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THREE-DIMENSIONAL MODELLING OF THERMAL STRESSES IN A PLANAR SOLID OXIDE FUEL CELL OF A NOVEL DESIGN

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Abstract. The presented modelling investigation was carried out to analyze thermal stresses and expansion in an anode supported planar Solid Oxide Fuel Cell (pSOFC). The temperature distribution was based on previously developed thermo-electrochemical model predicting fuel cell operation. The design of a single pSOFC consisted of three ceramic layers of membrane electrode assembly: anode, electrolyte, cathode and two cross-flow bipolar plates with 26 ribs. The gases flowed diagonally from one cell corner to the opposite one. The fuel and air flows were cross-wise opposed on each bipolar plate side. The study allowed to indicate the most vulnerable to thermal damage area of the fuel cell in the operating conditions. The results will be useful in further design modification and performance optimization of the SOFC.

Keywords: planar Solid Oxide Fuel Cell, thermal stresses, residual stresses, Finite Element Method, Computational Fluid Dynamics

MODELOWANIE 3D TERMICZNYCH NAPRĘŻEŃ W PŁASKIM STAŁOTLENKOWYM OGNIWIE PALIWOWYM O NOWATORSKIEJ KONSTRUKCJI

Streszczenie. Przeprowadzone symulacje numeryczne miały na celu analizę termicznych naprężeń i ocenę stopnia wydłużenia płaskiego stałotlenkowego ogniwa paliwowego typu pSOFC (ang. planar Solid Oxide Fuel Cell). Rozkład temperatury w ogniwie wyznaczono w oparciu o wcześniej opracowany model termiczno-elektrochemiczny [11]. Nowatorskie rozwiązanie ogniwa typu pSOFC objęło ceramiczną konstrukcję, w skład której weszły porowate elektrody – anoda i katoda, elektrolit oraz dwie płytki bipolarne z 26-cioma żebrami. Przepływ paliwa i powietrza odbywał się krzyżowo i przeciwnieprądowo, po przekątnej ogniwa. Wyniki symulacji pozwoliły na określenie obszarów ogniwa narażonych na uszkodzenie w wyniku wysokich wartości naprężeń termicznych. Uzyskane rezultaty FEM umożliwią dalszą modyfikację konstrukcji płaskiego ogniwa w celu optymalizacji wydajności pSOFC.

Słowa kluczowe: płaskie stałotlenkowe ogniwo paliwowe, naprężenie termiczne, naprężenie szczątkowe, Metoda Elementu Skończonego, Numeryczna Mechanika Płynów

Introduction

Nowadays renewable and clean energy sources are more and more popular as a result of the ecological awareness and the need of pollutant emission reduction. Fuel cells, particularly the Solid Oxide Fuel Cells (SOFCs), are taken into account in a future plan of power systems due to their capabilities of efficient usage for stationary and mobile energy generators [10, 12]. The SOFCs are characterized by high performance in comparison to other fuel cells. Moreover, SOFCs are quite fuel flexible. Both hydrogen as well as hydrocarbons, such as natural gas, may be used as fuel [7].

However, currently the key challenges are short fuel cell life duration and high SOFC fabrication costs. One of the main causes of high cell degradation rates is structural failure. The SOFC operates at high temperature, which is often more than 700°C. This influences thermal stress generation in the cell structure, which can lead to its damage. The stress is due to a spatial temperature gradient and thermal expansion coefficients mismatch of the fuel cell components [8]. Therefore, it is so important to be able to define areas of thermal stress occurrence and its values. This knowledge allows to save time, design and fuel cell production costs in a wide range of material parameters and operating conditions. A risk assessment of fuel cell damage and improvement of SOFC design can be performed with the help of numerical coupled approaches such as Computational Fluid Dynamics (CFD) and Finite Element Method (FEM) codes.

Therefore, the purpose of this study was to investigate thermal stresses in the anode-supported single planar Solid Oxide Fuel Cell (pSOFC) with an innovative design based on 3D CFD/FEM simulations.

1. Mathematical model

The computational method consisted of two components: a multi-physics electrochemistry model and a structural mechanics model. A coupled of Computational Fluid Dynamics (CFD) and Computational Structural Mechanics (CSM) with Finite Element Method (FEM) analyses were performed using the commercial ANSYS software: Fluent with SOFC module and Mechanical.

