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CONSTITUTIVE AND NUMERICAL MODELING OF CHEMICAL AND MECHANICAL PHENOMENA IN THERMAL BARRIER COATINGS FOR GAS TURBINE BLADES OF AIRCRAFT ENGINES

Виконано моделювання хімічних і механічних явищ, та розроблені узагальнені визначальні співвідношення, які можуть бути використано для розрахунків залежних від часу розподілень напружень та пошкоджуваності термоізоляції лопаток газових турбін авіаційних двигунів. Розроблені визначальні співвідношення впроваджено в формі структурних моделей для аналізу пошкоджуваності в часі термоізоляції лопаток газових турбін авіаційних двигунів, для аналізу міцності та тривалої міцності, для забезпечення безпечної роботи лопаток газових турбін авіаційних двигунів.

Выполнено моделирование химических и механических явлений, разработаны обобщенные определяющие соотношения, которые могут быть использовано для расчетов зависимых от времени распределений напряжений и повреждаемости термоизоляции лопаток газовых турбин авиационных двигателей. Разработанные определяющие соотношения внедрены в форме структурных моделей для анализа повреждаемости во времени термоизоляции лопаток газовых турбин авиационных двигателей, для анализа прочности и длительной прочности, для обеспечения безопасной работы лопаток газовых турбин авиационных двигателей.

Introduction. In this paper a comprehensive theoretical and computational investigation will be carried out with the main focus directed at the understanding of the relationships between electron beam physical vapour deposition (EB-PVD) parameters, characteristics of high-temperature coating systems such as multilayer composition, interface failure, crystal structure, defect chemistry and microstructure, and multicomponent material properties related to diffusion of ionic species and oxidation as well as at the understanding on how these material characteristics, oxygen chemical potential gradient, transport phenomena, swelling, oxidation, fatigue and high temperature creep affect degradation and lifetime reduction for thermal barrier coating systems for gas turbine blades of aircraft engines. Furthermore, focus is put on how the EB-PVD parameters, coating characteristics, diffusion processes, swelling, oxidation, creep deformation as well as the creep/fatigue damage growth due to microstructuctural changes in the materials over time may be controlled using developed constitutive modeling tool in order to reduce degradation, improve oxidation protection, optimize coating design and operating conditions, and extend lifetime of thermal barrier coating systems for gas turbine blades of aircraft engines. The interdisciplinary approach proposed in this project involves new knowledge developed in Mechanical Engineering, Material Science, Mathematical Theory of Diffusion and Computational Mechanics.

The specific objectives of the present paper are:

- to identify the mechanisms of chemical, thermal and structural degradation processes that affect the lifetime reduction of thermal barrier coatings systems, including the columnar ceramic layer made by EB-PVD, the metallic bond coat, the thermally grown oxide and the Ni-based superalloy substrate,
- to incorporate mathematical theory of diffusion into analysis of oxidation and diffusion induced stresses in the thermally grown oxide of thermal barrier coatings system,
- to develop an integrated micro-meso-macro constitutive framework that will then be used to calculate the time dependent and diffusion induced stress distribution, and the creep/fatigue damage growth in thermal barrier coating systems for gas turbine blades of aircraft engines under transient operating conditions as a function of the EB-PVD parameters and coating properties as well as operating conditions, and additionally to predict the lifetime of thermal barrier coating systems working at a harsh environment and exposed to very large oxygen chemical potential gradients at high temperatures and under severe service loading conditions,
- to establish a relation between EB-PVD parameters, coating properties, oxidation phenomenon, swelling, high temperature creep and creep/fatigue damage in thermal barrier coatings system, and diffusion induced stress evolution in thermal barrier coating system under high temperature and its degradation over time,
- to enter into the constitutive model the experimental data of the crystal structure, composition, defect chemistry and microstructure, and material properties related to diffusion of ionic species for thermal barrier coating systems,
- to incorporate an integrated micro-meso-macro constitutive model proposed in this project into in-house developed software as well as into the ANSYS codes in a form of the computer-based structural modelling tool for analyzing time dependent and diffusion induced stress distributions in thermal barrier coating systems for gas turbine blades of aircraft engines and its degradation over time, for durability analysis and lifetime predictions, and for improving the performance of thermal barrier coating systems,
- to formulate practical recommendations based on the results of computational modeling and simulation for thermal barrier coating systems on how to modify the EB-PVD parameters and coating properties, and improve oxidation protection and operating conditions in order to reduce degradation of thermal barrier coating systems for gas turbine blades of aircraft engines, and extend its lifetime.

