International Advance Journal of Engineering Research (IAJER)
*Volume 08, Issue 02 (**February - 2025**), PP 06-12*
ISSN: 2360-819X
www.iajer.com

Research Paper **Open Access**

Requirements Imposed On the Structural Properties Of Materials Used In SOFC Design Practice

R.A. Hasanov[1], S,A. Musevi[2], G.S. Kheyrabady[3]

[1,2,3] *Faculty of engineering, Azerbaijan State University of Oil and Industry, email: ramiz.hasanov52@gmail.com, saida.musevi@mail.ru, qazala.kheyrabadi@mail.ru*

ABSTRACT:- The thermo-mechanical analytical model proposed for different solid oxide fuel cell (SOFC) designs addresses the deformation behavior and mechanical stability of SOFCs at various thermal stresses, specifically the creep resistance and the long-term endurance beyond the elastic limit.
The model considers the deformation of multi-layer SOFC in the temperature range of 600–800°C and presents the combination of the correlated parameters for SOFC performance evaluation, stability and long-term endurance under realistic operating conditions and temperature gradients. The numerical analysis of the thermo-mechanical properties of the SOFC materials is presented in terms of mechanical behavior at failure conditions and the influence of rheological and structural properties on SOFC long-term endurance. The SOFC thermal behavior, creep parameters of the SOFC materials and long-term stability are analyzed in terms of stresses, deformations and displacements.

Keywords: Modelling, materials, performances, operating temperature, design of compatibility.

I. INTRODUCTION

Conventional energy sources such as gasoline (diesel), coal and hydro source are the main sources for power generation. However, these conventional energy sources are being depleted, and are also unfriendly to the environment. Alternative energy sources such as renewable energy (RE) systems are becoming more popular in power generation applications. RE sources include solar energy, wind energy, photovoltaic (PV) cell energy, fuel cell etc. which are very effective in reducing the greenhouse gas emissions. In the near future, large portions of increase in electrical energy demand will be met through widespread installation of distributed generation (DG). Many advantages are considered for application of DG, i.e., increased service reliability, reduction of the need for grid reinforcement, generation expansion and power factor correction. Furthermore, it is possible to improve voltage regulation and local power quality more precisely using DGs in comparison to conventional centralized generators. DG sources comprise of direct energy conversion sources producing DC voltages or currents such as fuel cells and photovoltaic sources, high-frequency sources such as micro turbines, and variable frequency sources such as wind energy. Power generation from solar energy sources and wind energy sources is unpredictable, because solar power depends on the availability of sun light and wind energy system depends on the wind. Since fuel cells have no geographical limitations, they are preferred for small scale power generation. Power generation in fuel cells depends on the hydrogen input which is available in abundance. Further, fuel cells are known for their low to zero emissions, high efficiency (35-60%) and high reliability because of the absence of moving parts.

There are six main types of fuel cell: alkaline fuel cell (AFC), phosphoric acid fuel cell (PAFC), molten carbonate fuel cell (MCFC), polymer electrolyte membrane fuel cell (PEMFC) and direct methanol fuel cell (DMFC), solid oxide fuel cell (SOFC).
Fuel cells are static energy conversion devices that partially convert the chemical energy of fuels directly into electrical energy and produces water as its byproduct.

Among different types and scale power generation systems, fuel cells have received more attention, because they can provide also both heat and power. The successful utilization of materials requires that they satisfy a set of properties. These properties can be classified into thermal, optical, mechanical, physical, chemical, and nuclear, and they are intimately connected to the structure of materials. The structure, in its turn, is the result of synthesis and processing. A schematic framework that explains the complex relationships in the field of the mechanical behavior of materials, shown in Figure 1, is Thomas's iterative tetrahedron, which contains four principal elements: mechanical properties, characterization, theory and processing. Interrelationships among

structure, properties, and processing methods, the most important theoretical approaches, and the most-used characterization techniques in materials science today.