1.1. Multi-physics electrochemistry model

A full numerical model used in this study, based on the coupled equations for thermal, fluid, electrochemistry and electrical transport, was presented in details in a paper [11].

1.2. Structural mechanics model

The applied structural mechanics model assumed that fuel cell materials undergo linear thermoelastic deformation. Total strain consisted of elastic and thermal contributions as follows:

$$\{\varepsilon\} = \{\varepsilon_{el}\} + \{\varepsilon_{th}\} \quad (1)$$

Thermal strain was calculated from Eq. (2):

$$\{\varepsilon_{th}\} = \{\alpha, \alpha, \alpha, 0, 0, 0\} \cdot (T - T_{ref}) \quad (2)$$

where: α was the coefficient of thermal expansion (CTE), T was the temperature obtained from the thermo-fluid model in the first stage of simulation, T_{ref} was the stress free temperature.

Stress-strain relationship for an isotropic, linear elastic solid material was computed as:

$$\begin{Bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{Bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{(1-2\nu)}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{(1-2\nu)}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{(1-2\nu)}{2} \end{bmatrix} \begin{Bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{xz} \\ \varepsilon_{xy} \end{Bmatrix} \quad (3)$$

$$- \frac{E \cdot \alpha \cdot \Delta T}{1-2\nu} \begin{Bmatrix} 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{Bmatrix}$$

where: E was the Young's modulus, ν was the Poisson's ratio of the model material.

The equivalent von Mises stress was described by Eq. (4):

$$\sigma_{vM} = \sqrt{\frac{1}{2} \cdot [(\sigma_{xx} - \sigma_{yy})^2 + (\sigma_{yy} - \sigma_{zz})^2 + (\sigma_{zz} - \sigma_{xx})^2] + 3 \cdot (\sigma_{xy}^2 + \sigma_{yz}^2 + \sigma_{xz}^2)} \quad (4)$$

1.3. Model geometry

The model geometry was based on the design of a single planar SOFC proposed by Bossel [1]. It consisted of three MEA layers (membrane electrode assembly – anode, electrolyte, cathode) and two cross-flow bipolar plates with 26 ribs. Bipolar plates acted as flow channels and as current collectors. The gas flows were diagonal from one cell corner to the diagonally opposed corner and the fuel and air flows were cross-wise opposed on each bipolar plate side.

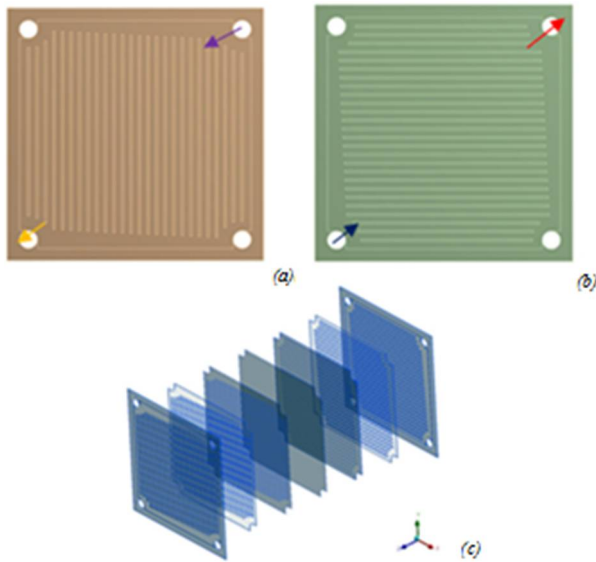


Fig. 1. The proposed planar SOFC design: a) bipolar plate, view from the cathode side, b) view from the anode side, c) single planar SOFC geometry divided into separate layers

The schematic of the analysed design is shown in Fig. 1. In Fig. 1a, ribs of bipolar plates from the cathode side are shown, while in Fig. 1b an anode side view is presented. The pSOFC geometry presented in Fig. 1c was divided into separate layers, sequentially from the left side: cathodic bipolar plate, air channel, LSM (Strontium-doped Lanthanum Manganite) cathode, YSZ (Yttria-Stabilized Zirconia) electrolyte, Ni-YSZ cermet anode, fuel channel and anodic bipolar plate. Arrows in Fig. 1a and b indicate gas flow directions: the purple arrow means the air inlet, and the orange arrow – the air outlet, the blue and red arrows indicate the fuel inlet and outlet, respectively.