2. State of the art. For structures working at a harsh environment, coating may be applied to protect the material from direct exposure to the environment (Fig. 1) [1-7]. For example, thermal barrier coating (TBC) must operate in the most demanding high temperature environment of aircraft, because it may protect the materials from environmental attacks and increase wear resistance. In this way, the TBCs can substantially improve the application potential of rotating blades for gas turbines of aircraft engines (Fig. 2) [8, 9]. The TBC system has very complex structure and generally consists of several intermediate layers with spatial variance in properties, namely the columnar ceramic layer made by electron beam physical vapour deposition (EB-PVD), the metallic bond coat, the thermally grown oxide (TGO), and the Ni-based single crystall superalloy substrate (Fig. 3) [10].

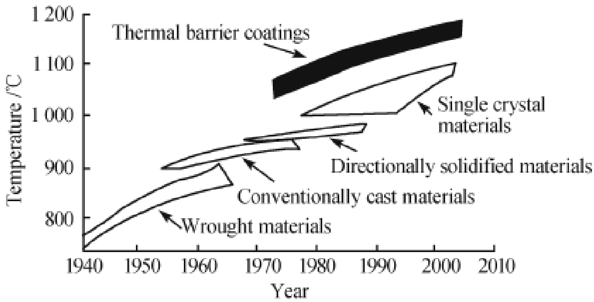


Fig. 1. Temperature improvements of gas turbine alloys in Rolls-Royce engines [1]

Fig. 2. The TBC system for gas turbine blade

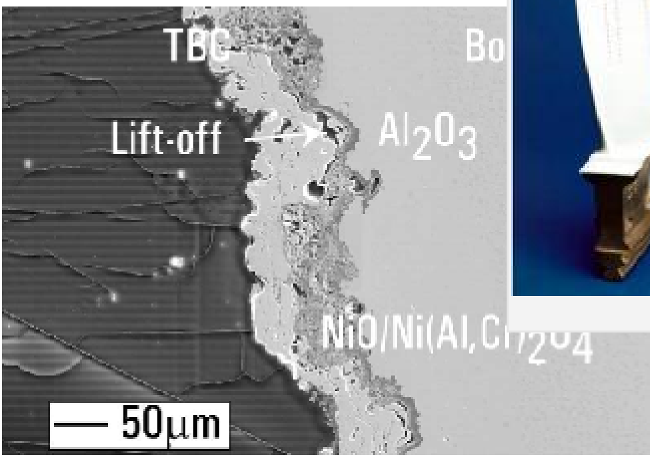


Fig. 3. Cross section of a TBC coated superalloy [10]

The TBC systems, which comprise metal and ceramic multilayers (Fig. 4), insulate turbine components from the hot gas stream and improve the durability and energy efficiency of aircraft engines [11-13]. The advantages of ceramics and metals are combined in utilizing ceramic thermal barrier coated metallic substrates. Usage of only 0.2 mm thick ceramic thermal barrier coating on the surface of gas turbine blade made by the EB-PVD gives the possibility to reduce the surface temperature in the order from 100 to 150°C, the specific fuel consumption of about 2 to 3 % as well as the corresponding emission. The extremely low thermal conductivity and good phase stability makes yttrium - stabilized zirconia (YSZ) the most successful ceramic top-layer, when combined with a metallic interlayer. This metallic interlayer acts on the one hand as a bond coat and on the other hand as an oxidation and corrosion protection barrier. This bond coat consists frequently of MCrAlY or PtAl alloys which, under service conditions, produce a thermally grown oxide (TGO) scale of alumina. The lifetime of TBC systems is mainly restricted by the growth of TGO. As a metal oxidizes, oxygen diffuses through the oxide to react at the metal-oxide interface and create more oxide.

