 Xiyuan Ave, West Hi-Tech Zone, 611731 Chengdu, Sichuan, PR China
[b] Center for Applied Chemistry, University of Electronic Science and Technology of China, 2006 Xiyuan Ave, West Hi-Tech Zone, 611731 Chengdu, Sichuan, PR China
[c] Department of Energy Sciences, Faculty of Engineering, Lund University, P.O. Box 118, SE-221 00 Lund, Sweden

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ABSTRACT

A 3D model is developed to investigate solid oxide fuel cells (SOFCs) contacting with optimized interconnect designs and the results indicate that the current density and thermal stress are closely related to both the shape of tip in interconnects and the depth of it in the cathode. The interconnect with triangular rips can yield the best electrochemical performance compared to those with tips of rectangle and trapezium, and the current densities increase with the depth of tips in cathodes, except the trapezoidal ribs, which shows a concaving change with the depth. The 1st principle stress reaches around 21.9 MPa and 16.6 MPa at the interfaces of electrodes and electrolytes, but it rises to 60 MPa and 18 MPa for the rectangular tips at the air and fuel inlets, respectively, which sharply decreases to nearly 25 MPa and 10 MPa with the depth in cathodes approaching 5 μm. The maximum shear stresses are found to reach 34.4 MPa and 32.1 MPa at the two interfaces, and the triangular tips will induce the most intensive stresses at electrolyte-cathode interface. The resulting conclusions are beneficial to optimize interconnect design to improve the efficiency of current collection and also reduce the risk of generation of remarkable thermal stresses.

1. Introduction

The solid oxide fuel cells (SOFC) is a promising power generator that can directly convert chemical energy in fuels to electricity [1,2], and the efficiency and stability depend mostly on the conductivities of materials [3,4], catalyst activity [5–7], the compositions of fuels [8,9] and the design of interconnects [10,11]. The interconnect is not only used to connect single solid oxide fuel cells in series in a stack, but it also acts as gas channels to transport air and fuels, which can thus strongly affect both the efficiency of current collection and the whole stack's stability due to mechanical mismatches between components. The optimization of interconnect can be thus a significant part in research and development of SOFCs [12].

The patterns of interconnect contacting cathodes can strongly affect the power density and stability of a SOFC stack [13,14]. It is reported that the maximum power output increased from 0.07 W cm^{-2} to 0.1 W cm^{-2} with the tip of interconnect increasing from 40 to 60 cm^2 [15]. Moreover, the tip area and its depth in cathode can strongly affect the power density and degradation [16], which also confirms that the optimum tip contact area was 45% (accounting for the whole area of an interconnect) and its depth in the cathode was 105 μm for achieving the best performance and duration property. Besides, Liu et al. studied effect of the interconnect rib width on the cell performance [17], which presented that the rib surface contact contributed to the ohmic polarization and the optimal rib width was linear to the pitch width.

Based on previous experimental results, it can be concluded that the shape and size of tip or rib in interconnects tend to affect the performance and durability of a stack. The contact area and the depth of tip or rib in cathodes are both expected to be large for more efficient current collection. However, there are mechanical mismatches between the metal interconnects and ceramic cathodes, which will induce thermal stresses in a single cell. Thermal stresses in single SOFCs were widely studied as functions of the operation conditions [18–20], cell configuration [21], porosity in electrodes [22] and sealing design [23], but there is lack of detailed investigations into stresses stemming from the patterns of the interconnect-electrode contact.

We previously evaluated distributions of thermal stresses by changing the interconnect-electrode contact area and the results demonstrated that a larger contact area is beneficial to effectively reduce the 1st principle stress close to the corner of interconnect-cathode contact region at the fuel inlet and a wider rib at the anode

* Corresponding author at: School of Materials and Energy, University of Electronic Science and Technology of China, 2006 Xiyuan Ave, West Hi-Tech Zone, 611731 Chengdu, Sichuan, PR China.

E-mail address: litingshuai@uestc.edu.cn (T. Li).