The basic physical parameters of the pSOFC materials are included in Tab. 1. The stress free temperature for SOFC was widely assumed as the sintering temperature, at which different layers were joined.

Tab. 1. The physical parameters of the SOFC materials

material	Ni-YSZ anode	YSZ electrolyte	LSM cathode	Crofer 22 APU bipolar plate
CTE $\cdot 10^{-6}$ [1/K]	12.2 [4, 9]	10.3 [2]	11.7 [4, 6]	10.3-12.7 (473–1273 K) [3]
Young's modulus [GPa]	57 [4, 9]	215/185 (298/1073 K) [7]	35 [4,6]	214-44 (298–1073 K) [3]
Poisson's ratio [-]	0.28 [9]	0.32/0.313 [9]	0.36 [6]	0.29 [3]
Density [kg/m ³]	7740 [13]	6000 [2, 6]	5300 [13]	7700 [3]
Thermal conductivity [W/m K]	6 [13]	2.7 [13]	10 [13]	24 [3]
Specific heat [J/kg K]	600 [13]	400 [13]	607 [13]	660 [3]
Tensile yield strength [MPa]	115 [7, 9]	332/256 [9]	155 [5]	291 [3]
Compressive strength [MPa]	100	1000 [7]	100 [7]	345 [3]
Stress free temperature [K]	1623 [6]	1623 [6]	1473 [6]	-

2. Results and discussion

In the first modelling stage, temperature distribution was calculated for 0.7 V operating voltage based on the CFD model. Then, the obtained temperature was imported into the Mechanical module in order to achieve the stress and expansion distributions in the single planar SOFC. The residual stress was calculated during a cooling down process using the stress free temperature of MEA.

2.1. CFD results

In this study, only one case at the operating voltage equal to 0.7 V was considered. The temperature distribution is shown in Fig. 2a. The temperature distribution estimated during the CFD simulation was imported to the ANSYS Mechanical module. Temperature profiles imported to the second step FEM simulation is presented in Fig. 2b.

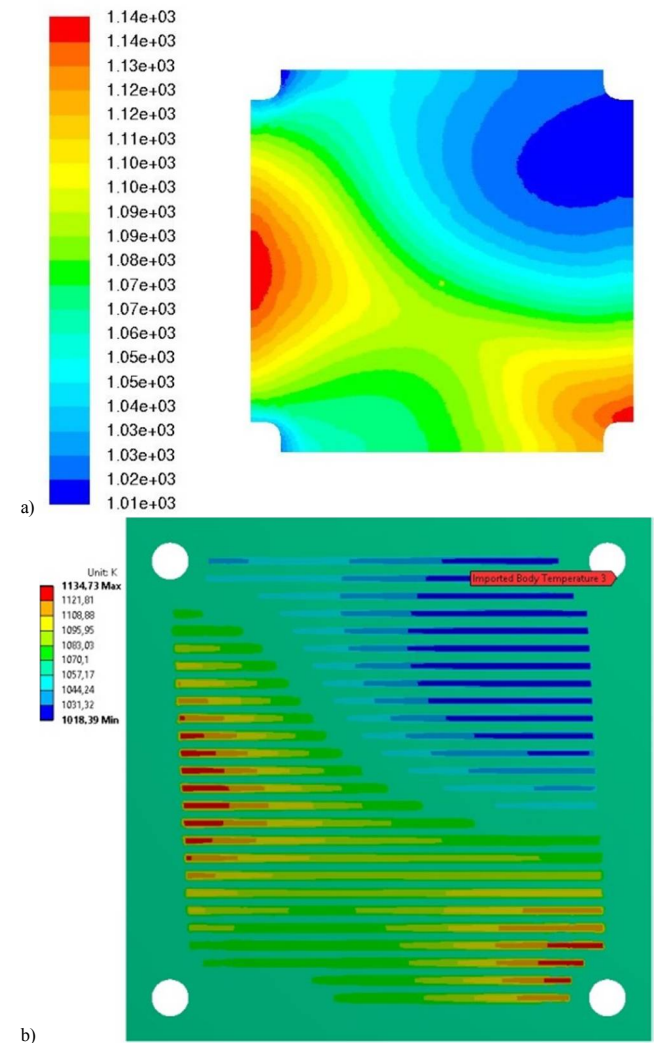


Fig. 2. Temperature distribution [K]: a) at electrolyte, CFD model, b) imported at bipolar plate, FEM model

2.2. Structural mechanics results

Both gradients of the operating temperature and the manufacturing process temperatures of the MEA layers were taken into account during thermal stresses generation. The operating stress resulted as the first factor from the temperature distribution imported from CFD calculation of the single planar SOFC at 0.7 V. Distributions of the deformation and operating von Mises stresses are shown in a diagonal cross-section views in Fig. 3.

