## DIFFUSION CREEP ANALYSIS IN PEROVSKITE THICK-WALLED CYLINDER UNDER **RADIAL OXYGEN VACANCIES GRADIENT**

# ANALIZA DIFUZIONOG PUZANJA U DEBELOZIDOM CILINDRU OD PEROVSKITA POD DEJSTVOM RADIJALNOG GRADIJENTA PRAZNINA KISEONIKA

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Abstract	Izvod

#### Abstract

In the present paper, the nonlinear problem of diffusion creep and stress evolution has been formulated for tubular perovskite-type membranes of a high-temperature catalytic membrane reactor. For this purpose, the impact of point defects (oxygen vacancies) and volume microstructural defects (voids) of perovskites on the creep deformation of a thick-walled hollow cylinder is analysed at high temperatures and under generalized plane strain in conditions of radial oxygen vacancies gradient. Transport of oxygen vacancies through the membrane thickness is described by Fick's second law. The constitutive equation of diffusion creep and damage evolution equation for voids have been specified for perovskites under complex stress state. The analytical-numerical method has been discussed for solving the initial-boundary value problems of the diffusion creep for thick-walled hollow cylinder, taking into account damage development in a form of oxygen vacancies and voids. An example of creep analysis of perovskite-type thick-walled hollow cylinder is considered under radial oxygen vacancies gradient and, additionally, under radial temperature gradient with the assessment of its long-term strength.

## INTRODUCTION

Modern trends in the application of alternative energy sources are directly connected to the development of perovskite-type membranes of the high-temperature catalytic membrane reactor. Such membranes, usually of tubular or planar design, referred to as ceramic membranes with mixed oxygen ion and electronic conductivity, are main elements of a reactor for the production of synthesis gas (a mixture of carbon monoxide and hydrogen). It is known /1, 2/ that synthesis gas serves as the basis for the production of synthetic fuels.

When using this membrane technology at high temperatures (1073-1223 K), one surface of the membrane is exposed to a feed air while the other is at equilibrium with a sweep gas (for example, methane). The use of perovskites as membrane materials with a difference in the partial oxygen pressure between the two surfaces of the membrane makes it possible to combine into a single physicochemical

U ovom radu je formulisan nelinearni problem difuzionog puzanja i razvoja napona kod cevaste membrane tipa perovskit visokotemperaturnog katalitičkog membranskog reaktora. U tu svrhu se analizira uticaj tačkaste greške (praznine kiseonika) i zapreminskih mikrostrukturnih grešaka (šupljina) perovskita na deformaciju puzanja debelozidog šupljeg cilindra pri visokim temperaturama i pri generalisanom ravnom stanju deformacija u uslovima radijalnog gradijenta praznina kiseonika. Transport praznina kiseonika kroz debljinu membrane se opisuje drugim Fikovim zakonom. Konstitutivna jednačina difuznog puzanja i jednačina evolucije oštećenja za praznine su određene za perovskite u složenom naponskom stanju. Data je diskusija o analitičkonumeričkoj metodi za rešavanje problema sa početnim i graničnim uslovima difuzionog puzanja debelozidog šupljeg cilindra, uzimajući u obzir razvoj oštećenja oblika praznina i šupljina kiseonika. Primer analize puzanja debelozidog šupljeg cilindra tipa perovskita se razmatra pod radijalnim gradijentom praznina kiseonika i, dodatno, pod radijalnim gradijentom temperature sa procenom njegove dugotrajne čvrstoće.

process the separation of oxygen from the air on one side of the membrane, the diffusion of oxygen ions through the thickness via vacancies, and the conversion of methane to synthesis gas on the opposite side of the membrane. The commercialization of this technology will significantly reduce the total capital cost of the traditional method of producing synthesis gas using the Fischer-Tropsch process /1, 2/. Unfortunately, the insufficiently high long-term strength of tubular and planar membranes made of modern perovskite-type materials limits the commercialization of this technology, /3/.

The functioning of perovskite-type membranes under conditions of oxygen ion diffusion, high temperature, and oxygen vacancies gradient through the membrane thickness is accompanied by the appearance of chemically induced expansion of the ceramic material /4, 5/, as well as a significant dependence of the creep process in oxide ceramics on oxygen ion concentration /6, 7/. Such phenomena, established experimentally, can have a significant impact on the

change in the stress-strain state in membranes over time, and, therefore, on their durability. In this regard, the phenomena under discussion (chemical expansion and diffusion creep) should be taken into account and adequately reflected. First, in the constitutive equations, and then, in the formulation of the initial-boundary value problems for membranes under consideration.

The analysis of stresses in perovskite-type tubular membranes, as well as, in the cathode of a solid oxide fuel cell, due to the gradient of oxygen vacancies through the thickness and inhomogeneous distribution of chemical expansion is carried out in an elastic formulation in /8-13/. The creep of perovskite-type tubular membranes is considered in /14/ without taking into account the dependence of creep deformation on the concentration of oxygen ions. The creep of the module of solid oxide fuel cells, presented as a threelayer thick-walled cylinder, due to the radial temperature gradient is studied in /15, 16/ without any consideration of the effect of diffusion on creep. Thus, at present, in literature there is no approach for modelling the diffusion creep in perovskite-type tubular membranes.

In general, there are two main physical mechanisms of creep for polycrystalline materials, such as, the motion of linear defects (dislocations) through the crystal lattice and diffusion of atoms or ions (transport of point defects, known as vacancies). The tubular membrane of the reactor is a hollow thick-walled cylinder, and the dislocation creep of a cylinder made of metallic and ceramic materials is studied in a number of papers, for example, in /17-20/. As the distribution of stresses in a cylinder at any given instant in time strongly depends on material properties and operating conditions, conclusions and recommendations derived from stress analyses of dislocation creep cannot easily be transferred to the case of diffusion creep even for one and the same cylinder geometry. Therefore, the purpose of the paper is to develop the constitutive equation for diffusion creep of perovskite-type materials, to provide the formulation of initial-boundary value problems on its basis for determining the stress-strain state at any given instant in time in tubular membranes, by taking into account the diffusion of oxygen ions, chemical expansion and creep, as well as, to predict the long-term strength of membranes under study.

#### CONSTITUTIVE MODEL

Consider a perovskite-type material represented symbolically by the formula ABO<sub>3- $\delta$ </sub>, under complex stress state with tensor  $\sigma_{ij}$ , where A is a cation (cations) larger than the cation (cations) B; O is an oxygen anion;  $\delta$  is oxygen nonstoichiometry. It is assumed that components of strain tensor  $\varepsilon_{ij}$ are composed of elastic components  $\varepsilon_{ij}^e$ , determined by the generalised Hooke's law, thermal components  $\varepsilon_{ij}^T$ , chemically induced components  $\varepsilon_{ij}^{ch}$ , as well as components of the irreversible creep strain tensor  $\varepsilon_{ij}^c$ . Therefore,

$$\varepsilon_{ij} = \varepsilon_{ij}^e + \varepsilon_{ij}^T + \varepsilon_{ij}^{ch} + \varepsilon_{ij}^c \,. \tag{1}$$

Thermal and chemically determined components of the strain tensor are calculated using formulas:

$$\varepsilon_{ij}^{T} = \alpha (T - T_0) \delta_{ij}; \quad \varepsilon_{ij}^{ch} = A(\delta - \delta_0) \delta_{ij}, \qquad (2)$$

INTEGRITET I VEK KONSTRUKCIJA Vol. 21, br. 1 (2021), str. 57–62 where: *T* is temperature;  $\alpha$  and *A* are coefficients of thermal and chemical expansion;  $T_0$  and  $\delta_0$  are values of temperature and oxygen non-stoichiometry at the reference state of the material;  $\delta_{ij}$  is the Kronecker delta;  $\delta_{ij} = 1$  if i = j, and  $\delta_{ij} = 0$  otherwise.

Assuming the initial isotropy and damage in a form of oxygen vacancies, as well as, neglecting the influence of the kind of stress state /21/, the constitutive equation of diffusion creep has been written for perovskite-type non-stoichiometric materials as follows,

$$\dot{\varepsilon}_{kl}^{c} = \frac{3}{2} \frac{B}{d^{p}} \exp\left(-\frac{Q}{RT}\right) \lambda(\omega) \frac{\nu(\sigma_{i})}{\sigma_{i}} s_{kl} , \qquad (3)$$

where:  $s_{kl}$  is the stress deviator;  $s_{kl} = \sigma_{kl} - (1/3)\sigma_{nn}\delta_{kl}$ ;  $\sigma_i$  is stress intensity,  $\sigma_i = \sqrt{\frac{3}{2}s_{kl}s_{kl}}$ ; the dot above the symbol

denotes the derivative with respect to time t; d is characteristic grain size of the ceramic material; Q is activation energy; R is the universal gas constant;  $\omega$  is the Kachanov-Rabotnov damage parameter /22, 23/, which is increasing with time from the initial value  $\omega = \omega_0$  at the reference instant of time to the final value  $\omega = 1$  at the instant of rupture; parameters B and p as well as specific expressions for functions  $\lambda(\omega)$  and  $\nu(\sigma_i)$  can be found using data from basic creep experiments. The latter, as a rule, represent tests of thin-walled tubular specimens under conditions of uniaxial compression with stress  $\sigma$  = const in a gas medium with oxygen partial pressure  $P_{O2} = \text{const}$  and temperature T =const. Analysis of the results of a series of these tests with different values  $\sigma$ ,  $P_{\rm O2}$  and T /6, 7/ allows us to conclude the absence of unsteady and accelerated stages on the diffusion creep curves of perovskite-type materials. It was also found /6, 7/ that a decrease in partial pressure of oxygen significantly intensifies the creep process.

The law of one-dimensional axial creep of perovskite under uniaxial compression has a form /6/

$$\left|\dot{\varepsilon}^{c}\right| = \frac{B_{0}}{d^{p}} \exp\left(-\frac{Q}{RT}\right) P_{O_{2}}^{-m} \left|\sigma\right|^{n}.$$
(4)

The relationship between  $P_{O2}$  and  $\delta$  in basic experiments can be represented as /10, 24/

$$P_{O_2} = K \left(\frac{3}{\delta} - 1\right)^{\xi},\tag{5}$$

where:  $B_0$ , K,  $\xi$ , m, and n are some material constants. Taking into account Eq.(5), we rewrite Eq.(4) as

$$\left|\dot{\varepsilon}^{c}\right| = \frac{B}{d^{p}} \exp\left(-\frac{Q}{RT}\right) \left(\frac{\frac{\delta}{3}}{1-\frac{\delta}{3}}\right)^{m\zeta} \left|\sigma\right|^{n}, \quad (6)$$

where

Then, taking into account the identity of Eqs.(3) and (6) in the case of uniaxial compression, when  $\sigma_{11} = -|\sigma|$  and  $\varepsilon_{11}^c = -|\varepsilon^c|$ , we can take

 $B = B_0 K^{-m}.$ 

$$\omega = \frac{\delta}{3}; \ \omega_0 = \frac{\delta_0}{3}; \ \lambda(\omega) = \left(\frac{\omega}{1-\omega}\right)^{m\xi}; \ \nu(\sigma_i) = \sigma_i^n . \tag{8}$$

STRUCTURAL INTEGRITY AND LIFE Vol. 21, No 1 (2021), pp. 57–62

(7)

Thus, the constitutive model of diffusion creep for perovskite-type nonstoichiometric materials is represented by Eqs. (3) and (8). In this case, the temperature and nonstoichiometry are assumed to be given or known from solving the problems of unsteady heat conduction and oxygen transport, respectively.

### FORMULATION OF THE PROBLEM

The tubular membrane of the reactor can be considered as a hollow thick-walled cylinder operating under conditions of generalised plane deformation /8, 10/. The membrane deformation is analysed in a cylindrical coordinate system  $(r, \theta, z)$ , where r is the radial coordinate,  $\theta$  corresponds to the circumferential direction, and z is the axial coordinate, under the assumption of symmetry around z axis. The outer surface of the cylinder, defined by r = b, is at equilibrium with feed air, and the inner surface, r = a, is exposed to sweep gas. The pressure of gaseous media on both surfaces of the cylinder is assumed to be atmospheric. Temperature T and oxygen nonstoichiometry  $\delta$  in a cylinder are only functions of the radial coordinate and time. In this case, nonzero stresses  $\sigma_r$ ,  $\sigma_{\theta}$ ,  $\sigma_z$  and strains  $\varepsilon_r$ ,  $\varepsilon_{\theta}$  are only functions of radial coordinate and time. Also, axial strain  $\varepsilon_z$  does not depend on coordinates, but can only depend on time.

Equations (1) and (2) can be represented for a cylinder as

$$\varepsilon_{r} = \frac{1}{E} \Big[ \sigma_{r} - \nu(\sigma_{\theta} + \sigma_{z}) \Big] + \alpha(T - T_{0}) + A(\delta - \delta_{0}) + \varepsilon_{r}^{c},$$
  

$$\varepsilon_{\theta} = \frac{1}{E} \Big[ \sigma_{\theta} - \nu(\sigma_{r} + \sigma_{z}) \Big] + \alpha(T - T_{0}) + A(\delta - \delta_{0}) + \varepsilon_{\theta}^{c},$$
  

$$\varepsilon_{z} = \frac{1}{E} \Big[ \sigma_{z} - \nu(\sigma_{r} + \sigma_{\theta}) \Big] + \alpha(T - T_{0}) + A(\delta - \delta_{0}) + \varepsilon_{z}^{c}, \quad (9)$$

where: E is modulus of elasticity; v is Poisson's ratio. From the third formula in Eq.(9) we have

$$\sigma_{z} = \nu(\sigma_{r} + \sigma_{\theta}) + E \left[ \varepsilon_{z} - \varepsilon_{z}^{c} - \alpha(T - T_{0}) - A(\delta - \delta_{0}) \right], \quad (10)$$

and from the first two in Eq.(9), we obtain

$$\sigma_{r} = \frac{E_{1}}{1 - v_{1}^{2}} \left[ \varepsilon_{r} - \varepsilon_{r}^{c} + v_{1}(\varepsilon_{\theta} - \varepsilon_{\theta}^{c}) + v_{1}(\varepsilon_{z} - \varepsilon_{z}^{c}) \right] - \frac{E_{1}}{1 - v_{1}} \left[ A_{1}(\delta - \delta_{0}) + \alpha_{1}(T - T_{0}) \right],$$

$$\sigma_{\theta} = \frac{E_{1}}{1 - v_{1}^{2}} \left[ \varepsilon_{\theta} - \varepsilon_{\theta}^{c} + v_{1}(\varepsilon_{r} - \varepsilon_{r}^{c}) + v_{1}(\varepsilon_{z} - \varepsilon_{z}^{c}) \right] - \frac{E_{1}}{1 - v_{1}} \left[ A_{1}(\delta - \delta_{0}) + \alpha_{1}(T - T_{0}) \right], \quad (11)$$

where

$$E_{1} = \frac{E}{1 - \nu^{2}}; \quad \nu_{1} = \frac{\nu}{1 - \nu}; \quad \alpha_{1} = \alpha(1 + \nu); \quad A_{1} = A(1 + \nu). \quad (12)$$

The stresses satisfy the equilibrium equation

$$\frac{\mathrm{d}\sigma_r}{\mathrm{d}r} + \frac{\sigma_r - \sigma_\theta}{r} = 0.$$
 (13)

Kinematic equations can be represented as

$$\varepsilon_r = \frac{du}{dr}; \quad \varepsilon_\theta = \frac{u}{r}; \quad \varepsilon_z = \frac{dw}{dz},$$
 (14)

where: *u* and *w* are radial and axial displacements, in respect.

INTEGRITET I VEK KONSTRUKCIJA Vol. 21, br. 1 (2021), str. 57-62

Substituting the expressions for stresses in Eq.(11) into Eq.(13) and taking into account the first two relations in Eq. (14), we arrive at the governing equation

$$\frac{d^2u}{dr^2} + \frac{1}{r}\frac{du}{dr} - \frac{u}{r^2} = (1 - v_1)\frac{\varepsilon_r^c - \varepsilon_\theta^c}{r} + \frac{d}{dr}(v_1\varepsilon_\theta^c + \varepsilon_r^c) + \frac{d}{dr}\left\{(1 + v_1)\left[A_1(\delta - \delta_0) + \alpha_1(T - T_0)\right] - v_1(\varepsilon_z - \varepsilon_z^c)\right\}.$$
 (15)

#### METHOD OF SOLUTION

Integrating Eq.(15), we obtain the radial displacement in the cylinder

$$u = \frac{1}{r} \int_{a}^{r} \left[ \varepsilon_{r}^{c} - v_{1}\varepsilon_{z} + v_{1}\varepsilon_{\theta}^{c} + v_{1}\varepsilon_{z}^{c} + (1 - v_{1})\int_{a}^{r} \frac{(\varepsilon_{r}^{c} - \varepsilon_{\theta}^{c})}{r} dr \right] r dr + \frac{1 + v_{1}}{r} \int_{a}^{r} \left[ A_{1}(\delta - \delta_{0}) + \alpha_{1}(T - T_{0}) \right] r dr + c_{1}r + \frac{c_{2}}{r}, \qquad (16)$$

where:  $c_1$  and  $c_2$  are constants to be determined from boundary conditions. Then, using Eq.(14) and taking into account Eq.(12), we obtain from Eq.(11) the radial and circumferential stress

$$\sigma_{r} = \frac{E}{1-\nu} \frac{r^{2}-a^{2}}{2r^{2}} (A\delta_{0} + \alpha T_{0}) - \frac{E}{(1-\nu)r^{2}} \int_{a}^{r} (A\delta + \alpha T) r dr + + \frac{E\nu}{1-\nu^{2}} \frac{r^{2}-a^{2}}{2r^{2}} \varepsilon_{z} + \frac{E}{1+\nu} I_{1}(r) - \frac{E(1-2\nu)}{1-\nu^{2}} \frac{I_{11}(r)}{r^{2}} - - \frac{E}{1-\nu^{2}} \frac{I_{2}(r)}{r^{2}} + \frac{E}{1+\nu} \left( \frac{c_{1}}{1-2\nu} - \frac{c_{2}}{r^{2}} \right), \sigma_{\theta} = \frac{E}{1-\nu} \frac{r^{2}+a^{2}}{2r^{2}} (A\delta_{0} + \alpha T_{0}) + \frac{E}{(1-\nu)r^{2}} \int_{a}^{r} (A\delta + \alpha T) r dr - - \frac{E}{1-\nu} (A\delta + \alpha T) + \frac{E}{1+\nu} \left( \frac{c_{1}}{1-2\nu} + \frac{c_{2}}{r^{2}} \right) + \frac{E(1-2\nu)}{1-\nu^{2}} \frac{I_{11}(r)}{r^{2}} + + \frac{E}{1-\nu^{2}} \left[ \frac{r^{2}+a^{2}}{2r^{2}} \nu \varepsilon_{z} + \nu I_{1}(r) + \frac{I_{2}(r)}{r^{2}} - \varepsilon_{\theta}^{c} - \nu \varepsilon_{z}^{c} \right],$$
(17)

where: for convenience, the following notation is introduced

$$I_{1}(r) = \int_{a}^{r} \frac{(\varepsilon_{r}^{c} - \varepsilon_{\theta}^{c})}{r} dr ; \quad I_{11}(r) = \int_{a}^{r} I_{1}(r) r dr ;$$
$$I_{2}(r) = \int_{a}^{r} \left[ (1 - v)\varepsilon_{r}^{c} + v\varepsilon_{\theta}^{c} + v\varepsilon_{z}^{c} \right] r dr . \tag{18}$$

Using Eq.(17) in Eq.(10), we obtain the axial stress

$$\sigma_{z} = -\frac{E}{1-\nu} \Big[ A(\delta - \delta_{0}) + \alpha (T - T_{0}) \Big] + \frac{E\nu}{1-\nu^{2}} I_{1}(r) + \frac{2E\nu}{1+\nu} \frac{c_{1}}{1-2\nu} + \frac{E}{1-\nu^{2}} \varepsilon_{z} - \frac{E}{1-\nu^{2}} (\nu \varepsilon_{\theta}^{c} + \varepsilon_{z}^{c}) .$$
(19)

