ASSESSMENT OF THERMOMECHANICAL BEHAVIOUR OF SOFC EXECUTIVE DESIGN ELEMENTS

Ramiz Hasanov, Javahir Gasimova
•
Azerbaijan State Oil and Industry University
ramiz.hasanov52@gmail.com
gasymova1974@list.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, thermal strain stresses

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 green house 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. 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.

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 Fig. 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.

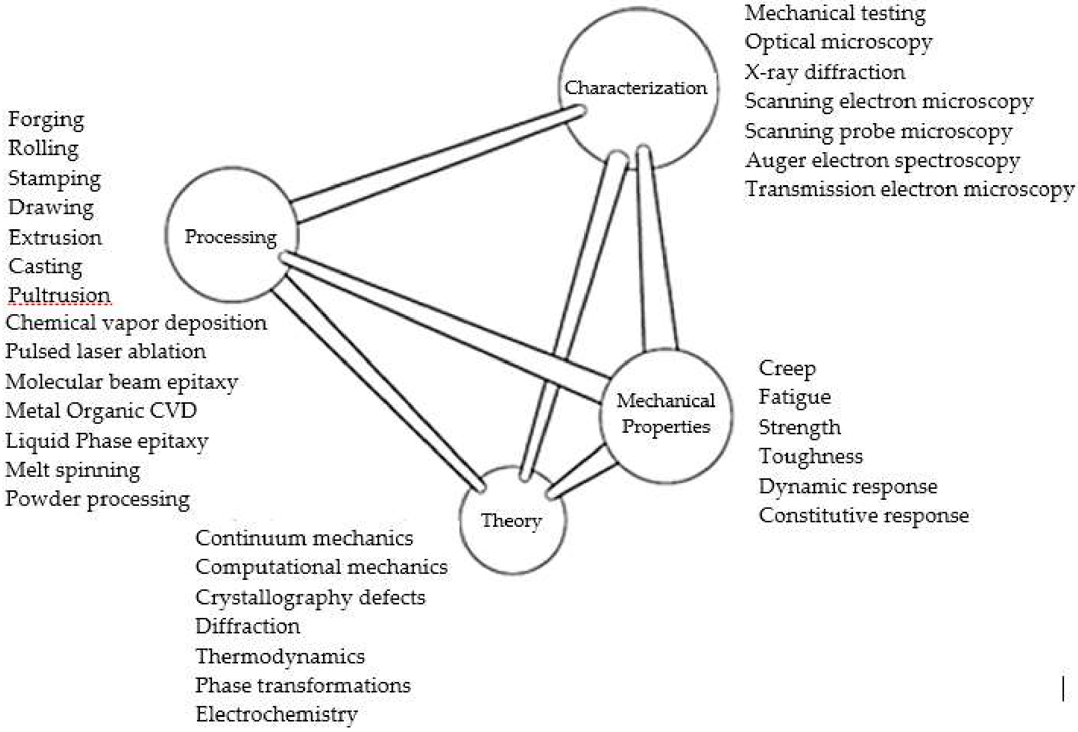

Fig. 1: *Tetrahedron, which contains four principle elements*

This entry will endeavor to answer the question whether SOFC technology is now ready for the market or perhaps put in another way: Is the market ready for SOFC technology and which challenges still need to be addressed?

The entry will describe how SOFC technology can contribute to solving the energy challenges in the future. The current status of the SOFC technology and industry will be briefly discussed and the possible markets described. Three main challenges on the road to competiveness – **life- time, reliability, and cost – are addressed.** Technoeconomic studies of the different market segments are used to define the threshold for market entry. The entry ends by looking ahead and concluding that the SOFC technology is ready for the market with respect to the projected cost and lifetimes, but that reliability under real-life conditions still remains to be demonstrated. The learning investments needed, however, do not appear to be prohibitive considering the benefits which this game - changing technology has to offer.

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).

Among different types and scale power generation systems, fuel cells have received more attention, because they can provide also both heat and power.

Advantages of SOFC Fuel Cells are:

- Higher electrical efficiency. The SOFC technology will be able to provide an electrical efficiency of up to 60%. This efficiency is very high compared to worldwide power plants operating at average electric efficiencies of 30–35% and to existing decentralized, smaller power generation equipment (engines and generators) operating at as low as 5–10% for engines and 15–25% for generators. Application of SOFC units with higher electrical efficiency will result in substantial savings in fuel and money, and for operation on fossil fuels also in a proportional reduction in CO_2 emissions.