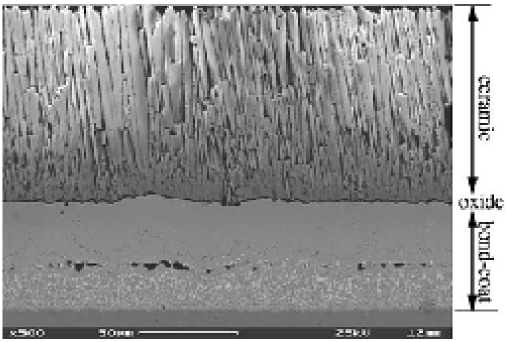


Fig. 4. SEM micrograph of an as-received TBC system [11]

3. Degradation features. Degradation of the TBC systems over time can be investigated experimentally at the laboratory conditions under thermal cycle loading (Fig. 5). Typical sample geometries are pins, plates, disks or turbine blades.

First, as its known [14], high thermal stress can be a source of cracking in the TBC system.

Second, it was experimentally established that the growth of the oxide layer and its stability as well as the embrittlement of the material due to incorporation of oxygen are of major importance [15].

Third, the creep response of the TBC system under the complex stress condition is another important issue concerning such novel multicomponent material system [16-18]. In this regard, it is necessary to take into account the top coat creep, bond coat creep and Ni-based single crystall superalloy creep.

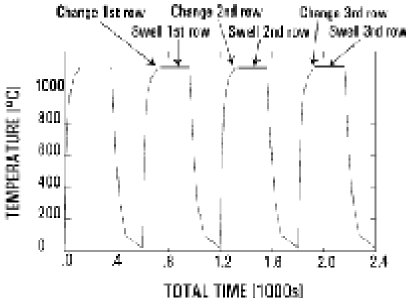


Fig. 5. Thermal cycle loading of the TBC systems [10]

Fourth, materials in the TBC systems operating under conditions of large oxygen chemical potential gradients combined with high temperatures for a prolonged period of time exhibit creep deformation considered as a time-dependent irreversible deformation process. Even in the initial stages of the creep process in metal and ceramic multilayers, dislocations, impurity atoms and voids accumulate at the grain boundaries to form grain boundary cavitation. For example, Fig. 6 shows the formation of the Kirkendall voids beneath the bond coat of the TBC system after 100 h of isothermal exposure at 1150°C [19].

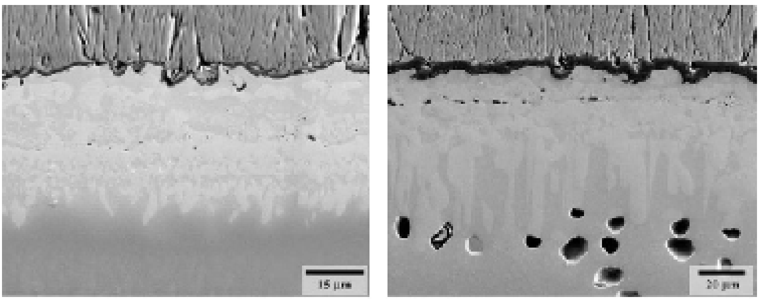
As microscopic cavities at the grain boundaries get larger and coalesce, dislocations, impurity atoms and voids move out to grain boundaries, and microcracks along the grain facets begin to be formed. Growth and coalescence of