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Nomenclature

i	current density, A m^{-2}
σ	electric/ionic conductivity, S m^{-1}
Φ	electric/ionic potential, V
V	volume fraction, –
T	temperature, K
V	working voltage, V
E^{OCV}	open circuit voltage, V
E_0	ideal voltage before partial pressure consideration, V
R	gas constant, 8.314 J mol^{-1} K^{-1}
F	Faraday constant, 96,485 C mol^{-1}
p	gas partial pressure, Pa
E_{eq}	equilibrium potential for anode/cathode, V
L	characteristic thickness, m
i_v	volumetric current density, A m^{-3}
i_0	exchange current density, A m^{-2}
A_i	pre-exponential factor, S m^{-2}
E_a	activation energy, J mol^{-1}
k	permeability, m^2
ρ_g	gas density, kg m^{-3}
$\vec{u}$	velocity vector, m s^{-1}
$\vec{F}$	volume force vector, N m^{-3}
x_i	mole fraction for species i, –
b_n	constant for viscosity calculation, –
D_i^T	thermal diffusion coefficient, kg m^{-1} s^{-1}
$D_{eff,ij}$	effective binary diffusion coefficient, m^2 s^{-1}
S_j	mass source term for species j, kg m^{-3} s^{-1}
D	diffusion coefficient, m^2 s^{-1}
M_{ij}	reduced molar mass, kg mol^{-1}
l_{ij}	characteristic length, Å
Ω	diffusion collision integral, –
M	mole mass, kg mol^{-1}
r	radius of pores, m
r	reaction rate, mol m^{-3} s^{-1}
m	mole concentration, mol m^{-3}
$c_{p,g}$	specific heat at constant pressure, J kg^{-1} K^{-1}
Q_h	heat source term, W m^{-3}
ΔS	entropy change, J mol^{-1} K^{-1}
ΔH	enthalpy change of reaction, J mol^{-1}
C	elasticity matrix, Pa

Greek symbols

η	polarizations, V
β	transfer coefficient, –
μ	dynamic viscosity, Pa S
ε	porosity, –
ϵ	strain, –
ψ	viscous stress tensor, Pa
ω	mass fraction, –
τ	tortuosity for gas transfer, –
τ	tortuosity for ion/electron transfer, –
λ	thermal conductivity, W m^{-1} K^{-1}
ε	stress, Pa
α	thermal expansion coefficient, K^{-1}

Subscribes

l	ion
s	electron
eff	effective
a	anode
c	cathode
act	activation
con	concentration
b	boundary between gas channel and electrode
g	gas
re	reversible
p	polarizations
R	reactions
M	methane
W	water
th	thermal
ref	reference

Abbreviations

SOFC	solid oxide fuel cell
TPB	triple phase boundary
ASL	anode support layer
CSL	cathode support layer
AAL	anode active layer
ASA	active specific area
MSR	methane steam reforming
WGSR	water gas shift reaction
PEN	positive electrolyte negative
FI	fuel inlet
AI	air inlet
FEM	finite element method
PDE	partial differential equation
OCV	open circuit voltage
EA_i	interface of electrolyte-anode
EC_i	interface of electrolyte-cathode

side can lower thermal stresses [24]. Although the proper contact area and depth are required to enhance the cell performance, the effects of the tip shape and depth on thermal stresses are not revealed, which will be significantly related to the durability. Therefore, we develop a 3D model of a unit SOFC using the COMSOL Multiphysics (Version 5.3) to study the thermal stresses resulting from different patterns of the interconnect-cathode contact, aiming to optimize the interconnect design in lights of shape, size and depth of the tips that are embedded in cathodes.

2. Mathematic model

Three typical contact modes as shown in Fig. 1 are discussed in this study, in which Dr, Dm and De mean the contact depth for the rectangular, trapezoidal and triangular tips. We set depths of the tips in cathodes to zero as a standard case, whose outline can be seen in Fig. 2 and the corresponding geometry parameters are listed in Table 1. Five groups of partial differential equations (PDE) are selected as governing equations that describe the ion/electron, mass, momentum and heat transport, and thermal expansion, which include:

(1) Ion and electron transport

Hydrogen as fuel in the anode and oxygen as oxidant in cathode are considered in the electrochemical reaction, which is the source of electricity (in Eq. (1)) and the rink of electron (in Eq. (2)) [25]:

$$H_2 + O^{2-} \rightarrow H_2O + 2e^- \tag{1}$$

$$\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-} \tag{2}$$

Ohm's law is used as the governing equation of ion/electron transport: