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MODELLING OF MECHANICAL PERFORMANCES FOR PLANAR SOFC DEVELOPMENT

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ABSTRACT

In the present work the thermo mechanical stability of planar is considered. For determination of the stable SOFC structures and prevention of complications during the operation a theoretical model of the deformation behavior was developed and solved. According to the results of the numerical interpretation of the received model a rational ratio of geometric relations of the planar SOFC design is determined. For classification of the planar SOFC deformation behavior and evaluation of the mechanical and reological properties of the SOFC electrode elements materials .on influence of different levels of operating temperatures the experimental studies are conducted. Experimental studies were conducted on a specially prepared and equipped installation with appropriate devices. Taking into account the capabilities of the experimental setup and the appropriate test targeting a program and methodics of experiments for conducting in conditions of high loads and operating temperatures is developed. Based on the methodology and in accordance with a program of experimental studies the mechanical behavior of materials proposed for the manufacture of electrode systems of developed SOFC designs in the form of charts and graphs are analyzed and presented.

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INTRODUCTION

As it is known in all cases loading type of FC various constructive design, characterizing by duration, variability in time and coordinates, is thermal (Noda *et al.,* 2002; Lowrie and Rawling, 2000; Nakajo *et al.,* 2006) and determines the mechanical behavior of design, i.e. deformability and vitality. The same is typical for fuel elements of planar design and this constructive design is not exception. It should be mentioned if a lot of electrochemical and material questions of development and exploitation of SOFC -for existing constructive makings have been solved, then problems of mechanical behaviour in generating high temperatures of separate cell represented solid composites with various deformation behaviour of elements and also their use in stack require accurate definition. It is explained by the fact that scientists, power specialists, physics, chemists are mainly interested in improving problems of exploitation and commercial characteristics of fuel elements. But SOFC, as more practical and effective class of fuel elements equally with the main problems of their development and exploitation. What happens with solid body foliated macro compositions by which electrode system of fluid elements are modeled? In long thermal loadings in the course of time plastic deformations occur, they depend on time and creeping deformation appears. In such deformation behaviour showings of construction elements efficiency in connection with others have to be evaluated taking into account properties of the materials and their changings during the loading period. Both single layers of layered structure and construction, including planar SOFC as a whole, react to thermal loading especially and differently. Difference in mechanical behaviour of multilayered construction' layers promote for various deformational complications for the period its exploitation. Deformational complications are characterized by invertibility property. They become apparent as:

- Formation and cracks germination of various sizes, direction and extension on anode and cathode surfaces;
- Formation of cavity as a result of connectedness disturbance of multilayered construction' layers of SOFC design (pairs, accordingly anode-electrolyte, electrolyte-cathode);

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- Formation of curvature and swelling at the expense of advance mechanical fragility of single layers and construction as a whole.
- In conclusion manifestations of deformational complications in multilayered constructions as planar SOFC depend on mainly:
- Structural-mechanical and thermo-physical material properties' layers, as well as existing in their structure initial defects (heterogeneity, Assuring, etc.);
- Stress condition of multilayered macro composite construction caused by thermal loading and concomitant factors;
- Physico-chemical properties and kinetic characteristics of delivery and circulation working substances in systems of fuel and air delivery, etc.;

High profile in manifestations of deformational complications has also the shape of constructive SOFC design and combination its geometrical characteristics. Consequently, the right choice and rational combination of geometrical characteristics with the shape of constructive design as well as conditions and modes of exploitations are directions of prevention various deformational complications.

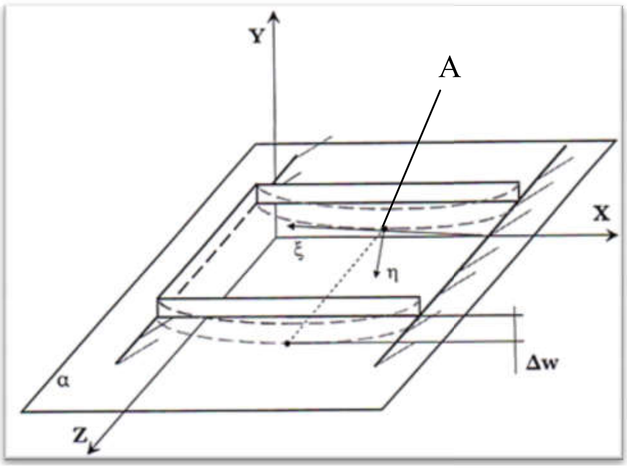

Figure 1. Mechanical model of single SOFC element.

1. **Problem AIM:** There is given a problem decision on determination stable in mechanical behaviour of SOFC planar design and rational combination of geometrical design parameters with regime-technological for preventions of deformational complications in this part.
2. **Problem setting:** The mechanical model is shown on the fig. 1 as multilayered plate deformable under influence of temperature loading.

Assumed that (see figure) plate fixed and limited by side surface. The plate is under impact of gravity force. The chosen system of coordinate (X,Y, Z) has combined beginning with low point of bended plate. Also assumed that the point with coordinates (x,0) before deformation occupies position with following coordinates (ξ,η|) after deformation process. The vectors of movement coordinates U(x) the following point marked as u(x), v(x), w(x).

Problem solution

For a start determines new coordinates of point "A", which moves due to deformation process of plate, in mobile combined with Euler coordinates depictured as:

$$\xi = X + U(x); \qquad \eta = W(x), \tag{1}$$

where $\xi, \eta|$ - coordinates of Euler system; x, y, z - coordinates of Lagrange system.

Then taking into account boundary conditions are shown the equation control of elemental section deformed plate with limited condition

$$W'(x=0)=0; \qquad \frac{d\eta}{dS}\int_{x=0} = 0 \text{ depictured as} \tag{2}$$

$$T\frac{1+u(x)}{\sqrt{(1+u(x))^2+w^2(x)dx}} = H;$$

$$T\frac{w(x)}{\sqrt{(1+u(x))^2+w^2(x)dx}} = q_0 x,$$

where T - tighting force directed to axis at a tangent to ds; q - weight unit of plate length. On the basis of equilibrium equations (2) taking into account boundary conditions after simple transformations determined displacements of elemental section as shown below (Hasanov *et al.,* 2007):

$$x + u(x) = \frac{H}{E}x + a\ln\left(\frac{x}{a} + \sqrt{1+\frac{x^2}{a^2}}\right);$$

$$w(x) = \frac{q_0}{2E}x^2 + \sqrt{a^2+x^2} - a, \tag{3}$$

where

$a^2 = H^2 \ / q_0^2$

E - multiplication of Yung module to area of cross section of plate; H - integral constant for determination. For three layered construction with thickness of layers 2hl, 2h2, 2h3, similar to SOFC (as 1 - anode, 2 - electrolyte, 3 - cathode) the axial movements of extreme cross sections of internal layers depictured:

First layer - $w\left(\frac{l}{2}\right) = (h_1\alpha_1 + h_2\alpha_2)T;$ (4)

Third layer $w\left(\frac{l}{2}\right) = (h_2\alpha_2 + h_3\alpha_3)T;$

where *l* - the length of plate.

Considering the equation of system (4) in each external layer and condition of plate jamming by the ends u(*l*/2)=0 derived the system of equations for determination of integral constant "H" and pressure force "q" between layers as shown:
- first layer (anode):

$$(h_1\alpha_1 + h_2\alpha_2)T = \frac{q_1}{2E}\frac{l^2}{4} + \sqrt{\frac{H^2}{q_1^2} + \frac{l}{4}} - \frac{H}{q_1};$$

$$\frac{Hl}{2E} + \frac{H}{q_1}\ln\left(\frac{lq_1}{2H} + \sqrt{1+\frac{l^2q_1^2}{4H^2}}\right) - \frac{l}{2} = 0 \tag{5}$$

third layer (cathode):

$$(h_2\alpha_2 + h_3\alpha_3)T = \frac{q_3}{2E}\frac{l^2}{4} + \sqrt{\frac{H^2}{q_3^2} + \frac{l^2}{4}} - \frac{H}{q_3}; \tag{6}$$

$$\frac{Hl}{2E} + \frac{H}{q_3}\ln\left(\frac{lq_3}{2H} + \sqrt{1 + \frac{l^2 q_3^2}{4H^2}}\right) - \frac{l}{2} = 0.$$

The solution of equation systems (5) - for first layer, anode, and (6) - for third layer, cathode after simple transformation and numerical interpretation of intermediate results for forces determination, applied to medium layer with electrolyte to external layers, corresponding to anode and cathode derived the following equations:

For anode: $q_1 = \dfrac{4{,}8E_1(h_1\alpha_1 + h_2\alpha_2)T}{l^2}$ (7)

For cathode: $q_3 = \dfrac{4{,}8E_1(h_2\alpha_2 + h_3\alpha_3)T}{l^2}$

where E_i, $h_i a_i$; - correspondingly to the module of elasticity, thickness and coefficient thermal expansion of i-numbered layer.

Using, for reasons of physics, the flexure approximation for researched constructive scheme (accordingly, hinged and rigid fixing of end section of SOFC) and developed variation principle have been determined the efforts and. appropriate critical value of temperature loading (see previous reports for April and October 2007). According to results of investigation the obtained dependences is determined the values of critical temperatures depend on value of the root of cubic equation as given below:

for hinged fixed plate: $A_1C_1^3 + A_2C_1^2 - A_3 = O;$ (8)

for rigid fixed plate: $A_4C_1^3 + A_5C_1^2 - A_6C_1 + A_7 = O,$ (9)

Where

$$A_1 = \frac{\pi}{4}\frac{b}{a};$$

$$A_2 = \frac{3}{4}\left(1 - \frac{h_2\alpha_2}{h_1\alpha_1}\right)\frac{9{,}6(1+\nu_1)(1-2\nu_1)}{2\pi(1-\nu_1)};$$

$$A_3 = \frac{1}{6}\left(\frac{h_1\pi}{a}\right)^2\left(1 + \frac{h_2\alpha_2}{h_1\alpha_1}\right)\frac{9{,}6(1+\nu_1)(1-2\nu_1)}{2\pi(1-\nu_1)};$$

$$A_4 = 3\left[4\left(1 + \frac{h_2\alpha_2}{h_1\alpha_1}\right)\frac{h_1\pi}{a}\frac{9{,}6(1+\nu_1)(1-2\nu_1)}{2\pi(1-\nu_1)}\right];$$

$$A_5 = 4\left[1 + \left(1 + \frac{h_2\alpha_2}{h_1\alpha_1}\right)1 - \frac{h_2\pi}{a}\frac{9{,}6(1+\nu_1)(1-2\nu_1)}{2\pi(1-\nu_1)}\right];$$

$$A_6 = 16\left(\frac{h_1\pi}{a}\right)^2\left[\frac{h_1\pi}{a}\frac{9{,}6(1+\nu_1)(1-2\nu_1)}{2\pi(1-\nu_1)}\right];$$

$$A_7 = 43\left[\left(1 + \frac{h_2\alpha_2}{h_1\alpha_1}\right)\left(\frac{h_1\pi}{a}\right)^3\frac{9{,}6(1+\nu_1)(1-2\nu_1)}{2\pi(1-\nu_1)}\right].$$

The equations (8) and (9) in any setting have at least one real root. Determination their roots was realized at simplification (special cases are considered):

1. When $C_1^3 \to 0$, i.e. equations are solvable squared.
2. When comparative volume change at the expense of outside forces influence equal to zero, i.e $1 - 2\nu_1 = 0$, accordingly,

$$\mu_1 = \frac{9{,}6(1+\nu_1)(1-2\nu_1)}{2\pi(1-\nu_1)} = 0$$

Some numerical calculations by obtained analytical expressions and their interpretation

Quantity calculations are carried out for below mentioned initial data [ ] on layers of multilayer plate:

- longitudinal size, accordingly layers – a_1 (anode)=a_2(electrolyte)=3,8 mm;
- CTE accordingly, $a_1$anode) =$1{,}22\cdot10^{-5}k^{-1}$; a_2(electrolyte) = $1{,}08 \cdot 10^{-5}k^{-1}$
- thickness, accordingly h_1(anode) = 0,04mm; h_2(electrolyte) = 0,15mm;
- Puasson coefficient, accordingly
- $\mu_1 = \dfrac{4{,}8(1+\nu_1)(1-2\nu_1)}{\pi(1-\nu_1)} = 1{,}069;\quad H_1 = \dfrac{\alpha_2 h_2}{\alpha_1 h_1};\quad b_1 = \dfrac{h}{a}\cdot\pi = 1177{,}5$

Mentioned below variants of planar SOFC constructions design was used as calculation variants, as it shown above:

-hingedly joint construction design;
-hard support construction design.

Calculation in direct (when sizes are given and operation temperature in determined) and adverse (when operation temperature is limited and rational correlation of layer sizes are determined) organizations have been carried out.

Calculations for comparative evaluation of temperature stability of mono and poly layer constructions are also carried out. It has been determined that:

-polylayer constructions are stable in temperature influences in comparison with monolayer construction for =(52-5-58)%;
-for monolayer construction stability in operation temperature equal to 1000 K, is provided in size correlations

$$\gamma = \frac{a}{h} \leq 28$$

-for polylayer construction dependence operation temperature and size correlation is shown in the Fig. 2:

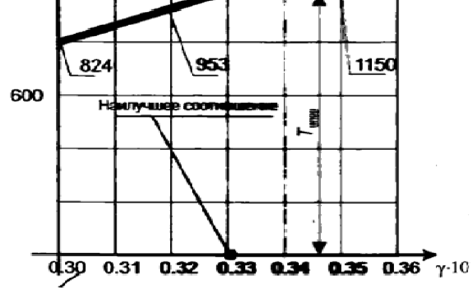

Figure. 2. Dependence of critical temperature of planar SOFC on geometrical characteristics

For the period of time after last report period for classification of deformational behaviour of planar SOFC in operational temperatures conditions was carried out experimental investigations on the samples, their layer as it is shown below:
-for determination of mechanical characteristics for producing material of SOFC layers (i.e. μ. - Poisson's coefficient, E - elasticity coefficient, σ_{np} - proportional limit, σ_T - fluidity limit, σ_n - durability limit), by testing on stress (strain) have been run curve $\sigma = \sigma(\varepsilon)$ this materials;

-for determination of reological properties of producing materials of SOFC layers (i.e. $\sigma_{np} = \sigma_{np}(t)$ $\sigma_T = \sigma_T(t)$ $\sigma_n = \sigma_n(t)$, necessary for studying in them relaxation phenomena and creeping phenomena have been run dependences $\sigma = \sigma(\varepsilon)$ at long-term loading.

Results of experimental investigations and their interpretation

With the purpose of determination the mechanical characteristics samples of electrolyte materials of various length, prismatic shape with cross section S=(4X4)MM^2 were subjected to testing. The tests on the especial equipped experimental devise was curried out (Hasanov *et al.,* 2007). Samples, produced from material 10SclCSZ, have been testing on compress both in cross and longitudinal locations (see Fig. 3) at room temperature. As a result of testing the values of destroying forces in cross (F_1) and longitudinal (F_2) locations was sharply differed and the ratio their values on average were found on equal to F2/Fi≈3,5. However manifestation of various resistibility of samples in mutually perpendicular locations was not signified the presence of anisotropic properties in structures of samples materials. Most likely it was result of poor processing of bearing surface of samples, thus was not correspondence their geometrical characteristics and shape of required relevant standards.

Results of carried out testing are shown in the Fig. 3. As it is shown material of testing samples right up to destruction behaves as a elastic body, and the destruction begins instantly, i.e. material is characterized by fragility. It is explaining by porous structure of producing material of sample.

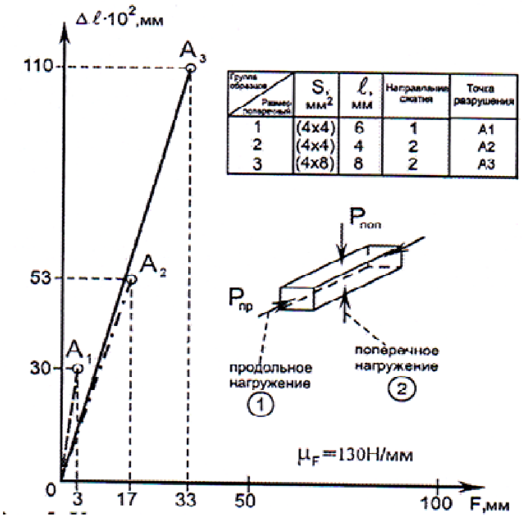

Figure. 3: Characteristics of deformational behaviour of producing materials of electrolytes

1. At longitudinal loading of sample with characteristics of cross section S=(4x4)mm^2; l=6mm
2. At cross loading of sample with characteristics of cross section S=(4x4)mm; l=4mm

By testing results was stated the values of mechanical characteristics of testing samples material:

- Durability limit at room temperature $\sigma_{np} = 1{,}38 \cdot 10^8$ Pa
- YUNGA'S module, i.e. elastic resistibility pf material E= (7-8)·10^8Pa;
- Value of deformation in destruction time ε_{np}= σ_{np}/E=0,172. For metals this parameter is equal to ε_{np}≈0,001. It means that for testing materials value this user exceed values by metals in 100 times. This parameter testifies to availability of useful porousity (≈20%) in materials of testing samples.

Next stage of experimental investigations were method development and testing program in the conditions of influence of loading and high temperature, processing their results with the purpose of determination reological properties of producing materials of electrodes FC. As mentioned above, were investigated such reological properties of producing materials FC as creeping in the conditions of fluctuation operating loading and high operational temperatures, loading relaxation, elastic aftereffect, etc.

Therefore, main factors, excited manifestation of reological processes in producing materials of electrodes FC, are high values and fluctuation of operational temperatures. It means that electrode system (or single electrode) may be shown as object of mechanical model, subjected to long-term thermal mechanical loading in operation process. At once it should be noted that all attempts to organize and carry out tests of the given samples on strain (compression) in the conditions of high temperatures were unsuccessful.

The reason was vulnerability of capturing junctions of developed devices to influence of high temperature. Poor capture in current configuration of samples was caused creeping and depressurizing of junction, and at strong - samples were broken in the capture place, that disabled loading of samples and taking off necessary characteristics of deformational behavoiur (there were tested more capturing devices which were made useless). Therefore taking into account rather small both cross and longitudinal geometrical characteristics of testing samples (cross section - S=4x4 mm, sample length - 1=40 mm) were produced devices for studying reological properties of materials by results one-point deformation of bend.

Testing Program consists of two test type, exactly short- term and long-term tests. The main objective of these tests were determination of dependences of durability characteristics on temperature factors and creeping characteristics, including long durability and creeping limits of producing materials of FC.

Results of experimental investigations in both setting for samples of square and round crosses are shown in the fig. 4 and 5.

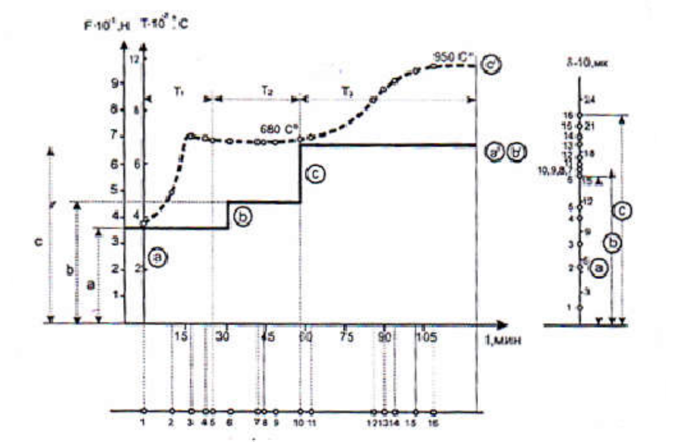

Figure 4. Mode factors of testing samples with square cross section

a, b, c - accordingly, mechanical loading at 3,5; 4,5; 6,5 H:
a', b', c' - appropriate to mechanical thermal loading at changes:

for 350<a'<680° C; for b'<680° C=Const; for 680<c'<1000° C. Properly from fig. 4 tests were carried out at 3 modes of mechanical and thermal loadings. According to proposal methodic by results of bend deformation of testing samples for various levels of temperature and mechanical loadings were obtained creeping ε=ε(t), as it is shown in the Fig-5:

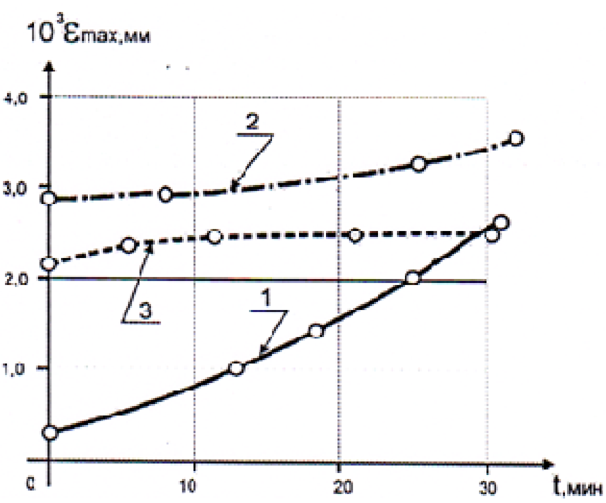

Figure 5. Creeping curve e=e(t), obtained by results of bend deformations of square (1,2) and round sections (3)

1-at mechanical loadingϬ=24,6 МПа and temperature T=680°C;
2-at mechanical loading Ϭ=45,7 МПа and temperature T=900°C;
3-at mechanical loading Ϭ=40,4МПа and temperature T=750°C.

Calculations pointed to creeping rate with loading increasing (in this case from Ϭ=24,6 МПа and T=680°C tillϬ=45,7 МПа and T=900°C) is decreased more 3 times (from v_ε=0.075·10^3l/min. - for the first mode till v_ε=0.026-10^{-3}l/min. - for the second mode). It is explained by presence large porosity in the material structure of testing samples. However, as tests shown, samples mainly were destroyed at more intensive and hard modes of loading. Thus for samples of square section the destruction correspond to loading mode Ϭ=49, 2 МПа and T=900°C, and appropriate deformation at the same time amounted to the limit ε_{max}=3,911·10^{-3} mm. Similar tests were carried out for sample of round sections (see Fig. 5 and 6) with diameter d=4,2 mm. Tests modes are shown in the Fig. 6.

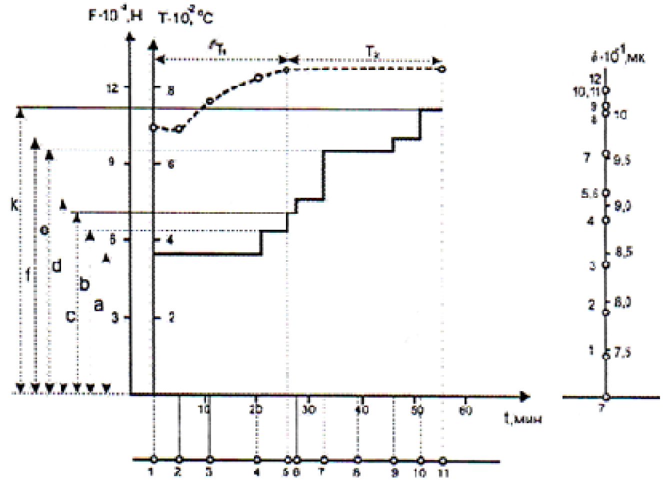

Figure 6. Mode factors of tests program with samples of round section

a, b, c, d, e, k - limits of mechanical loading,
T_1 and T_2 - modes of thermal loading.

Creep curves of testing samples, obtained at various temperature constant mechanical modes of loading, are shown in the fig. 7.

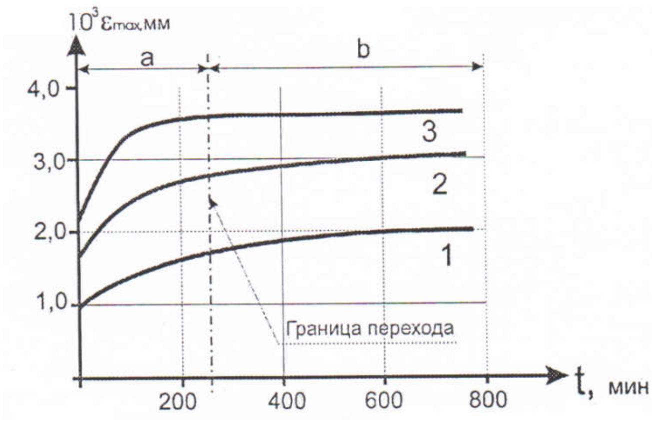

Figure 7. Creep curves at various temperature modes:

1 - 100°C; 3 - 400°C; 5 - 800°C.
a - transitional creep space;
b - damped creep space.

Analyses of curves shows that creeping deformation development (Bernshtein and Zaymovskiy, 1979) irrespective of temperature mode of loading occurs in two stages: in the stage of transitional creep, rate of which is slowed down, and in the stage of damped creep with constant deformation rate. However in all cases because of porous structure of samples takes place their viscocreeping deformation. The behaviour of curves shows that temperature mode of tests essentially impact on quantitative parameters of creeping deformation, resulted in samples softening. Thus at equal conditions the temperature increasing in 7-8 times increases the deformation in 2,5-3 times. At that should notice with temperature increasing at constant mechanical loading the creeping deformation rate are risen. From creep curves may be obtained dependence Ϭ=f(ε,t) by reconfiguration of coordinates strain-deformation. As at constant loading the deformation is increased in time so various values ε(t) will be correspond to its definite value (see fig. 8). In that way comes in curves family, each of which corresponds to definite time. Vital importance at this has density of samples producing and characteristics their porosity (samples are produced and supplied by Ukrainian part and therefore we haven't such opportunity). However, because of supposed structure softening of samples as a result of creeping deformation (see Fig. 7) should to make conclusion that for more dense and less porosity of samples dependences Ϭ=f(ε,t) will be having large steepness also with relaxation effect demonstration of loading. Besides, high-cycle loading of testing materials in the operational process, as well as naturally strong relaxation of thermal loading will be providing for resistibility reduction of design elements and their thermal mechanical fatigue breakdown. Fatigue breakdown circulation in consequence of creeping and thermal fatigue will be lasting till appearance of deformation kind complications in design elements and stopping of operational cycle.

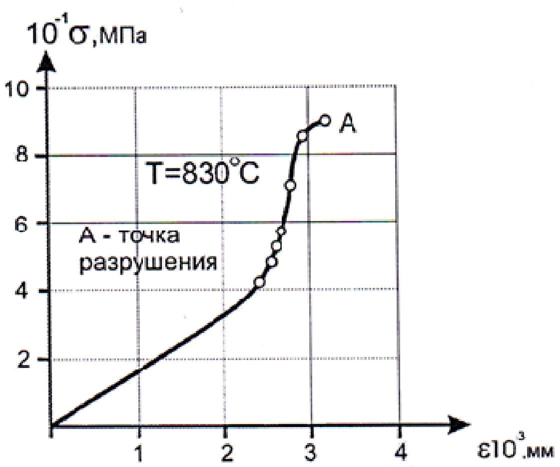

Figure 8. Dependence Ϭ=f(ε,t)

Conclusion

1. As a result of analytical investigations conducting of layered planar designs thermal stability found that their stability at an operating temperature of 1000 K can be provided at a ratio of the geometric dimensions
$Y = a./h$ 28, where a, h - respectively, the longitudinal dimension and thickness of the design;

2. On the basis of the developed methods and programs for determination of the mechanical and rheological properties of SOFC materials in a high mechanical and temperatural loads experimental studies of given samples are curried out.

3. According to the results of tests assessed value: A. Mechanical properties of test samples, namely: — strength at a room temperature
$\sigma_{st} = 1{,}38 \cdot 10^2 MPa;$

- elastic resistance of the material, i.e Young's modulus
$E = (7 \div 8) \cdot 10^2 MPa;$

- the strain at the moment of destruction- ε_{st}= 0,172 ;

B. Structural characterization of the material samples:
- porosity - no more than 20%;

C. Rheological properties of materials in the form of creep curves at different temperature regimes. Found that the development of creep strain, regardless of the temperature regime of loading occurs in two stages, namely:

- stage of the transient creep rate which decreases with time;
- stage of fading creep with constant strain rate.

4 It was established that under the same conditions, the increase of temperature indicator 7÷8 times the deformation increases 2,5÷3 times.

5 Because of the rather large porosity of the material and its relatively low mechanical strength, and in consequence of which a strong relaxation of thermal stresses will reduce the resistance of design elements from this material and further the thermo-mechanical fatigue destruction.

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