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Моделювання оперативного лікування остеопорозу у людей старшого віку після первинного ендопротезування кульшового суглоба/ М.А.Шимон, В.В.Литвак, А.А.Шерегій, О.В.Веретельник, М.А.Ткачук // Вісник НТУ «ХПІ». Серія: Машинознавство та САПР. – Х. : НТУ «ХПІ», 2014. – № 29 (1072). – С. 177-182. – Бібліогр.: 12 назв. ISSN 2079-0075.

На сьогоднішній день одним из самых актуальных вопросов в травматологии и ортопедии является восстановление функций движения в суставах. Лечение переломов шейки бедра у больных пожилого возраста – это эндопротезирование. Оно эффективно и доступно для больного, который в кратчайшие сроки становится трудоспособным. Предлагается методика моделирования и исследований процесса оперативного лечения пациентов. Проведен тестовый расчет интактной модели.

Ключевые слова: остеопороз, эндопротезирование, реабилитация, метод конечных элементов, эквивалентные напряжения, напряженно-деформированное состояние

Today, one of the most pressing issues in traumatology and orthopedics is to restore the functions of motion in the joints. Treatment of hip fractures in elderly patients is joint replacement. It is effective and available to the patient, which rapidly becomes employable. The methods of modeling and process studies of surgical treatment of patients. Test calculations intact model.

Keywords: osteoporosis, hip replacement, rehabilitation, finite element method, the equivalent stress, stress-strain state

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DAMAGE ACCUMULATION IN MULTILAYER THIN FILMS ON GAMMA TITANIUM ALUMINIDES

The present paper involves comprehensive investigations towards an understanding on how aggressive environments, high service temperatures and long dwell times affect damage growth and lifetime reduction of different components

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of automotive combustion engines and aero-engines made out of gamma titanium aluminides with protective coatings. The outcome of this paper is related to the practical recommendations on how damage growth at high temperatures in multilayer thin films on gamma titanium aluminides under thermal cyclic conditions and multiaxial stress state may be controlled in order to reduce environmental degradation, optimize the protective coating and extend lifetime of a component for automotive, energy and aerospace applications.

Keywords: Gamma titanium aluminide; Creep; Fatigue; Damage; Multilayer thin film; Stress

Introduction. At present, researchers have focused their attention on evaluating gamma titanium aluminides (γ -TiAl) for components of automotive combustion engines and aero-engines, such as turbine airfoils, turbocharger wheels, valves or compressors [1]. This new class of lightweight alloys has been intensively developed over the last two decades, because density of γ -TiAl is equal to half the density of steel or nickel-based superalloys [2]. In this regard, γ -TiAl alloys could be used at high temperatures in gas turbines of aero-engines instead of the heavy nickel-based superalloys in order to increase the speed of aircraft. For structures working at a harsh environment up to temperatures in excess of 900°C, coating may be applied to protect the material from direct exposure to the environment. In this way, protective coatings are required for both environmental protection and thermal insulation of the structural material [3]. Thus, protective coating can substantially improve at high temperatures the application potential of gas turbine blades of aircraft engines made out of γ -TiAl alloys.

A European Project INNOVATIAL (2005-2009) [4] supported within the Sixth Framework Programme for Research and Technological Development was directed at the development of protective coatings for γ -TiAl alloys using four different coating strategies, namely, nanoscale multilayers, nanocomposites, intermetallic coatings and thermal barrier coatings (Table 1). Twenty two international research organizations and industrial partners led by the German Aerospace Center (Project Coordinator Prof. Christoph Leyens) were involved into extensive collaborative research within 54 months. INNOVATIAL coatings were applied to various components, such as aero-engine airfoils, engine valves, gas turbine buckets, gassier components, rollers and dies [4].