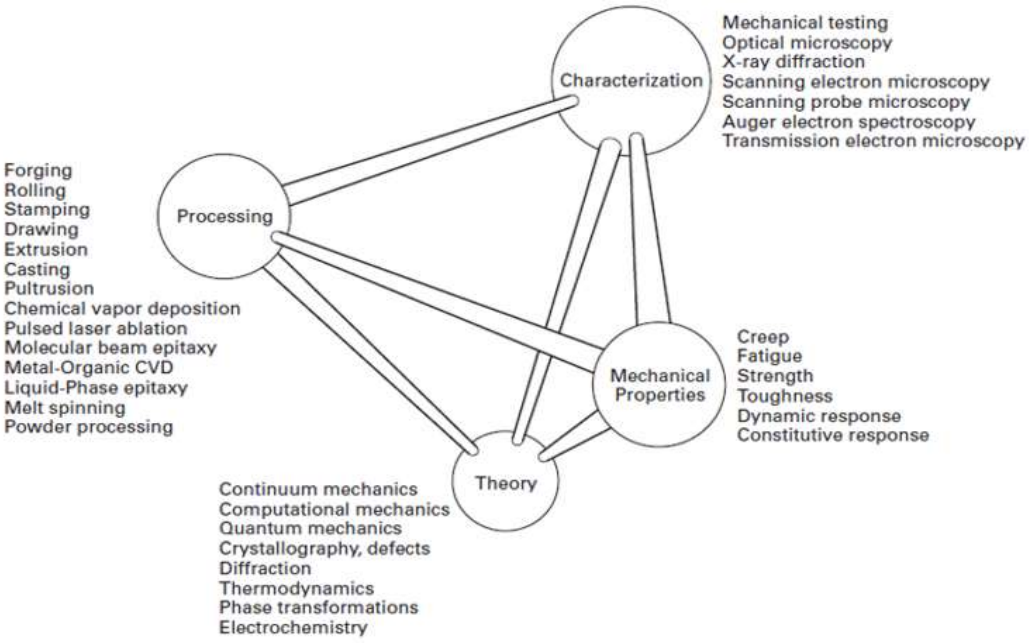

Figure 1. Tetrahedron, which contains four principal elements

According to the work is planned to study materials of different structural content exposed to operating temperature during the operation of the facility, namely (Figure 2):

1. Dense structure, based on zirconium (Zr);
2. Porous structure, based on titanium (TI);
3. Materials based on transition metals, so-called MaxPhase in different chemical composition.

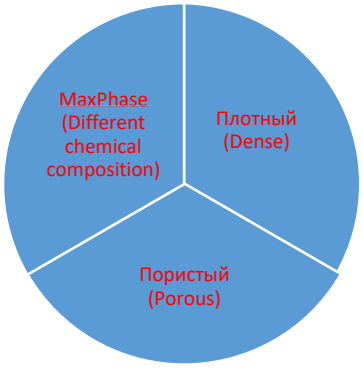

Figure 2. Materials with structure

Creation of materials with given and desired properties to ensure a higher consumer quality of devices by synthesizing compatible combinations of the indicated disciplining factors and structural properties of materials [7, 8]