these microcracks lead to the creep rupture in the final stage of the creep process with formation of macrocrack with some preferential orientation, often, direction perpendicular to the maximum principal stress. Thus, creep deformation changes the microstructure of metal and ceramic multilayers by introducing dislocations, impurity atoms and voids in the initial stages, microscopic cavities in the following, and microcracks in the final stage of the creep process, all of them, at the grain boundaries with some preferential orientation. Furthermore, the velocity of the growth of already existing grain boundary microscopic cavities and microcracks, and of the nucleation of new ones essentially depends on the intensity of creep deformation. On the other hand, creep deformation of metal and ceramic multilayers is influenced by the growth of microscopic cavities and microcracks. This influence begins at the primary and secondary stages of the creep process, and can be visible in the tertiary stage due to possible increasing of the creep strain rate, preceding the creep rupture. The creep rupture case without increase in the creep strain rate can be also observed. Thus, creep deformation and material deterioration in the TBC systems due to growth of creep damage occur parallel to each other, and they have a reciprocal effect. Obviously, creep damage growth in metal and ceramic multilayers leads to the mechanical and structural degradation of the TBC systems over time. However, to the best of the authors' knowledge, up to now no investigations exist for creep damage development over time in the TBC systems for gas turbine blades of aircraft engines.

Finally, the fatigue damage development in the TBC systems over time is important for durability analysis of gas turbine blades of aircraft engines [20].

4. Modeling of TBC system. The interdisciplinary approach proposed in this paper includes:

- the simultaneous consideration of oxidation and oxygen bulk diffusion, thermoelaestic deformation and swelling, as well as, high temperature creep process and creep damage development in the TBC systems for gas turbine blades of aircraft engines,
- modelling of oxygen diffusion process in TGO with determination of the chemical diffusion coefficient using the Fick's second law,
- constitutive modeling of thermal, diffusional and mechanical phenomena under consideration,
- structural analysis of the TBC systems for the typical laboratory sample geometries, such as pins, plates, disks and turbine blades, using in-house developed software as well as the ANSYS codes and constitutive model developed,
- computational modeling and simulation, and the quantitative analysis of the TBC systems degradation over time,
- comparison of the lifetime predictions against the experimental results obtained at the laboratory conditions under thermal cycle loading.



(a) (b)

Fig. 6. The microstructures of the coatings on Ni-based alloy in the as-received condition (a) and following 100 h of isothermal exposure at 1150°C (b) [19]

Total strains in the TBC system are composed of an elastic part, thermal part, diffusional part [21] and a part due to creep [22] related to a continuum damage parameter by Kachanov-Rabotnov-type [22] reflecting microstructural changes, material deterioration and TBC system degradation. Constitutive model considered in this paper takes into account different properties of ceramic top-layer under tension and compression (Fig. 7).

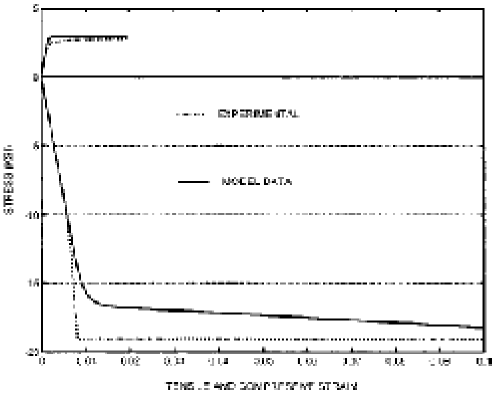


Fig.7. Stress-strain diagram for yttrium- stabilized zirconia at 1150°C °C under tensile and compressive loading types [17]

The infinitesimal creep strain tensor p_{kl} will be defined [22] as

$$\dot{p}_{kl} = s_e^{m}\left(1-\frac{f}{f_*}\right)^{-q}\left(\frac{AI_1 d_{kl}+Bs_{kl}}{s_2}+a\,Cm_k m_l\right),$$

$$\dot{f} = s_e^{m+1}\left(1-\frac{f}{f_*}\right)^{-q} \qquad (1)$$

with

$$s_e = s_2 + a\,s_1,\; s_1 = Cs_{\max},\; s_{\max} = s_{kl}m_k m_l,$$
$$s_2 = \sqrt{AI_1^2 + BI_2},\; I_1 = s_{kl}d_{kl},\; I_2 = s_{kl}s_{kl},$$
$$\dot{f} = s_{kl}\dot{p}_{kl},\; f \in [0, f_*]$$