Table 1 – Four different coating strategies to protect γ -TiAl against environmental attack [4]

Coating	Deposition technique	Coater	Thickness (μ m)	Operation performance
Nanoscale multilayer coatings				
TiAl ₂ O ₃ /TiN + Al ₂ O ₃	JBM	HALZER	3.5	2000h / 950°C
SiAlN/TiN	JBM	SHJ	3	2000h / 850°C
SiAlN/TiN	HRMS	SHJ	3.5	1000h / 950°C
TiAl ₂ O ₃ /TiN + Al ₂ O ₃	HRMS / JBK	SHJ / HALZER	3.5	2000h / 850°C
Nanocomposites				
TiAl ₂ O ₃	JBK	MUL	4	1000h / 750°C
SiAlN	JBK	MUL	4	1000h / 750°C
Intermetallic layers				
Al ₂ O ₃	JBK	MUL	4	1000h / 850°C
TiAl ₂ O ₃	JBK	DLF	10	1000h / 850°C
TiAl ₂ O ₃ /Ni	JBK	DLF	10	1000h / 900°C
TiAl ₂ O ₃ /Cr	JBK	DLF	20	1000h / 850°C
TiAl ₂ O ₃ /ZrO ₂	HRMS	SHJ	7	1000h / 1000°C
TBC systems				
SiAlN/TiN + SiO ₂	HRMS / EB-PVD	SHJ / DLF	4.5 / 10	1000h / 750°C
SiAlN + SiO ₂	JBK / EB-PVD	MUL / DLF	4 / 10	1000h / 850°C
TiAl ₂ O ₃ + SiO ₂	JBK / EB-PVD	DLF / DLF	10 / 10	1000h / 900°C
TiAl ₂ O ₃ + SiO ₂	JBK + EB-PVD	DLF / DLF	10 / 10	1000h / 850°C

The technology adopted from nickel-based superalloys [1, 3] was used at the German Aerospace Center (DLR) and was focused on the development of improved oxidation protective coatings in combination with thermal barrier coatings on the γ -TiAl alloys for high temperature applications (Fig. 1).

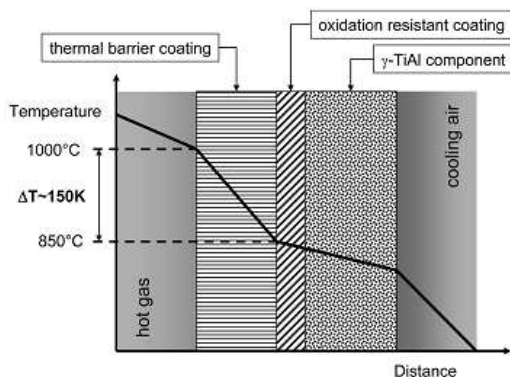


Fig. 1 – A schematic of protective coating applied to γ -TiAl alloys [3]

Conventional Pt modified aluminides and MCrAlY coatings (M = Ni and/or Co) are not suitable as protective coatings for γ -TiAl due to the poor coating–substrate compatibility [5]. In this regard, intermetallic Ti–Al–Cr layers with small additions of Si, Zr, W and Y were deposited on the γ -TiAl substrate by magnetron sputtering technique, and coating thickness ranged between 20 μm and 30 μm [1, 3]. This intermetallic coating remarkably improves the oxidation resistance of γ -TiAl alloy, and exhibits an excellent chemical and physical compatibility with γ -TiAl substrate [5]. In the following, coated substrate was pre-oxidized to form an alumina scale [3]. Intermetallic layer serves also as a suitable bond coat for thermal barrier coatings ($\text{ZrO}_2 - 7-8 \text{ wt } \% \text{ Y}_2\text{O}_3$) due to the excellent adherence of zirconia top coats to alumina scales and represents the most effective oxidation resistant INNOVATIAL coating [4]. Thermal barrier coating was deposited on the pre-coated γ -TiAl substrate using electron beam- physical vapor deposition (EB-PVD), and coating thickness was 150–190 μm [3]. These coating systems exhibited lifetimes exceeding the maximum exposure length of 1000 cycles with 1 h dwell time at 950°C, but failed at 1000°C [6]. Failure was caused by degradation of the intermetallic layers resulting in spallation of the thermally grown oxides.