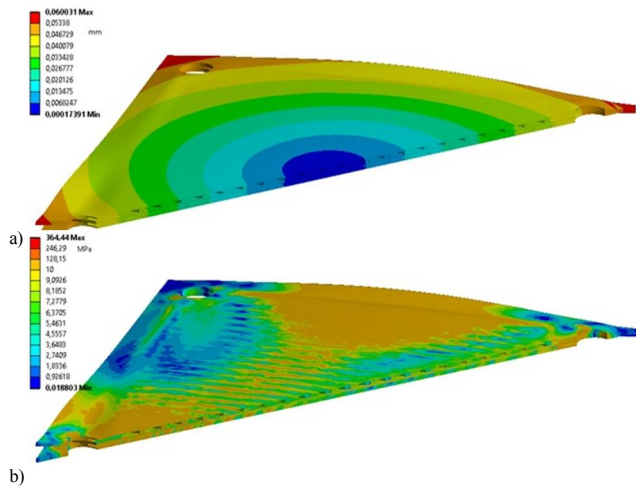


Fig. 3. Operating distribution of: a) total displacement [mm], b) von Mises stress [MPa]

Fig. 4 presents the contour maps of maximum principal stress in the local scale for each part of the planar SOFC.

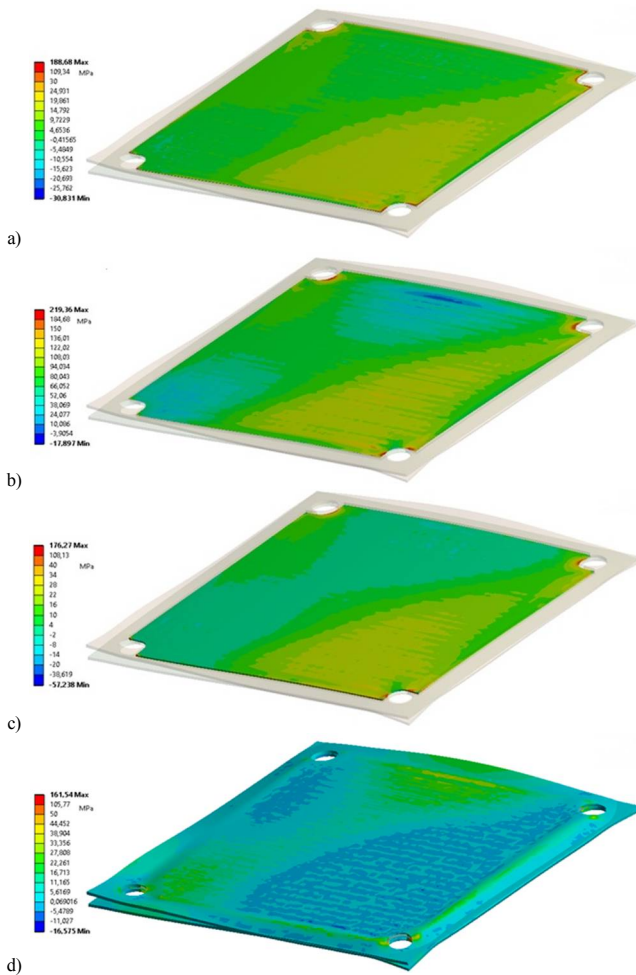


Fig. 4. Operating maximum principal stress [MPa]: a) in cathode, b) in electrolyte, c) in anode, d) in bipolar plates

The MEA residual stress was developed during the sintering process of the MEA layers. It was assumed in this study that only one stage of the cooling down process from 1623 K to 298 K [6] is considered. Due to a constant temperature profile in this approach, the residual stress varied only along the vertical direction. Therefore, the stress results are shown in zoomed view of a diagonal cut of MEA parts in Figs. 5 – 6. Fig. 5a shows the total displacement of MEA under sintering process.