- High efficiency for all capacities. The SOFC technology is scalable and can cover the complete range from 1 kW to 1 MW, or even higher, with almost no loss of efficiency. The technology offers a very competitive output per weight or volume compared to power plants. Because of this, the SOFC technology addresses a wide range of applications and finds use both in urban and remote areas and both for stationary and mobile purposes.

- Fuel flexibility. The SOFC technology is (together with MCFC) the only technology among the different fuel cell technologies which is able to effectively generate power directly based on the fossil fuels in use today, and at the same time, the technology has a clear path to renewables and CO2-neutral energy systems. This is due to the higher operating temperatures and the superior ability of the SOFC to convert hydrocarbon in the fuel cell stack.

- Lower maintenance cost. The SOFC system provides a highly effective and direct electrochemical conversion of fuel to power. The only rotating parts in the system are a fuel pump and a small air blower. Accordingly, maintenance costs are expected to be substantially lower, and operating periods between overhauls are substantially longer than conventional technologies (see Fig. 2).

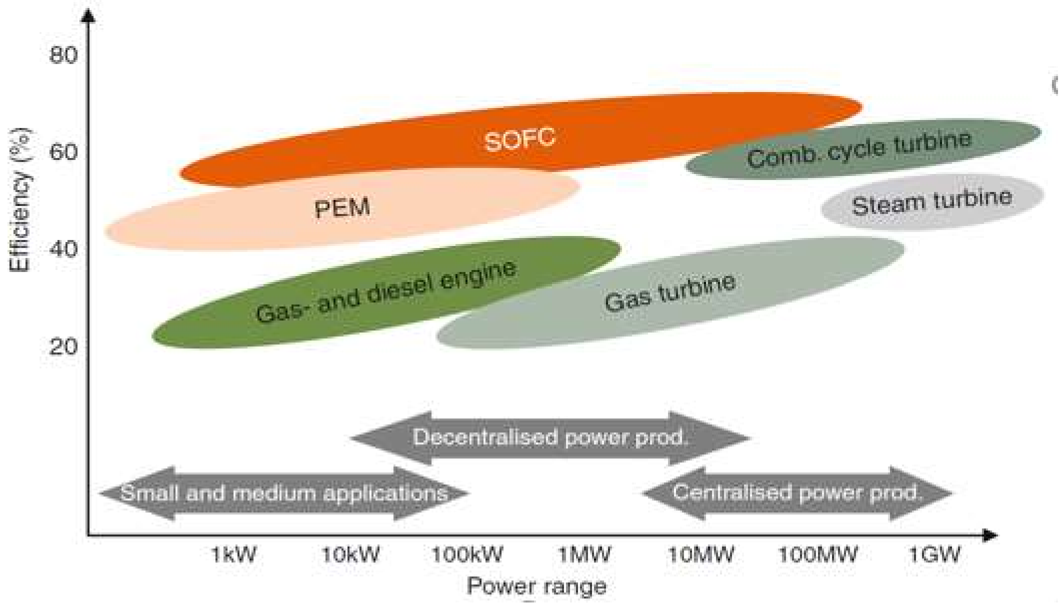

Fig. 2: *SOFC compared with other power production technologies (illustrative figures)*

II. New approach to risk forecasting

The increasing penetration of renewable energy sources (RES) and distributed generation (DG) technologies introduces significant uncertainties related to reliability, lifetime, and structural endurance of energy systems. Traditional risk forecasting methods, which primarily rely on statistical performance data of conventional power plants, are insufficient for technologies such as Solid Oxide Fuel Cells (SOFCs), photovoltaic systems, or wind turbines. These systems operate under highly dynamic loading conditions, where thermal, mechanical, and rheological properties of materials play a decisive role.

The proposed new approach to risk forecasting integrates thermomechanical modeling, rheomechanical behavior analysis, and structural endurance assessment. Unlike conventional reliability analysis, this methodology explicitly accounts for:

- Coupled stress–strain–temperature interactions in multilayer SOFC structures;
- Creep and plastic deformation effects under prolonged operation at elevated temperatures;
- Anisotropy and nonlinearity of material properties**, including imperfections and manufacturing deviations;
- Dynamic operational risks arising from fluctuating loads in renewable energy integration.

By applying the developed energy theory of deformation and incorporating experimental creep-core parameters, the model enables quantitative estimation of critical operational thresholds, such as the onset of plastic deformation, buckling time, and long-term endurance limits. This predictive framework allows for risk-informed design of SOFC systems, providing more accurate forecasts of reliability and lifetime under real operating conditions.

Such a forecasting methodology forms the foundation for technoeconomic risk evaluation, ensuring that decisions on large-scale deployment of SOFCs and other advanced energy technologies consider both their mechanical stability and economic feasibility. Ultimately, this new approach supports the safe and efficient integration of next-generation power generation systems into modern energy infrastructures.

III. Engage experts

Structural strength of materials – a set of mechanical properties that ensure reliable and long-term operation of the material under operating conditions depend on a number of factors (see Fig.3)

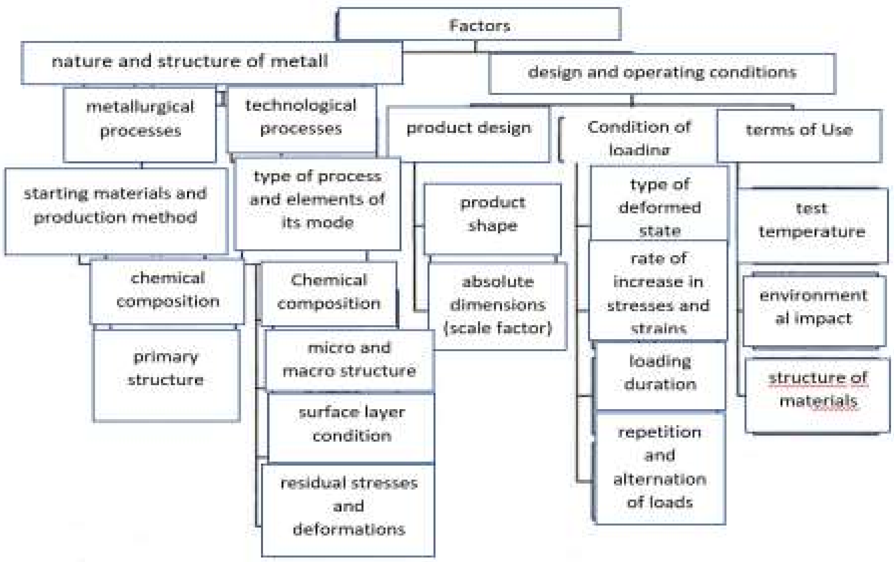

Fig. 3: *Factors define reliable and long-term operation of the material*

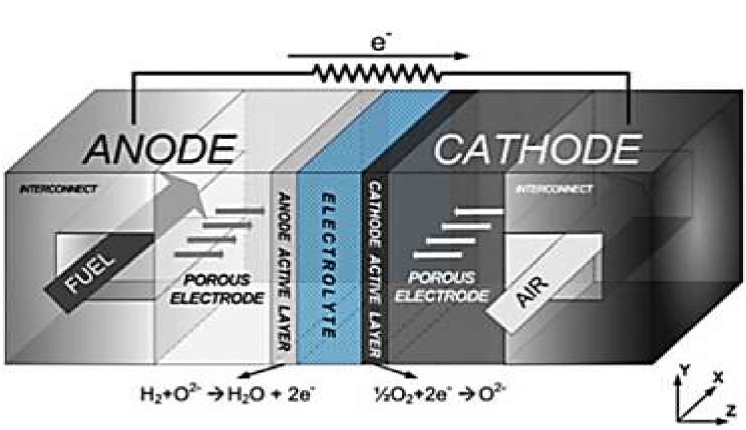

Fig. 4: *Schematic of the basic operation principles of a SOFC (I. Bonis 2012)*

Depending on the location of the loading path to the yield surface, as well as on the radius of the yield surface and the location of its center, different deformation behaviors can occur. This behavior depends on various parameters, the clarification of which will make it possible to determine the degree of correlation between the elastic and plastic parts of the total deformation (see Fig. 5 and 6).

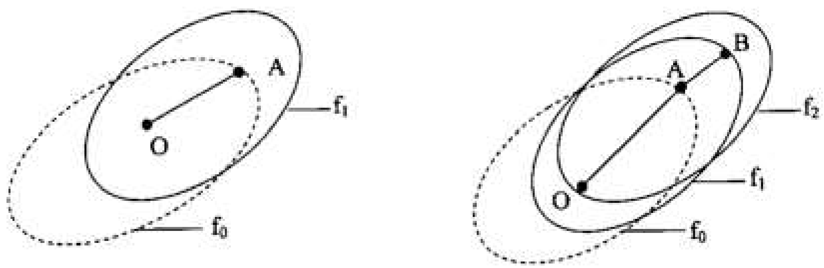

Fig. 5: *Elastic deformation behavior:*
f_1 - yield surface under repeated loading; f_2 - is the limit state yield surface corresponding to destruction; OAB - trajectory of the path of active loading; Point "O" - a geometric place with zero stresses

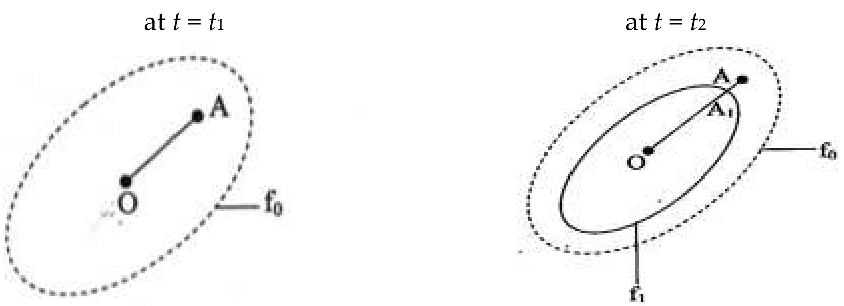

Fig. 6: *Creep deformations ($t_1 < t_2$)*

Therefore, a brief review of recent studies confirms the fact that the simplifications adopted in the preparation of mechanical and theoretical models for the rheomechanical properties of materials and their changes, loading modes and deformation state significantly affect attempts to determine and evaluate SOFC performance and quality indicators, taking into account operational conditions. Therefore, in our opinion, in order to fill this void, it was necessary to develop a theory and an appropriate research methodology that would allow modeling deformation behavior and creating strength conditions for real structures, taking into account real operating conditions.

Such a theory, called energy theory, was developed, which was based on a hypothesis that characterizes both physically and mathematically the deformation processes under repeated loading and has the following content.

The work of the total elastic deformation in the stress space for the case of any static loading in opposite directions is a constant value. Mathematically, this means that: If the point with coordinates "σ_{ij}" in the stress space is on the yield surface, then the point with coordinates - $\sqrt{\frac{\sigma_{1T}^2+\sigma_{2T}^2}{J_1+2(1+V)J_2}-1}\cdot\sigma_{ij}$ is also on the yield surface. Graphic representation of the mathematical value of the proposed theory (see Fig. 7):

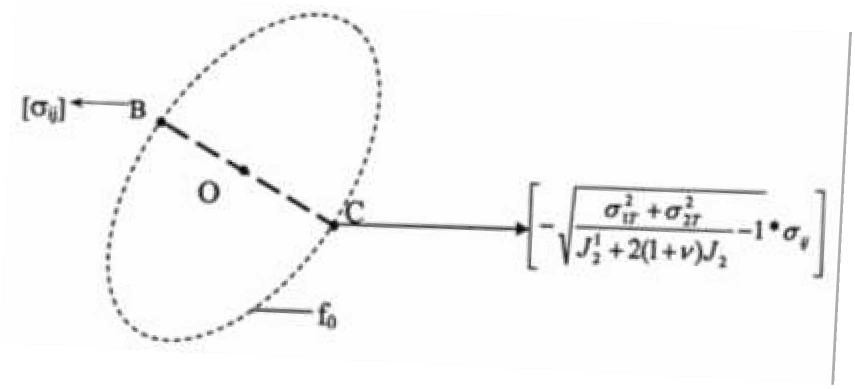

Fig. 7: *Graphical representation of the mathematical significance of the proposed energy theory*

From this, the yield surface equation is obtained in the for

$$\bar{J}_1^2+2(1+\nu)\bar{J}_2=\bar{\sigma}_T^2,$$

where σ_{1T} and σ_{2T} – respectively, the tensile yield strength and compression; J_1 and J_2 - respectively, the first and second invariants of the tensor stresses; σ_{ij} (i, j = 1,3) – stress tensor components; ν – коэффициент Пуассона; $\bar{J}_1$ и $\bar{J}_2$ – respectively, the first and second invariants of the tensor stress differences $(\sigma_{ij}-\sigma_{ij}^1)$, σ_{ij}^1 – coordinates of the yield surface center; J_1^0 and J_2^0 – respectively, the first and second invariants of the tensor stresses at the end of the active loading path;

$$\bar{\sigma}_T^2=\left(J_1^{02}+2(1+\nu)J_2^0\right)\left(\frac{K_0+1}{2}\right)^2;$$

$$K_0=\sqrt{\frac{\sigma_{1T}^2+\sigma_{2T}^2}{J_1^{02}+2(1+\nu)J_2^0}-1};$$

$$\sigma_{ij}^1=\frac{1-K_0}{2}\sigma_{ij}^0$$

The implementation of these phenomena makes it possible, on the basis of appropriate strength conditions, to evaluate and calculate the bearing capacity of structural elements of the SOFC type, taking into account the structural and rheomechanical properties and changes in their material support under operating conditions, loading modes, deformation anisotropy, geometric nonlinearity (finiteness of deformations during buckling) and etc. for the following deformation states:

- elastic state with stable and changing physical and mechanical properties of materials;
- elastic-plastic state, taking into account changes in the physical and mechanical properties of materials and deformation anisotropy;

- elastic-viscous-plastic state, when changes in the mechanical properties of materials contribute to the occurrence of creep deformation.

A method has been developed for studying the stress-strain state of structural elements, taking into account geometric nonlinearity in the absence (presence) of initial imperfections (manufacturing errors). Here, the subjects of study are the time of onset of plastic deformation, the critical time of onset of buckling, the critical load of buckling, etc. In this case, the rheological properties of materials are characterized by the corresponding model of the creep core and its parameters (to determine them, it is necessary to conduct appropriate experimental studies).

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.

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.

The numerical analysis of thermo physical 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.

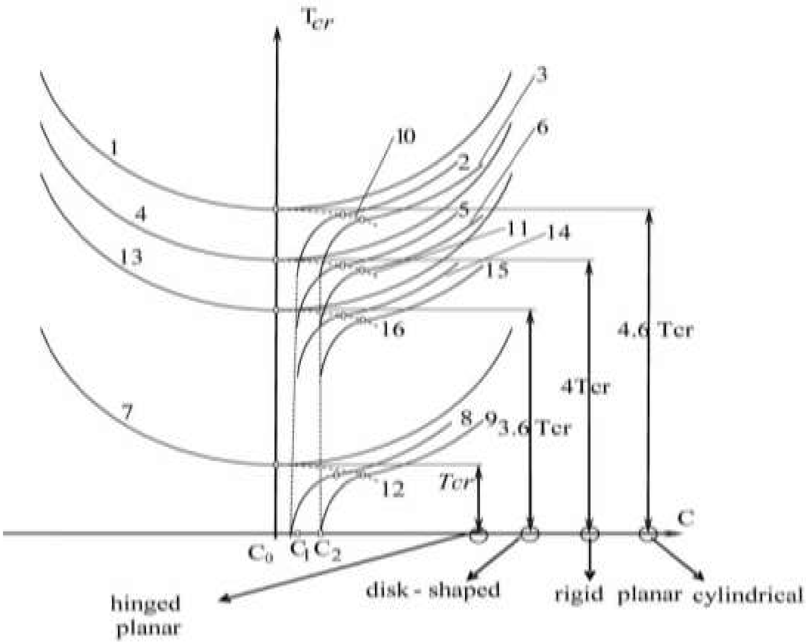

Fig. 8: *Critical temperature (T_{cr}) changes vs. surface irregularity for different SOFT design:*
C_0, C_1, C_2 – Initial surface irregularities; Tier - critical temperature for rigid planar design; $3.6T_{cr}$ – critical temperature for disc shaped design; $4T_{cr}$ – critical temperature for hinged planar design; $4.6T_{cr}$ – 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 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.