Here s_{kl} is the Cauchy stress tensor, f_* is a critical value of the specific dissipation energy f that corresponds to creep rupture time, I_1 and I_2 are the first and the second invariants of the stress tensor, a is a weight coefficient, d_{kl} is the Kronecker delta, and the dot above the symbol denotes a derivative with respect to time *t*. Material parameters *m*, *q*, *A*, *B* and *C* can be found using the experimental results under uniaxial tension

$$\dot{p}_{11} = K_+ s_{11}^{m} \left(1 - \frac{f}{f_*} \right)^{-q}, \quad f = s_{11} p_{11} \tag{2}$$

uniaxial compression

$$\dot{p}_{11} = -K_- \, | s_{11} |^{m} \left(1 - \frac{f}{f_*} \right)^{-q}, \; f = s_{11} p_{11} \tag{3}$$

and pure torsion

$$2\dot{p}_{12} = K_0 s_{12}^{m} \left(1 - \frac{f}{f_*} \right)^{-q}, \quad f = 2 s_{12} p_{12} \tag{4}$$

with the material constants K_+, K_- and K_0.

In order to investigate the oxygen bulk diffusion, the consideration of the Fick’s second law with hydrostatic pressure dependence of oxygen concentration in TGO has been given for the purpose of oxidation analysis. Describing the fatigue damage growth has been given using the continuum damage mechanics model proposed in [23]. Analysis of stress distributions in the multicomponent layers and TBC system degradation over time as well as life-prediction studies in this paper are related to the consideration of the physically nonlinear initial/three-dimensional boundary value problem. Therefore, in-house developed software as well as commercial software with ANSYS codes has been used for structural analysis, computational modeling and simulation, when the constitutive model proposed in the present paper has been implemented into software.

Some examples of the finite element models of TBC systems under discussion that have been considered using ANSYS are given in Figs. 8 and 9.

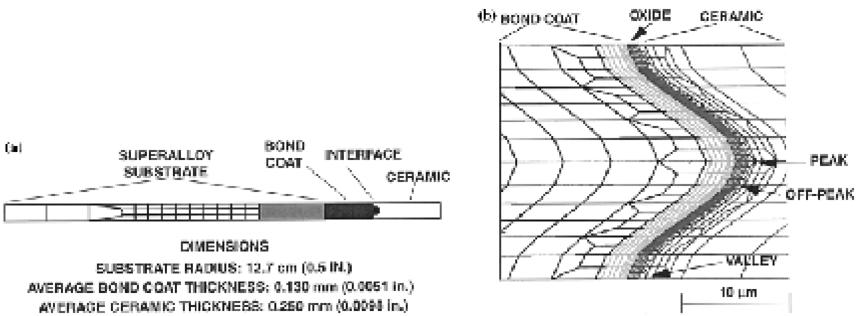
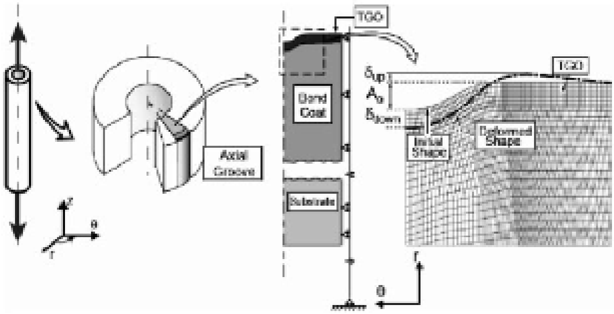


Fig. 8. Finite element mesh geometry for TBC model in the form of disk showing overall geometry of the system (a) and detail view of the interface region (b) [15]

The main feature of the kinematic model of the in-house developed modeling tool for analysis of TBC systems given in Figs. 8 and 9 using the recently proposed shear deformation theory [24, 25] compared with the classical shell theory based on the Kirchoff-Love assumptions is that the differential equations of this refined theory are of the tenth order while the classical theory has the eighth order. Thus, since the separate boundary condition corresponds to each of five generalized degrees of freedom of the normal element (three displacements and two angles of rotation), the boundary conditions in the proposed shear deformation theory are formulated more naturally.