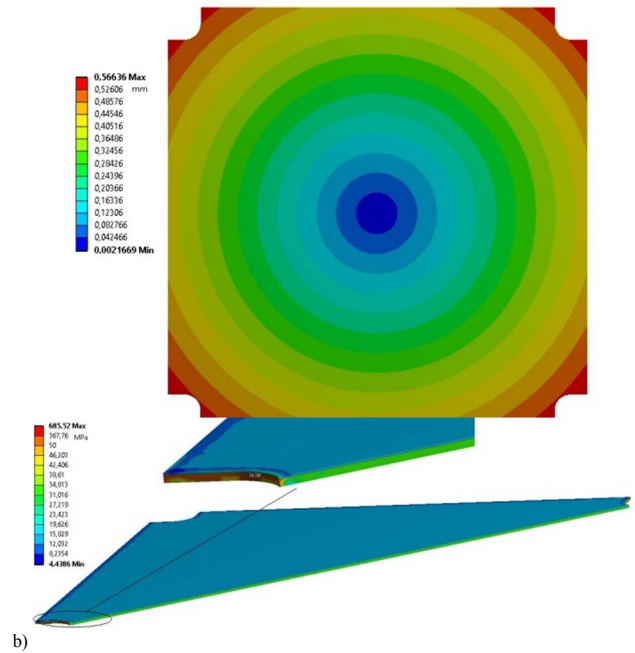


Fig. 5. Fabrication impacts: a) total displacement [mm], b) von Mises stress of MEA [MPa]

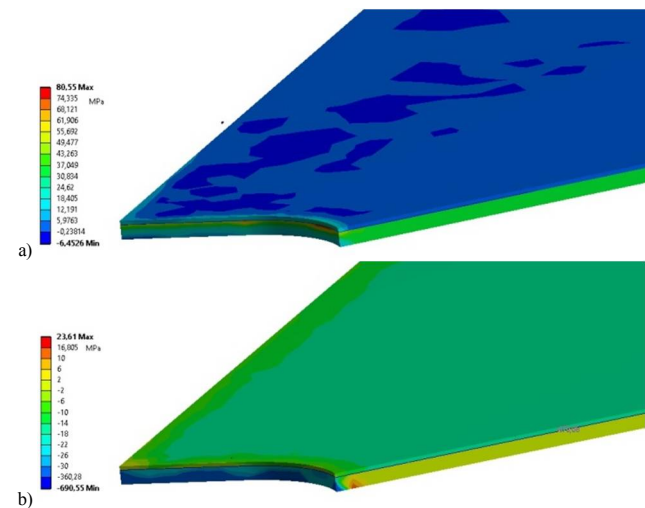


Fig. 6. Fabrication impacts: a) maximum principal stress [MPa], b) minimum principal stress of MEA [MPa]

Fig. 7. shows the total principal stress, which was defined as a sum of both the residual and operating stresses. The highest total stress was noticed in the electrolyte and it was equal to -670 MPa, i.e. it was the compression stress.

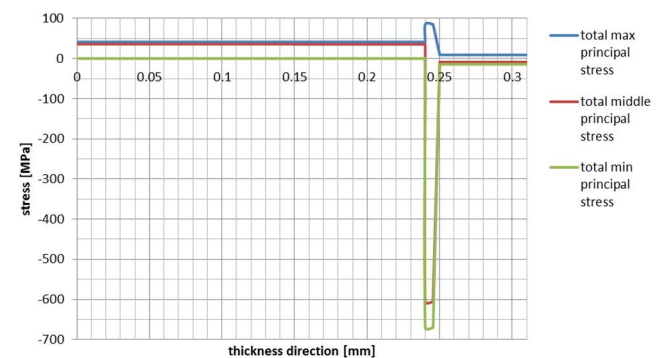


Fig. 7. Total principal stress in the planar SOFC along the vertical centerlines in the center point of geometry

3. Conclusion

The stress state in the anode supported planar SOFC of the innovative design was predicted using a coupled CFD and CSM analysis. Both operating temperature and that of the manufacturing process of the MEA layers were taken into account in generating the thermal stresses.

The highest total stress value of -670 MPa was noticed in the electrolyte, while -14.5 MPa was created in the cathode and 41.5 MPa in the anode layer. Based on this numerical investigation it can be concluded that the residual stress due to the manufacturing process has a major influence on thermal stress distributions.

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