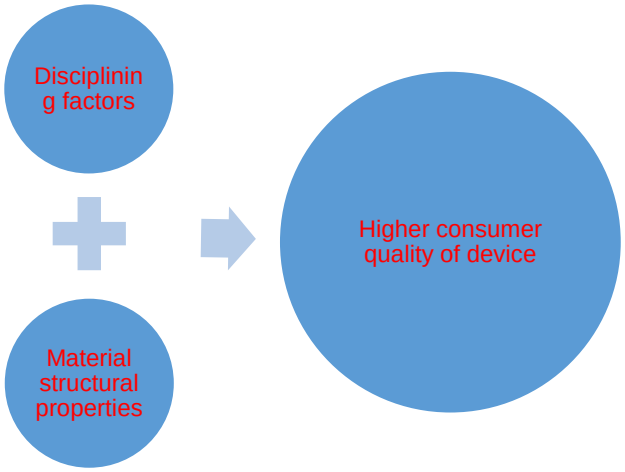

Figure 3. Creation of materials with given and desired properties

II. STATEMENT OF PROBLEM

2.1. The task for a dense structure synthesis based on zirconium

1. The thermomechanical analytical model is assumed for studying the deformation behavior of SOFC at various operational temperatures; in particular, provide the resistance of creep and long-term endurance outside the elastic limit.
2. The model takes into account the deformation of the multilayer SOFC in the temperature range of 600-800°C and is a decision on long-term endurance in the process of real operating conditions.
3. The numerical analysis of thermophysical properties of SOFC materials and their changes, depending on the mechanical behavior their destruction are estimated taking into account the rheological and structural properties of materials for the long-term endurance of SOFC.
4. The results of modeling thermomechanical deformation behavior of SOFC allowed to develop an algorithm for a decision on synthesis of the materials properties and their characteristics outside the elasticity limit, which is significant for long - term operation of SOFC at elevated temperatures.
5. In the end, a technique has been developed for the synthesis of desired materials taking into account the operating temperature, topology surfaces, form, metric characteristics and thermophysical properties.

2.2. Solutions used for device design

The influence of the surfaces state on the deformation behavior of the device the constructive performance are considered for the irregularities range from C0 to C2 (C0 <C2). These results of poses have to make decisions according to the constructive characteristics and material support of the developed anode substrates - 1 - direction (Figure 4).

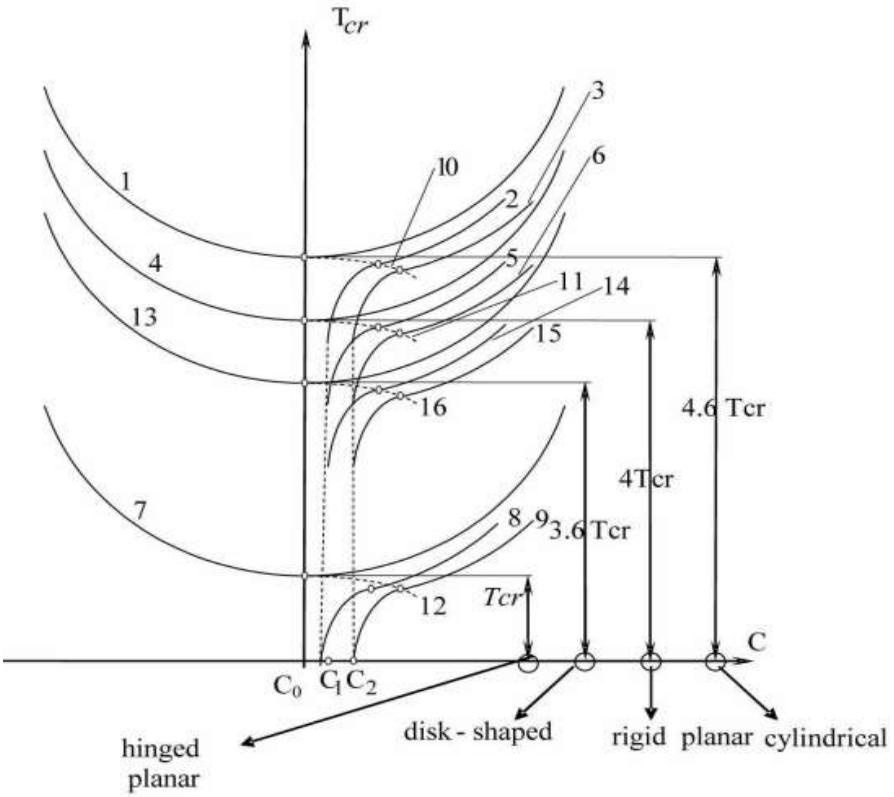

Figure 4. Critical temperature (T_{cr}) changes vs. surface irregularity for different SOFT design:
C_0, C_1, C_2 – Initial surface irregularities; Tier - critical temperature for rigid planar design; $3.6T_{1cr}$ – critical temperature for disc shaped design; $4T_{1cr}$ – critical temperature for hinged planar design; $4.6T_{1cr}$ – critical temperature for cylindrical design;
1 – SOFC cylindrical design with zero initial surface irregularity C=0;
2 – SOFC cylindrical design with initial surface irregularity C_1;
3 – SOFC cylindrical design with initial surface irregularity C_2;
4 – SOFC rigid planar design at initial surface irregularity C=0;
5 – SOFC rigid planar design at initial surface irregularity C_1;
6 – SOFC rigid planar design at initial surface irregularity C_2;
7 – SOEC hinged planar design at initial surface irregularity C=0;
8 – SOC hinged planar design at initial surface irregularity C_1;
9 – SOFC hinged planar design at initial surface irregularity C2;
13 – SOFC disc shaped design with zero initial surface irregularity C=0;
14 – SOFC disc shaped design with initial surface irregularity C_1;
15 – SOFC disc shaped design with initial surface irregularity C_2;
10, 11, 12, 16 – accordingly, surface irregularity characterizing the decrease of T_{cr} with approaching irregularity.