Taking, without loss of generality, the boundary conditions  $\sigma_r = 0$  for r = a and  $\sigma_r = 0$  for r = b, we get the constants  $c_1$  and  $c_2$  as follows:

$$c_{1} = \frac{(1+\nu)(1-2\nu)}{(1-\nu)(b^{2}-a^{2})}c_{3}; \quad c_{2} = \frac{a^{2}(1+\nu)}{(1-\nu)(b^{2}-a^{2})}c_{3};$$
$$c_{3} = \int_{a}^{b} (A\delta + \alpha T)rdr - (b^{2}-a^{2})\left(\frac{\nu}{1+\nu}\frac{\varepsilon_{z}}{2} + \frac{A\delta_{0} + \alpha T_{0}}{2}\right) + \frac{1}{2}c_{3}c_{3}$$

STRUCTURAL INTEGRITY AND LIFE Vol. 21, No 1 (2021), pp. 57-62

$$+\frac{1-2\nu}{1+\nu}I_{11}(b)-\frac{1-\nu}{1+\nu}I_{1}(b)b^{2}+\frac{1}{1+\nu}I_{2}(b).$$
 (20)

Thus, the stress state in a thick-walled hollow perovskitetype cylinder under radial oxygen vacancies gradient and creep conditions is determined by Eqs.(17)-(20). In this case, the axial deformation  $\varepsilon_{\tau}$  is assumed to be known. Also note that, despite the semi-analytical representation of stresses, Eqs.(17) and (19) are nonlinear.

A change in stress distribution of a hollow cylinder over time is influenced by chemical expansion and creep. Diffusion of oxygen ions in perovskite-type cylinders occurs rather quickly, and a steady state occurs within seconds (or minutes) /8, 10/, when creep deformation can be neglected. Then, Eqs.(17)-(20) can be accepted for a given time interval under assumption  $\varepsilon_r^c = \varepsilon_{\mathcal{E}} = \varepsilon_z^c = 0$ , and the problem of linear elastic deformation of cylinders under study should be supplemented by the Fick's second law, /10/:

$$\frac{\partial \delta}{\partial t} = D \left( \frac{\partial^2 \delta}{\partial r^2} + \frac{1}{r} \frac{\partial \delta}{\partial r} \right), \tag{21}$$

with an initial condition for t = 0:

 $\delta = \delta_0$ ,

as well as, with the boundary condition for r = a:

$$D\frac{\partial\delta}{\partial r} = \beta(\delta - \delta_1), \qquad (23)$$

and the boundary condition for r = b:

$$\delta = \delta_2 \,. \tag{24}$$

(22)

The initial-boundary value problem of oxygen transport given by Eqs.(21)-(24) can be solved numerically /8/ or analytically /10/. In this work, the distribution of nonstoichiometry over the membrane thickness at the steady state stage of oxygen ion diffusion is found by the formula /10/:

$$\delta = \delta_2 + (\delta_1 - \delta_2) a\beta \ln(b/r) / [D + a\beta \ln(b/a)]. \quad (25)$$

For time values greater than the instant of steady state oxygen transport, measured in hours (days or months) /6, 7/, it is necessary to take into account creep deformation described by Eqs.(3), (8) and (25). In addition, deformation of perovskite-type materials in the final stage of creep is accompanied by the appearance and growth of damage in the form of voids /7/. We represent the kinetic equation of creep damage due to voids as follows

$$\frac{d\psi}{dt} = \frac{L}{d^{q}(1-\psi)^{k}} \exp\left(-\frac{\Delta}{RT}\right) \left(\frac{\omega}{1-\omega}\right)^{\chi} \left(\frac{\sigma_{1}-\sigma_{0}}{\sigma_{b}-\sigma_{1}}\right)^{k}.$$
 (26)