The CrAlYN/CrN nanoscale multilayer coatings were studied instead of intermetallic Ti–Al–Cr layers as oxidation resistant coatings in combination with thermal barrier coatings (TBCs) on the γ -TiAl alloys [7]. It was established that the TBC systems with CrAlYN/CrN layers did not fail at 850 and 900°C during the maximum exposure time period of 1000 cycles of 1 h dwell time [7, 8].

Alternative coating strategy with nanoscale multilayers and without TBC was applied when TiAlYN/CrN and CrAlYN/CrN nanoscale multilayer coatings were deposited on the γ -TiAl specimens using magnetron sputtering techniques [9]. On some of the coated samples an additional alumina top coat was deposited too. The TiAlYN/CrN films exhibited poor stability at 850°C and rapidly oxidised, and therefore were not applicable for long-term protective coatings on the γ -TiAl alloys [9]. On the other hand, the Cr-based nitride films provided effective oxidation protection to γ -TiAl at 850°C. The alumina top coat did not significantly increase the oxidation resistance of γ -TiAl alloys with CrAlYN/CrN nanoscale multilayer coatings [9].

Environmental protection of γ -TiAl alloys by CrAlYN nanocomposites and thermal barrier coatings was investigated at 850 and 900°C under cyclic oxidation conditions [10]. Thin films of CrAlN + 2 mol.% YN were deposited on the γ -TiAl substrate by magnetron

sputtering technique while TBCs were deposited on the pre-coated γ -TiAl substrate using EB-PVD. The mixture of chromium and aluminium oxides was formed on the nitride coating. The EB-PVD zirconia top coat was well adherent to the mixed oxide scale of chromia and alumina formed on the degraded CrAlYN nanocomposite.

Direct applicability of thermal barrier coatings on the γ -TiAl alloys without oxidation resistant coating was studied by cyclic oxidation testing in air at 850 and 900°C [11, 12]. SEM micrographs of the thermally grown oxide scale revealed outer oxide mixture $\text{TiO}_2 / \text{Al}_2\text{O}_3$. For the γ -TiAl sample with TBC at 900°C, spallation was observed after 810 cycles [11]. Failure occurred in the thermally grown oxide. Thus, effective oxidation protection remains a major issue for high temperature applications of γ -TiAl alloys.

Diffusion coatings on the γ -TiAl alloys were produced using the pack-cementation process and annealing treatments [13]. In this case, the high temperature exposure resulted in the formation of TiAl_2 layer due to interdiffusion between TiAl_3 coating and γ -TiAl substrate. In the following, TBC was deposited on the pre-coated γ -TiAl substrate using EB-PVD. The oxidation behavior of the aluminized and annealed specimens with TBC was studied performing cyclic oxidation tests in the temperature range between 850 and 950°C. The lifetime of this TBC system at 950°C exceeded 1400 cycles, whereas an aluminized and annealed sample without TBC failed after 500 cycles occurring in the mixed oxide scale formed on the γ -TiAl phase. Thus, diffusion coatings on the γ -TiAl alloys provided an effective oxidation protection at 950°C due to the formation of a continuous alumina layer.

Obviously, preventing the formation of non-protective titanium oxide is the primary goal to improve the resistance of γ -TiAl alloys against oxidation. In this regard, Si-based and aluminum rich Ti-Al coatings produced by means of magnetron sputter technique were studied as oxidation resistant coatings for γ -TiAl alloys [14]. Both these coatings were tested at exposure temperatures up to 950°C for 1000 h resulting in very good oxidation behavior.

The specific objectives of the research reflected in the present paper are:

- to specify the mechanisms of thermal, chemical, mechanical and structural degradation of multilayer coating systems developed to protect γ -TiAl alloy against environmental attack involving four different coating strategies (nanoscale multilayers, nanocomposites, intermetallic coatings and thermal barrier coatings),
- to develop the constitutive laws of materials behavior and kinetic equations of damage for coated γ -TiAl substrates to describe elastoplastic deformation and creep under thermal cyclic conditions, transport phenomena, oxidation and chemical expansion, ratcheting and fatigue, wear, erosion and particle impact,
- to identify material parameters in the proposed constitutive model using different experimental data for multilayer thin films on the γ -TiAl alloys,
- to calculate the time-dependent stress distribution (finite element modeling, structural mechanics) and damage growth (continuum damage mechanics) in multilayer thin films on the γ -TiAl alloys under thermal cyclic conditions as a function of material and system parameters as well as operating conditions, and additionally to predict the lifetime of multilayer coating systems,
- to find the interrelationship between environment, protective coating, γ -TiAl substrate and degradation of multilayer coating system over time,
- to compare the lifetime predictions obtained in this research against experimental

data from the burner rig tests involving four different coating strategies for γ -TiAl alloys,

- to develop efficient instrumentation for durability analysis of multilayer coating systems with γ -TiAl substrate and new concepts that could change the way manufacturers design,
- to transfer new knowledge obtained in this research to scientific and industrial communities related to the development of the γ -TiAl components for automotive, energy and aerospace applications.

State of the art. The functionality and reliability of the γ -TiAl components with protective coatings for automotive, energy and aerospace applications are strongly related to the damage growth and stresses redistribution over time in the coating systems. A methodology for durability analysis of multilayer coating systems with γ -TiAl substrate is needed that complements experimental procedures for evaluation of coatings discussed above. There are various sources of stresses in coatings [15]:

- a) thermal induced stresses resulting from temperature changes and differences of the coefficient of thermal expansion of coating layers and substrate material;
- b) stresses resulting from coating growth. In this case it is necessary to distinguish between intrinsic growth stresses and geometrically-induced stresses. Intrinsic growth stresses are due to oxidation; chemical reactions, phase transformations, energetic particle bombardment, etc;
- c) stresses due to deformation of the coating systems under applied loading and environmental influence.

The consideration of thermoelastoplastic deformation in coating systems with γ -TiAl substrate, as well as, stresses resulting from temperature gradients and from external mechanical loading is vital in the structural analysis of the systems. However, this alone is not sufficient to understand the mechanisms of multilayer system degradation that affect damage growth and reduce the lifetime of the γ -TiAl components with protective coatings. Therefore, it is necessary to identify the time-dependent phenomena related to the chemical, mechanical and structural degradation of coating systems over time. These time dependent phenomena can be investigated experimentally.

In the following, several processes are described that are essential to understand and control for long term operation of the multilayer systems, but that are among the most challenging to master, which is probably a reason why relatively little literature on them has appeared so far. The considered processes are creep, chemical expansion, fatigue and erosion.

Creep of EB-PVD zirconia top coat. The EB-PVD zirconia top coat in the coating systems operating under severe service thermal and chemical conditions for a prolonged period of time exhibits creep deformation considered as a time-dependent irreversible deformation process. Even in the initial stages of the creep process in ceramics of TBC, dislocations, impurity atoms and voids accumulate at the grain boundaries to form grain boundary cavitation. As microscopic cavities at the grain boundaries get larger and coalesce, dislocations, impurity atoms and voids move out to grain boundaries, and micro-cracks along the grain facets begin to be formed. Growth and coalescence of these micro-cracks lead to the creep rupture in the final stage of the creep process with the formation of macro-cracks with some preferential orientation, often, direction perpendicular to the maximum principal stress. Thus, creep deformation changes the microstructure of the EB-PVD zirconia top coat by introducing dislocations, impurity atoms and voids in the initial stages, microscopic cavities in the following, and micro-cracks 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 cavi-

ties and micro-cracks, and of the nucleation of new ones essentially depends on the intensity of creep deformation. On the other hand, creep deformation of ceramics is influenced by the growth of microscopic cavities and micro-cracks. This influence begins at the primary and secondary stages of the creep process, and can be visible in the tertiary stage due to increase of the creep strain rate, preceding the creep rupture. The creep rupture case without increase in the creep strain rate can also be observed in ceramics.

Thus, creep deformation and material deterioration in the EB-PVD zirconia top coat due to growth of creep damage occur parallel to each other, and they have a reciprocal effect. Obviously, creep damage growth in TBC leads to the degradation of coating system on the γ -TiAl substrate over time. The creep deformation of yttria-partially stabilized zirconia ($ZrO_2 - 7-8 \text{ wt } \% Y_2O_3$) has been studied experimentally in [16-18].

Creep of γ -TiAl substrates. Experimental creep studying for three different compositions of γ -TiAl alloy shows three regimes of secondary creep behavior (Fig. 2). In the high stress region (Region I), dynamic recrystallization with small grains forming along grain boundaries takes place. In Region II, dynamic recrystallization is not observed. In Region III, the grain boundaries remain planar.

The relationship between the stress σ and the corresponding steady-state creep rate $\dot{\epsilon}^c$ can be expressed at the temperature T with a power law by Norton and an Arrhenius type dependence on temperature such as

$$\dot{\epsilon} = K \sigma^n \exp\left(-\frac{Q}{R T}\right) \quad (1)$$

where R is the universal gas constant. The creep deformation of γ -TiAl alloys is controlled by a dislocation creep mechanism, and the scopes of 3.5, 7.5 and 4.7 in Fig. 2 refer to the stress exponent n in Eq. (1).

The creep activation energy was determined to be $Q = 313 \text{ kJ/mol}$ for all three γ -TiAl alloys with different grain sizes (32-230 μm) for a temperature range of 707-927°C [19]. Creep of γ -TiAl alloys has been also studied experimentally in [20, 21]. Tertiary creep with rupture has been observed.

Creep of intermetallic Ti-Al-Cr layers. The creep deformation of intermetallic Ti-Al-Cr alloys with small additions of Si, Zr, W and Y up to rupture has been investigated experimentally in [21-23]. The strengthening effect of Cr at high stresses has been discussed. It was established that the main source of strengthening in intermetallic Ti-Al-Cr alloys is precipitation hardening. TEM studies of crept microstructures indicate extensive interaction between the precipitates and the dislocations at the interface [21]. Small additions of Si decrease the melt viscosity and may yield some improvements in oxidation resistance. Addition of W improved the creep resistance but reduced the ductility of intermetallic Ti-Al-Cr alloys.

Creep of oxide scales. Oxide scales located between oxidation resistant coating and

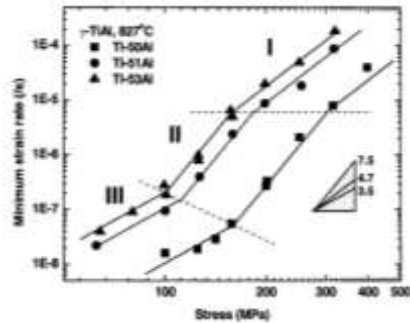


Fig. 2 – Minimum creep strain rates under uniaxial loading for γ -TiAl alloys [19]

TBC demonstrate strong creep behavior too. The creep deformation of Al_2O_3 has been studied experimentally in [24, 25]. It was established also [26] that high-temperature creep deformation of Al_2O_3 is sensitively affected by small amount of dopant cations, which tends to segregate along grain boundaries. The dopant oxides used in this study were TiO_2 , ZrO_2 and Y_2O_3 . Creep of Al_2O_3 is suppressed by Ti/Y or Zr/Y co-doping, and, in particular, Zr/Y co-doping improves the high-temperature creep resistance remarkably. On the other hand, the creep deformation in Ti singly co-doped Al_2O_3 is accelerated in comparison with undoped Al_2O_3 . Interaction between creep deformation and oxynitride scale growth in γ -TiAl alloys has been discussed in [19].

Chemical expansion. During cyclic oxidation, the thermal grown oxide (TGO) exhibits parabolic or exponential growth kinetics. When the TGO forms and grows, the grain size of the TGO grows from small grains (less than $0.1 \mu\text{m}$) to large grains (up to $2.5 \mu\text{m}$). The thickness of the TGO in the γ -TiAl coating systems can reach a size of $16 \mu\text{m}$ without fracture [3, 17]. The process under discussion can be termed as the chemical expansion of the TGO due to the diffusion of oxygen.

Fatigue and ratcheting of γ -TiAl substrates. Coating systems with γ -TiAl substrate used at high temperature are subjected to cyclic mechanical loading as well as periodic temperature variation during the start-up and shut-down of the engine, which gives rise to the so-called thermomechanical fatigue (TMF) and life limitation of the components. In many cases isothermal low cycle fatigue (LCF) tests were used to evaluate the TMF life because of expensive equipment and time-consumption for TMF test. Therefore, it is necessary to clarify TMF behaviors of the γ -TiAl components with protective coatings under the simulated service conditions in the laboratory for the safety and reliability of the used materials. Fully-reversed isothermal TMF tests for γ -TiAl alloys were performed in the temperature range of 550 - 850°C on a servohydraulic closed-loop machine [27]. At all temperatures tests were conducted under total strain amplitude of $\Delta\varepsilon/2 = 0.7\%$, while at service-relevant temperatures (i.e. 550 - 650°C) additional tests were run at total strain amplitudes of $\Delta\varepsilon/2 = 0.5\%$ and 0.6% .

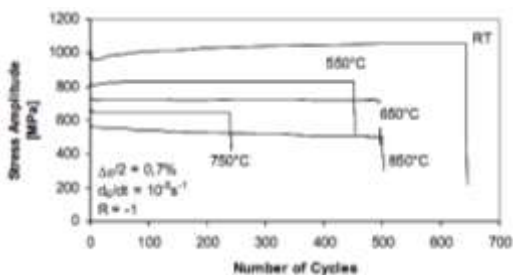


Fig. 3 – Stress amplitude vs. number of cycles for isothermally fatigued γ -TiAl alloy [27]

If in the low cycle TMF test the total strain amplitude is kept constant over a wide range of temperature, it may be expected that the amount of plastic strain is increasing with temperature. Therefore a shorter lifetime at elevated temperatures may be assumed, which will be even more pronounced when oxygen attack occurs. However, this is not the case for the γ -TiAl alloy investigated in [27]. While the stress amplitude is decreasing with temperature, lifetime

seems to be rather unaffected at elevated temperatures (Fig. 3). Quick decreasing of the stress amplitude at the fixed temperature with number of cycles occurs before failure.

TMF behavior of the γ -TiAl alloys was studied either in in-phase or out-of-phase [28]. In this regard, the influence of related microstructural instability during TMF process

on stress-strain response, fatigue life and fracture way under in-phase (IP) and out-of-phase (OP) loading mode was investigated. The variation of tensile load and compressive load counteracts each other, leading to almost constant cyclic stress amplitudes at various temperature portions (Fig. 4). Fig. 4 also shows that TMF life strongly depends on the mean stress as well as on the loading mode. At the same temperature portion, the fatigue life under IP mode is much longer than OP mode. The results are associated with the environmental embrittlement that influences the initiation of fatigue cracks during high temperature exposure to air. Under OP mode, the high tensile stress at minimum temperature acts on the specimen and fatigue cracks can easily nucleate on the oxide surface layer and/or brittle subsurface layer. In contrast to this, the tensile stress is lowered in IP condition because of the significant improvement of the deformability of the alloy at high temperature. As a result, the fatigue crack initiation on the brittle surface layer is delayed under IP mode.

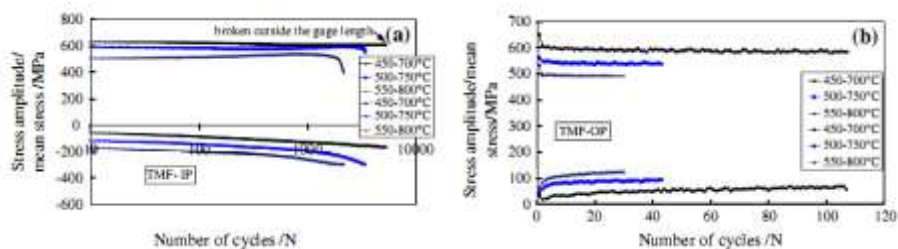


Fig. 4 – Change of cyclic stress amplitude and mean stress with temperature and number of cycles for fatigued γ -TiAl alloy: a – TMF-IP; b – TMF-OP [28]

It is interesting to note that such cyclic behavior of the γ -TiAl alloys shown in Figs. 3 and 4 can be described considering simultaneously fatigue and ratcheting of γ -TiAl substrates. The increase of mean stress with increasing test temperature and cyclic number enlarges the plastic strain accumulation (ratcheting) and promotes the TMF damage. Negative mean stress in OP condition causes the more early fatigue cracks' initiation on the oxidized surface layer than in IP condition, leading to shorter TMF life. Creep damage arising from grain boundary sliding contributes to the TMF failure under IP mode. Intergranular crack and transgranular cleavage crack in the coarse γ grains are the predominant ways of fatigue fracture under OP mode.

Fatigue of oxidation resistant coating. Shida & Anada [29] have demonstrated that at least 70 at.% Al is necessary in γ -TiAl alloys to obtain an alumina-only scale during high-temperature exposure. As discussed earlier, in recent years several coating systems have been developed in order to create sufficient oxidation resistance at temperatures larger than 700°C. Niewolak et al. [30] have shown that silver additions to TiAl can improve oxidation behavior tremendously. Therefore, a coating of the composition Ti-48Al-2Ag was deposited on the γ -TiAl specimens of TNB-V2 using magnetron sputtering technique [28]. In the fatigue test at 850°C it was investigated whether these beneficial properties may be transferred to fatigue conditions. A lifetime increase by a factor of about 2 was measured compared to the test of an uncoated specimen [28]. Thus, a Ti-48Al-2Ag coating is showing excellent oxidation resistance.

Fatigue and ratcheting of zirconia top coat. Ratcheting of ZrO₂ – 8 wt %

Y_2O_3 at high temperatures has been studied experimentally in [31]. Fatigue of TBC on the γ -TiAl alloy was investigated at 850 and 900°C [11, 12].

Erosion. TBCs are used to protect hot path components of gas turbines from hot combustion gases. In this way, TBCs of aircraft gas turbines, as well as, of stationary gas turbines can be exposed to erosion damage, leading to essential reduction of the aerodynamic efficiency of the gas flow over the airfoils and, finally, to structural failure of the blades [32]. Solid particle erosion is particularly important for aero gas turbines operating in sandy (or ashy) environments, but even for land based gas turbines, where air is filtered before entering the compressor stage, solid particle erosion can take place owing to particles escaped from filters, or produced either within compressor stages or in the combustion chamber, depending on the materials and on the operating conditions of the specific engine. Owing to their inertia, solid particles do not move along the flow streamlines and thus they impact on components eroding the protective coatings from the base materials. Pressure loss, change in blade geometry, overheating of γ -TiAl substrate and, finally, structural failure of the blades are the main effects of erosion in gas turbines [33].