The application of the form, metric characteristics and material execution of dense elements are considered for various operational temperatures and are presented in the logarithmic coordinates (Figure 5).

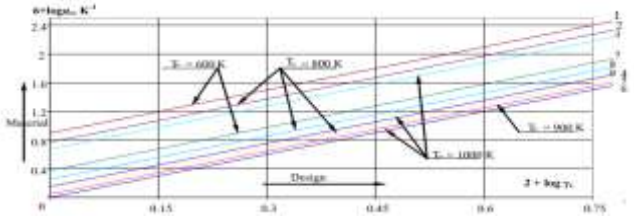

Figure 5. Materials properties vs. SOFC design:
1,2,3 – cylindrical$ 4,5,6 – planar;
7,8,9 – disk-shaped SOFC designs

The results obtained allow you to make decisions for the design of devices from dense materials with a different metric characteristic, form of execution and properties of material support.
Thus compatible combinations of these indicators for various operating temperatures might be determined.

2.3. Influence of the elements surface on the stability of the SOFC design

The third direction of work – to study of porous materials for use in the practice of designing a device as a whole and their elements. This issue has been discussed many times with project partners. With his great support and faith in the possibility of application in the practice of creating devices, the following task has been set and solved:

Development goal – the study of the deformation behavior of porous structure and the determination of an adequate deformation model for this behavior, taking into account mass transfer processes in a dynamic model for planning and effective implementation of various measures aimed at designing devices using of a similar material structure

Task content:

1. The problem of determining a mathematical model of deformation behavior and studying, on this basis, the stress-strain state of porous structure under quasi-static and dynamic loading is being solved.
2. The presence of mass transfer during loading, etc. the dynamism of porous structure distinguishes and is decisive for choosing their equations of state.

III. PROBLEM SOLUTION

The mathematical model of deformation behavior for studying the stress-strain state of any medium with a porous structure includes 21 equations, of which:

- 9 equations of the form ε= ε(u) define geometric ratios;
- 9 equations of the form σ= σ(ε) define physical ratios;
- 3 equilibrium equations (or equations of motion if dynamic loading is considered).

Source dependencies:

1. A porous structure is considered, inclu ding a solid phase from the skeleton of the structure and a phase of the filling pore.
2. Reduced modulus of elasticity porous structure is defined as [1,9]:

$$E_{pr} = \frac{m_s E_s + m_g E_g}{m} \quad (1)$$

where E_{pr} is the reduced modulus of elasticity; m, m_s, m_g are, respectively, the masses of the porous structure, the skeleton of the structure and medium fills the its pores; E_s and E_g – respectively, the Young's modulus of the skeleton and the medium that fills the pores under compression.

During operation, the porous structure is also deformed under the influence of external factors. This contributes to the migration of the medium filling the pores in the direction of the pressure gradient - P in the pores, as a result of which the volume of the medium filling the pores changes, i.e. as a view from (1) E_{pr} is a function of time and therefore

$$E'_{pr} = \frac{m_s(E_g - E_s)}{(m_s - m_g)} m'_g \quad (2)$$

Under quasi-static loading, which provokes a slow change in the stress state of the porous structure due to displacement, the mass of the medium filling the pores mg decreases (how many this is also question and must be defined!! This task is currently being studied)

Dependency analysis for E_{pr}:

1. It is assumed that only mg changes with time, i.e. $m_g < 0$;
2. For most porous structures $E_g < E_s$;
3. Then from (2) due to the fact that $m_s(E_g - E_s) < 0$ and $m_g < 0$, then $E_{pr} > 0$, which means that over time the reduced modulus of elasticity for a porous structure, containing a certain medium in the pores increases, t .e. the tension diagram between the normal stress "σ" and the relative strain ε for uniaxial tension in various modes (see Figure 1) will have the form (see Figure 2)