Here,  $\psi$  is the new Kachanov-Rabotnov damage parameter /22, 23/ in a range  $\psi \in [0, 1]$  which is equal to zero,  $\psi =$ 0, at the reference instant of time, and is equal to a critical value,  $\psi = 1$ , at the instant of creep rupture,  $t = t^*$ ; the material constants L, q, k,  $\Delta$ ,  $\chi$  can be found after the approximation of the long-term strength curves of samples with different grain sizes, tested at different temperatures and in a different environment; the maximal principal stress  $\sigma_1$  is accepted as equivalent stress in order to reflect the experimentally established fact /7/ of the orientation of grain boundaries with voids in the final creep stage perpendicular to the direction of action of the maximal principal stress,

and it is assumed that  $\sigma_1 \ge 0$ ,  $\sigma_1 \in [\sigma_0, \sigma_b]$ ; in the case when  $\sigma_1 < 0$  occurs after calculations, we take  $\dot{\psi} = 0$ ;  $\sigma_b$  is the short-term strength limit.

The main unknowns of the present problem are related to structural analysis of creep  $(\varepsilon_r^c, \varepsilon_\theta^c, \varepsilon_z^c)$  and creep damage  $(\psi)$  at an arbitrary point of the cylinder through thickness. In such a case, unknowns incorporated into Eqs.(3), (8) and (26) can be found from the numerical solution of the Cauchy problem in time for a given system of differential equations. The fourth-order Runge-Kutta-Merson's method of time integration with an automatic selection of the time step can be used effectively /25/ to solve the initial problem for Eqs. (3), (8) and (26). The practical application of the latter implies a fivefold use of linearised relations Eqs.(17) and (19) for stresses at each time step in accordance with the numerical scheme of Runge-Kutta-Merson's method. The initial conditions for the Cauchy problem with respect to the argument t include natural requirement  $\varepsilon_r^{\ c} = \varepsilon_{\ell}^{\ c} = \varepsilon_z^{\ c} =$  $\psi = 0$  and imply the use of stresses for elastic deformation of the cylinder at the steady stage of oxygen ion diffusion under the assumption of the nonstoichiometry distribution according to Eq.(25). The integrals in Eqs.(17) and (18) are calculated by the Gauss method.

### NUMERICAL RESULTS

As an example, a cylinder of sizes  $\frac{8}{a} = 2 \cdot 10^{-3}$  m and  $b = 3.25 \cdot 10^{-3}$  m made of perovskite La<sub>0.5</sub>Sr<sub>0.5</sub>CoO<sub>3- $\delta$ </sub> is considered. Parameters in a natural unstressed state are  $T_0 =$ 1423 K and  $\delta_0 = 0.144$ . The outer surface of the cylinder is heated to a temperature 1123 K in an air atmosphere ( $P_{O2} =$ 0.021 MPa). The inner surface, heated to 1073 K, is at equilibrium with argon ( $P_{O2} = 10^{-5}$  MPa). The temperature distribution over the thickness is assumed to be linear in the calculations. Coefficients of thermal and chemical expansion in the temperature range under study are  $\alpha = 30.7 \cdot 10^{-6} \text{ K}^{-1}$ and A = 0.035. Elastic constants are E = 86.0 GPa and v =0.25. Oxygen nonstoichiometry values are  $\delta_1 = 0.26$  and  $\delta_2 = 0.144$ . Diffusion constants are  $D = 3.10 \cdot 10^{-9} \text{ m}^2/\text{s}$  and  $\beta = 3.12 \cdot 10^{-5}$  m/s. Grain size and short-term tensile limit strength are accepted as d = 1.7 nm and  $\sigma_b = 181$  MPa /26/. Creep constants /26/ are m = 0.46; n = 1.32;  $B_0 = 5.793$ ·  $10^8 \text{ MPa}^{m-n} \text{m}^p \text{h}^{-1}$ ;  $K = 4.2301 \cdot 10^{-18} \text{ MPa}$ ;  $Q = 619.0 \text{ kJmol}^{-1}$ ;  $p = 1.28; \xi = 12.098;$  universal gas constant R = 8.3145 J.  $mol^{-1}K^{-1}$ . Constants in Eq.(26) to describe creep damage evolution are taken as  $L = 1.128 \cdot 10^{23} \text{ m'h}^{-1}$ ;  $\Delta = 566.0 \text{ kJ} \cdot 10^{23} \text{ m}^{-1}$  $mol^{-1}$ ; k = 1;  $q = \chi = \sigma_1 = 0$ , /27/.