(a) (b)

Fig. 9. Finite element model for TBC system in the form of cylinder showing overall geometry of the system (a) and detail view of the interface region (b) [20]

Furthermore, in the case of the refined theory under discussion for a moderately thick shell of revolution (model of a disc in Fig. 8 and a cylinder in Fig. 9) subjected to an axisymmetrically and statically applied diffusional and force loading leading to the meridional, transversal shear and torsional deformations it is necessary to find the 27 unknowns in the coordinate surface [24, 25]. They are the displacements u, v and w, total angles of rotation of a rectilinear element y_s and y_j, angles of rotation of the normal to the coordinate surface J_s and J_j, angles of rotation due to transversal shears g_s and g_j, forces N_s, N_j, N_{sj}, N_{js}, Q_s and Q_j, moments M_s, M_j, M_{sj} and M_{js}, components of the deformation of the coordinate surface e_s, e_j, k_s, k_j, w_s, w_j, t_s and t_j. A vector of resolving functions can be introduced as

$$\vec{Y} = \{ y_1, ..., y_{10} \}^{\mathrm{T}} = \left\{ \vec{N}, \vec{u} \right\}^{\mathrm{T}} \tag{5}$$

with

$$\vec{N} = \{ N_1, ..., N_5 \}^{\mathrm{T}} = \{ rN_s, rN_{sj}, rM_s, rM_{sj}, rQ_s \}^{\mathrm{T}},$$

$$\vec{u} = \{ u_1, ..., u_5 \}^{\mathrm{T}} = \{ u, v, y_s, y_j, w \}^{\mathrm{T}},$$

and the resolving system of nonlinear differential equations of the shell theory under discussion can be presented in the following vector form

$$\vec{Y'} = [P]\vec{Y} + \vec{f} \tag{6}$$

where *r* is the distance from a point of the coordinate surface to the axis of revolution *z*, j is the circumferential coordinate, S is the length of the coordinate meridian arc, the superscript 'T' denotes the transposition operation, $(\mathbf{K})' = \dfrac{\mathrm{d}(\mathbf{K})}{\mathrm{d}s}$, $r' = \cos q$, $z' = \sin q$, and $(p - q)$ is the angle between the normal to the coordinate surface and the axis *z*. The system (6) is complemented by the boundary conditions at the ends of the moderately thick shell

$$[G]\vec{Y} = \vec{g} \tag{7}$$

The matrixes $[P]$ and $[G]$ as well as the free-term vectors $\vec{f}$ and $\vec{g}$ used here have been discussed in [24, 25].

The components $e_{ss}, e_{jj}, e_{sj}, e_{sV}$ of the strain tensor as well as the angles of rotation q_s, q_j of the reference triad of orthonormal vectors due to its declination at any point of a shell with coordinate V across shell thickness are connected with corresponding parameters of the coordinate surface by the following relations [24, 25]:

$$e_{ss} = \frac{e_s + Vk_s}{a_s} \; (s, j), \quad 2e_{sj} = \frac{w_s}{a_s} + \frac{w_j}{a_j} + V\frac{t_s}{a_s} + V\frac{t_j}{a_j},$$

$$2e_{sV} = \frac{g_s}{a_s} \; (s, j), \quad q_s = y_s - \frac{g_s}{a_s} \; (s, j) \tag{8}$$

where $a_s = 1 + V k_s$, $a_j = 1 + V k_j$, k_s and k_j are the principal curvatures of the coordinate surface, the symbol (s, j) implies that the new equation follows from the equation under consideration by the cyclic substitution of the subscripts *s* and j.

It was established for the TBC systems good correlation of the numerical results obtained using in-house developed software with the analogous results based on the ANSYS codes .

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