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 thermo-physical properties.

The influence of the surfaces state on the deformation behavior of the device the constructive performance are considered for the irregularities range from C_0 to C_2 ($C_0 < C_2$). These results of poses have to make decisions according to the constructive characteristics and material support of the developed anode substrates - 1 - direction (see Fig. 8).

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 (see Fig. 9).

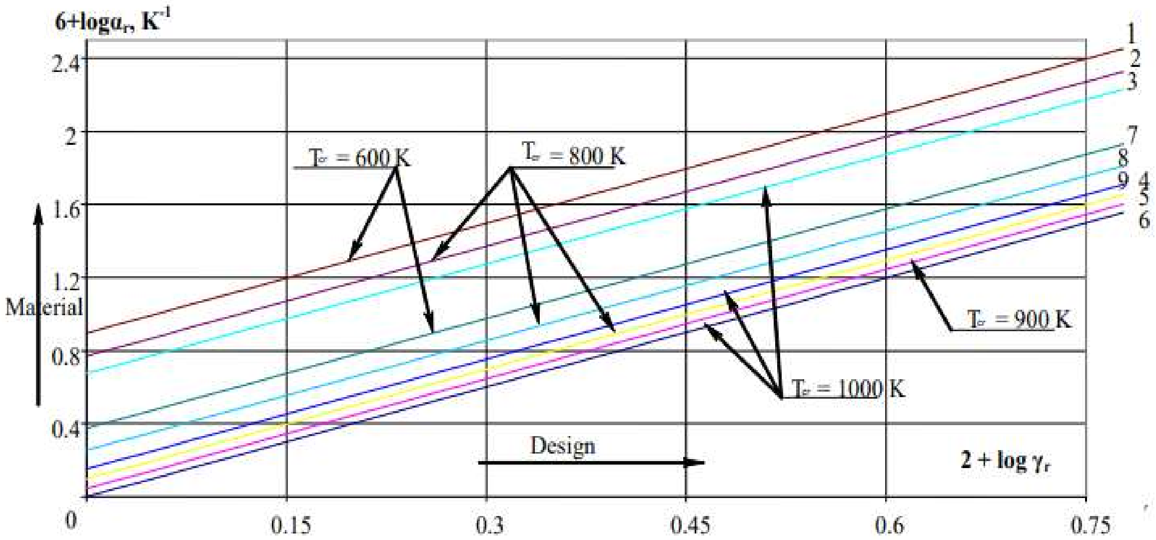

Fig. 9: *Application of shape, metric characteristics and material design of dense elements for different operating temperatures represented in logarithmic coordinates: 1,2,3 – cylindrical; 4,5,6 – planar; 7,8,9 – disk-shaped SOFC designs*

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.

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.

In all models the most commonly used materials were studied to analyze the distribution of thermal stress. The mechanic properties of materials were listed in Table 1 taken from Refs. properties of materials were listed in Table 1 taken from Refs [8, 23]. It should be noted that the material was assumed as linear elastic and isotropic. Fig. 10 showed the anode's coefficient of thermal expansion, which was a function of its porosity [30]. Moreover, the Young's modulus (GPa) and shear modulus (GPa) was a function of porosity, which was the main point all of investigations and could be calculated from the used for that experimentally obtained equations.