Considering the condition of zero force in the axial direction of a cylinder with free ends and taking into account Eqs.(19) and (20), we obtain the axial strain

$$\varepsilon_{z} = \frac{2}{(b^{2} - a^{2})(1 - v^{2})} \Big[ I_{3} - v(1 - 2v)I_{11}(b) + v(1 - v)I_{1}(b)b^{2} - vI_{2}(b) \Big] + \frac{2}{b^{2} - a^{2}} \int_{a}^{b} (A\delta + \alpha T)rdr - A\delta_{0} - \alpha T_{0}, \qquad (27)$$
  
where:  $I_{3} = \int_{a}^{b} \Big[ v\varepsilon_{\theta}^{c} + \varepsilon_{z}^{c} - vI_{1}(r) \Big] rdr.$ 

INTEGRITET I VEK KONSTRUKCIJA Vol. 21, br. 1 (2021), str. 57-62

As a result of calculations, it is found that the steady state stage of oxygen ion diffusion in the cylinder under consideration begins after 400 s, and the creep rupture time is equal to  $t^* = 1990$  h. The rupture occurs on the outer surface of the cylinder with tensile stresses. The influence of diffusion creep leads to a significant redistribution with time of stress components (Fig. 1a, b, c), as well as the stress intensity (Fig. 1d) over the membrane thickness.



Figure 1. Stresses: a) circumferential; b) axial; c) radial; and d) stress intensity at instants of time: 1-400 s; 2-100 h; 3-500 h; 4-1000 h; 5-1990 h.

Figure 2 demonstrates the relaxation of stress intensity in a cylinder, and the results shown here for t = 0 actually correspond to the time instant t = 400 s.



Figure 2. Stress intensity on the inner (solid line) and outer (dashed line) surface of the cylinder.

### CONCLUSION

A constitutive model for describing the diffusion creep and damage development in perovskite-type materials has been implemented into the stress analysis in tubular membranes of a high-temperature catalytic membrane reactor, as well as the lifetime prediction studies.

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### LCF9 - Ninth International Conference on Low Cycle Fatigue June 21-23, 2022, Berlin, Germany

Organisation

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#### Scope

With a further postponement, we do hope to assure a safe on-site event, enabling fruitful personal discussion as well as various networking opportunities. A permanent and growing interest of the scientific community in low-cycle fatigue, including thermome-chanical fatigue addresses a broad range of applications, e.g. in energy technology, ransportation, civil engineering, and several other topics. On the other hand, many scientific questions on fundamental deformation and damage mechanisms, influence of multiaxial stresses/strains, creep-fatigue and TMF/HCF interaction as well as crack initiation and growth are investigated with increasing experimental efforts.

As a bridge between fundamental research and application in component and structural design, simulation approaches for cyclic plasticity, crack initiation and growth have made impressive and continuing progress in recent decades: FEM-based deformation and life assessment models at different scales, from microstructure to macroscopic structures, are state-of-the art and under successful development, especially for reliable design of components undergoing complex thermomechanical loads. Current research activities show that LCF research is a hot topic in material research and in structural integrity considerations.

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#### Topics

Isothermal LCF, thermomech. fatigue (TMF) and multiaxial LCF Superimposed LCF/HCF & TMF/HCF loads and creep-fatigue interaction

In-situ fatigue testing

Microstructural aspects of cyclic plasticity, fatigue damage, crack initiation and growth

Influence of surface, environment and protective coatings

Advanced materials and case studies

Novel experimental methods and standardization

Deform. & damage modelling and simulation based life assessment Fatigue Research 4.0: Future approaches in data acquisition, handling and processing

Additive manufacturing

#### Timeline

May 1, 2022, deadline for submission of full papers and registration June 1, 2022, submission of power point presentations

#### Executive chairs

Tilmann Beck, Technische Universität Kaiserslautern, Germany Eric Charkaluk, Ecole Polytechnique, Palaiseau, France