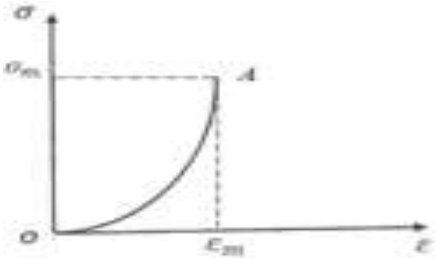

Figure 6. Tension diagram of a porous structure, the pores of which are filled with a medium, where σ_m, ε_m are the maximum values, respectively, of stress and strain

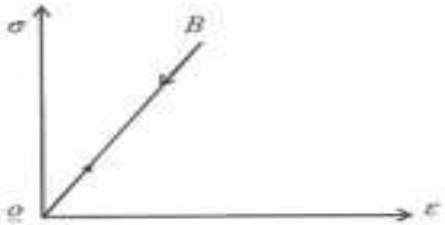

Figure 7. Tension diagram of a porous structure, the pores of which are filled with a medium (high-speed loading)

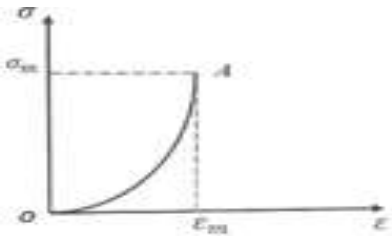

Figure 8. Tensile diagram for a non-porous elastic-plastic structure

Thus, we can conclude that when the stress-strain state of a porous structure is studied, depending on the loading rate, different equations of state should be used, i.e.:

1. With dynamic processes, i.e. under impulse loads, the dependence $\sigma = \sigma(\varepsilon)$ is represented by a straight curve, as a result of which the equation of state can be expressed by the Hook law.
2. Under quasi-static loading, i.e. for time-distributed loads, the application of the HUK law can lead to large inaccuracies (up to 80%). This is especially true for porous structures, in which the loading process is characterized by the presence of mass transfer and which have deformation characteristics that coincide with the characteristics for elastic-nonlinear bodies.

Thus, the equation $\sigma = f(\varepsilon)$ of the load diagram branches can describe both plastic and nonlinear elastic deformation of a body with a porous structure.

Hence, to obtain the equation of state for porous body, the equation of state for structures with an elastic-plastic characteristic can be used.

Consequently, as a result of the analysis of the dependence that determines the change in one of the mechanical indicators - the reduced modulus of elasticity for the porous structure, two possible variants of its loading, different in terms of deformation behavior, have been established, namely:

1. Quasi-static (the reduced modulus of elasticity E_{pr} increases);
2. Speed loading (the reduced modulus of elasticity E_{pr} remains permanent).

As the initial equation, the functional dependence for elastic media in the form of the stress tensor σ_{ij} on the components of the strain tensor ε_{ij} , the components of the metric tensor g_{ij} and external disturbances (temperature, pressure and radiation dose) in various combinations is used, which is represented by the dependence below:

$$\sigma_{ij} = f_{ij}\left(\varepsilon_{\alpha\beta}, g_{\alpha\beta}, T - M, D\right),$$
$$i, j, \alpha, \beta = 1,2,3$$

To determine the equation of state for elastic and elastic-plastic structures in a general form, the method of expansion in a Taylor series of the original above equation was used to study the functional dependence σ_{ij} and ε_{ij} at T, P = constants, D = 0, which is presented both for stresses and for deformations:

$$\sigma_{ij} = Pg_{ij} + Q\varepsilon_{ij} + R\varepsilon_{ik}\varepsilon_{kj}, \quad i, j = 1,2,3$$
$$\varepsilon_{ij} = Ag_{ij} + B\sigma_{ij} + C\sigma_{ik}\sigma_{kj}$$

where P, Q, R are functions of the invariants of the strain tensor and the stress tensor . In a particular case, it is assumed that $P = lq$, $Q = 2m$, $R = 0$, l, m – Lame coefficients; $q = e_{ij}\, g_{ij}$ – relative volume change or the first strain invariant

To describe the deformation behavior of elastic-plastic structure, an analogy was used between the deformation characteristics of elastic and plastic structures in the processes of loading and unloading, which is based on the assumption that there are no constant values of the elastic modulus and yield strength for deformable porous structures.