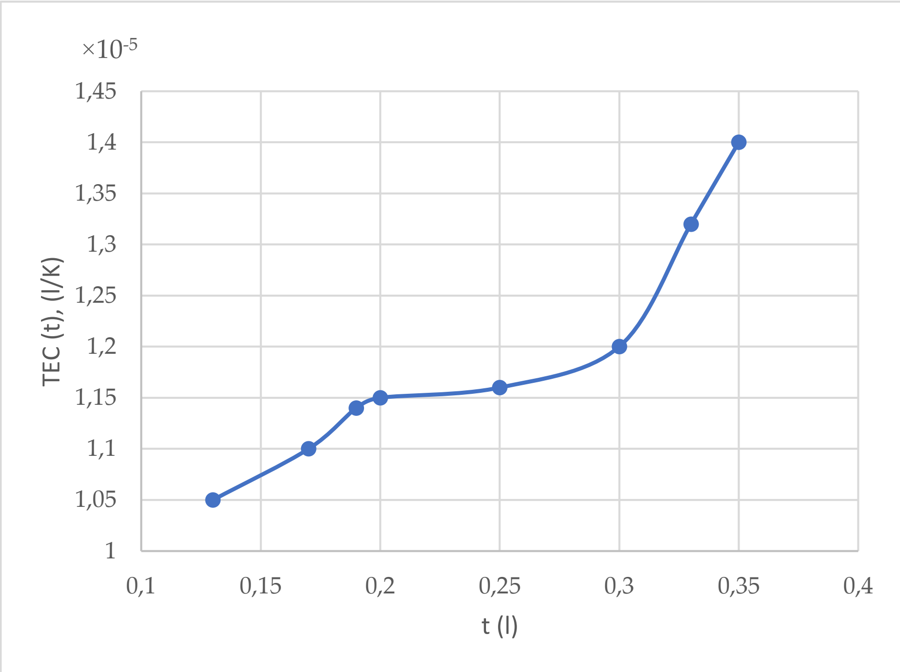

Fig. 10: *The relationship between porosity and TEC*

The thermal strain stress was enhanced when the temperature increased, which resulted in a thermal expansion, which was different for each material (Table 1). The thermal stress was proportional to the coefficient of thermal expansion (a) and the difference of the temperature distribution (T) and the reference temperature (Tref). The reference temperature was the sintered temperature for the cell’s materials and it was set as 800 C, i.e., the thermal strain stress only emerged when the temperature was higher than 800 C.

Table 1: *The key stress factors for the modeling SOFC*

Layer	Young’s Modulus [GPa]	Poisson’s ratio	Coefficiant thermal expantion (CTE), [$10^{-6}K^{-1}$]
Anod	220	0.3	12.5
Cathod	160	0.3	11.4
Electrolyte	205	0.3	10.3
Interconnect	205	0.28	12.3

V. Conclusion

1. A classifier has been compiled of factors that determine the load-bearing capacity and quality indicators of technological machines, and in general their effectiveness, having different material design in terms of structural, physical-mechanical and chemical-thermal properties, causing of vary deformation behavior in structural materials under various operating conditions and loads.
2. Isotropic and kinematic Mises plasticity curing rules are available, is confirming existing of isotropic and kinematic curing linear combination in the process of exploration under operating modes.
3. This allows for the existence of two systems of forces that contribute to changes in both the volume and shape of the structural material and causing mainly plastic deformation behavior.
4. Changing in both the volume and shape of the structural material contribute to changes in the radius, coordinates of the yield surface center, as well as the location of the active loading path in relation to its position.
5. A new method for determining coefficients of statical and dynamical plasticity (SCP and DCP) for various groups of materials is presented.
6. To determine the estimate of plasticity coefficients , the linear law of Hencky-Mises for materials hardening was used and for determining the static and dynamic hardening coefficients corresponding analytical expressions are obtained.
7. The obtained dependences of the plasticity coefficients make it possible to evaluate the properties of the plastic deformation behavior of structural materials individually and in combination with others, which have unequal plastic and structural-mechanical properties i.e. meaning of flat - shaped hybrid structure.
8. 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.
9. It has been proven that porous structures are characterized by nonlinear elastic behavior under quasi-static loadings developing in time.
10. 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.
11. 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.
12. 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.
13. 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 – 2025 years.

CONFLICT OF INTEREST.

Authors declare that they do not have any conflict of interest.

References

[1] Hasanov R., Vasylyev O., Smirnova A., Gulgazli A. Modeling design and analysis of multi-layer solid oxide fuel cells. USA: Hydrogen Energy, Vol. 36, 2011, pp.1671-1682.

[2] Kachanov L. M. Fundamentals of creep theory. M.: Nauka, 1969, 420 p.

[3] Handbook of physical constants of rocks. / Ed. S. Clark, M.: Peace, 1969, 544 p.

[4] Rabotnov Yu. N. Creep of structural elements, M.: Nauka, 1966, 780 p.

[5] Amenzade Yu. A. Theory of elasticity, M.: Higher School, 1976, 275 p.

[6] Nikolaevsky V. N., Basniev K. S., Gorbunov A.T., Zotov G.A. Mechanics of saturated porous media, M.: Nedra, 1970, 335 p.

[7] Milewski J., Wołowicz M., Bernat R., Szabłowski Ł., and J. Lewandowski, (2013) Variant analysis of the structure and parameters of SOFC hybrid systems. Applied Mechanics and Materials, 2013, Vol. 437, pp. 306–312.

[8] Jeon D. H. A comprehensive CFD model of anode-supported solid oxide fuel cells. Electrochimica Acta, 2019, Vol. 54, No. 10, pp. 2727–2736.

[9] Antman S. Nonlinear Problems of Elasticity.2nd edition, 2015, 838 p. – Springer.

[10] Baud P., Wong T. Shear-enhanced compaction and strain localization: inelastic deformation and constitutive modeling of four porous sandstones. Journal Geophysical Research, 2016, Vol. 111, is. B12, doi:10.1029/2005JB004101.

[11] Guliyev A., Kazymov B. Deformation of rocks and its influence on their filtrations-capacitor properties and on processes of a filtration and development of oil and gas deposits. Baku: Elm, 2019, 88 p.

[12] Delin T., Zheng Ch. On A General Formula of Fourth Order Runge-Kutta Method. Journal of Mathematical Science & Mathematics Education, 2012, 7, (2), pp.1-10

[13] Chan, A. A unified finite element solution to static and dynamic geomechanics problems. Ph. D. Thesis C/Ph/106/88, University College of Swansea, 1998.

[14] Chai, Z., Shi, B., Lu, J., Guo, Z. Non-Darcy flow in disordered porous media: A lattice Boltzmann study. J. Computers & Fluids 39, 2010, pp.2069–2077.

[15] Jeon D. A comprehensive CFD model of anode-supported solid oxide fuel cells, Electrochemical Acta, 2019, Vol. 54, No.10, pp. 2727–2736.

[16] Jones R. Deformation theory of plasticity. Bull Ridge Corporation, 2009, 622 p.

[17] Ju B. Mathematical model and numerical simulation of multiphase-flow in permeable rocks considering diverse deformation. Journal of Petroleum Science and Engineering, 2014, Vol.119, pp.149-155.

[18] Holm B., Ahuja R., Johansson B. Ab initio calculations of the mechanical properties of Ti3SiC2 Appl. Phys. Lett. 79:1450–52, 2001.

[19] Pietzka M., Schuster J. Summary of constitution data of the system Al-C-Ti. J. Phase Equilib.15:392–400, 1994.

[20] Vasilev A., Sotnik A. and Slis I. An influence of porosity of fracture toughness of brittle powder materials. Electron Microscopy and Strength of Materials, Institute for Problems of Materials, Kiyev, 1989.

[21] Yokokawa, H. Understanding materials compatibility, Annual Review of Materials Research, 2003, Vol. 33, pp. 581–610.

[22] Zenga S., Min Xua M., Parbeya J., Guangsen Y., Andersson M., Lic Q., Baihai Lia B., Lia T. Thermal stress analysis of a planar anode-supported solid oxide fuel cell: Effects of anode porosity, international journal of hydrogen energy, 2017, pp.1–10. www.elsevier.com/locate/he

[23] Norouz Mohammad Nouri Amin Mirahmadi, Majid Kamvar.A twodimensional numerical model of a planar solid oxide fuel cell. J. Iran. Chemical. Research. 3, 2010, pp. 257-269.

[24] Baykov Yu. A. Physics of condensed matter. M.: Knowledge Laboratory, 2013, 294 p. http://e.lanbook.com/books/element.php?pl1_id=56908.

[25] Yuskaev V. B. Composite materials. Sumy: SumSU, 2006, 79 p. http://essuir.sumdu.edu.-ua/bitstream/12345678 /1929/3/Kom.pdf.

[26] Rabotnov Yu. N. Introduction to fracture mechanics. M.: Science. Ch. ed. physics and mathematics lit., 1987, 80 p. URL:http://www.ph4s.ru/book_razrushenie.html