After carrying out a number of mathematical calculations, the equations of state of porous structures were ob-

tained for the variants of their loading, respectively, by quasi static (a) and dynamic loads (b):

$$\varepsilon_{ij} = (1 - k_0)\left(\frac{1+\nu}{E_{sek}}\sigma_{ij} - \frac{\nu I_1}{E_{sek}}g_{ij}\right) \qquad (a)$$

$$\varepsilon_{ij} = \frac{1+\nu}{E_{pr}}\sigma_{ij} - \frac{3\nu}{E_{pr}}\sigma_{ij} \qquad (b)$$

IV. CONCLUSIONS AND RECOMMENDATIONS

1. An algorithm has been developed for the synthesis of dense structure materials based on zirconium with properties that are compatible combinations with the operating temperature, shape and metric characteristics of devices from these materials;
2. It has been proven that porous structures are characterized by nonlinear elastic behavior under quasi-static loadings developing in time;
3. The equations of state are obtained and a mathematical model of the deformation behavior of porous structures is formulated to study their stress-strain state, taking into account the corresponding loading modes
4. It has been established that when Hooke's law is used as an equation of state to describe the deformation behavior of porous structures under quasi-static, i.e. loads distributed in time can contribute to 80% distortion of their stress-strain state.
5. The expansion in Taylor series of the original functional dependence was used, which determines the physical and geometric relationships in deformation behavior and, as a result, equations of state were obtained in general form for structure with elastic, elastic-plastic and nonlinear-elastic deformation character rustics.
6. The obtained dependences allow us to investigate various problems of studying the stress-strain state of porous structures under various loadings, determined taking into account the implemented technological measures in the process of generating electricity by fuel cells on an anode substrate.

ACKNOWLEDGMENT

The authors express their sincere gratitude for this work, which was carried out with the financial support of the project G5949 “Light-Weight 600 °C Solid Oxide Fuel Cells for Energy Security (LW – SOFC) of the NATO Science for Peace and Security Division during the period 2022 – 2024 years.

REFERENCES

[1]. R. A. Hasanov, O. Vasylyev, A. Smirnova, A. S. Gulgazli, *Modeling design and analysis of multi-layer solid oxide fuel cells*. USA: Hydrogen Energy, Vol. 36, pp.1671-1682, 2011.
[2]. Sharifullina E.R., Shveykin A.I., Trusov P.V. Review of experimental studies on structural superplasticity: Internal structure evolution of material and deformation mechanisms / PNRPU Mechanics Bulletin 3 (2018) 103-127 DOI: 10.15593/perm.mech/2018.3.
[3]. *Handbook of physical constants of rocks*. / Ed. S. Clark, M.: Peace, 544 p.,1969.
[4]. Yu. N. Rabotnov, *Creep of structural elements*, M.: Nauka, 712 p., 1988.
[5]. Ilyushin A.A. Plasticity. Ч.1. Elastic plastic deformations. – M.: Лoroc, 2004. – 388 c.
[6]. V. N. Nikolaevsky, K. S. Basniev, A.T. Gorbunov, G.A. Zotov, *Mechanics of saturated porous media*, M.: Nedra, 335 p.,1970.
[7]. J. Milewski, M. Wołowicz, R. Bernat, Ł. Szabłowski, and J. Lewandowski, “*Variant analysis of the structure and parameters of SOFC hybrid systems*, Applied Mechanics and Materials, Vol. 437, pp. 306–312, 2013.
[8]. D. H. Jeon, *A comprehensive CFD model of anode-supported solid oxide fuel cells*, Electrochimica Acta, Vol. 54, no. 10, pp. 2727–2736, 2009.
MECHANICS OF COMPOSITE MATERIALS. — 2021. — Vol. 57, No. 5. — P. 805—1022, ISSN 0203-1272
[9]. https://doi.org/10.22364/mkm.57.5.01

R.A. Hasanov, S,A. Musevi, G.S. Kheyrabady
Faculty of engineering, Azerbaijan State University of Oil and Industry,