Little information exists on the mechanisms that govern erosion of EB-PVD TBCs. Two types of mechanical responses have been identified and are outlined as *severe erosion by foreign object damage*, and *mild erosion by near surface cracking*. In the first case, large particles at high velocity cause the material to be susceptible to large-scale plastic deformation and densification around the contact site. The deformation zones develop over millisecond timescales, as the impacting particle decelerates to rest, prior to rebound. Within the densified zone, kink bands form and extend diagonally downward, toward the interface with the TGO. In some cases, the bands reach the interface with the TGO and lead to delamination within the TBC, just above the TGO. Such delaminations provide a mechanism for creating large-scale spalls.

Second mechanism of erosion corresponds to initial impact, when elastic waves are induced in the TBC columns. Over a time frame of nanoseconds, bending waves are induced at the top of the columns, and these cause flaws at the column perimeter to extend across the columns. The column-sized cracks link, leading to small amounts of material removal. Elastic waves also reflect off the bottom of the columns, becoming tensile waves that propagate back to the surface. These waves can also induce cracking across the columns, and at the interface between the columnar layer and the underlying TGO, particularly when the interface has been embrittled by segregation of contaminants such as sulphur.

Modeling. Thus, to the best of our knowledge, up to now no modeling tool exists for damage analysis of multilayer thin films on the γ -TiAl alloys under thermal cyclic conditions and multiaxial stress state. The goal of this research is to solve such an important problem. The present paper involves comprehensive investigations towards an understanding on how aggressive environments, high service temperatures and long dwell times affect damage growth and lifetime reduction of different components of automotive combustion engines and aero-engines made out of γ -TiAl alloys with protective coatings. The outcome will be how damage growth at high temperatures in multilayer thin films on the γ -TiAl alloys under thermal cyclic conditions and multiaxial stress state may be controlled in order to reduce environmental degradation, optimize the protective coating and extend lifetime of a component for automotive, energy and aerospace applications.

In order to study damage accumulation in multilayer thin films on the γ -TiAl alloys, which may occur in-service and limit the performance of turbine blades, two different test

specimens (Figs. 5 and 6) were subjected in the laboratory of the German Aerospace Center (DLR) to conditions, which simulate the in-service condition as close as possible. Testing of the tubular multilayer specimen (Fig. 5) realizes cyclic thermal and mechanical loading including a thermal gradient over the specimen wall. An applied mechanical loading by force N reproduces the centrifugal force acting on the turbine blade. Temperature T (Fig. 7) on the inner and outer surfaces of the tubular specimen, and load N can act over time under in-phase (IP) and out-of-phase (OP) loading mode. Second specimen under study (Fig. 6) is a rotating round multilayer plate. The applied test cycle for the surface temperatures of a plate is shown in Fig. 7. A heating period t_1 , a dwell time $t_2 - t_1$ and a cooling period $t_3 - t_2$ should be introduced so in order to represent damage growth in a turbine γ -TiAl blade with the protective coating during an entire flight of a jet engine.

An integrated approach to the analysis of damage accumulation in multilayer thin films on the γ -TiAl alloys of the two specimens (Figs. 5 and 6) with multiaxial stress state under thermal cyclic conditions (Fig. 7) has been developed. Thermal and chemical expansions, creep deformation, accumulated "ratcheting" straining, and damage development from creep and fatigue are considered. Total strains in the specimens are assumed to be composed of an elasto-plastic part, thermal part, chemical part, a part due to creep

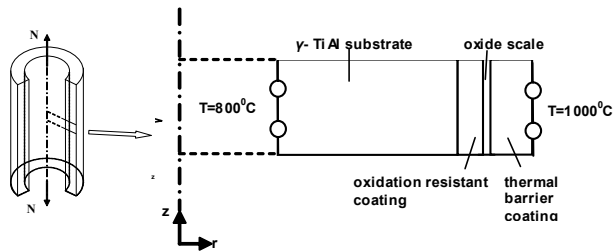


Fig. 5 – The model of the cylindrical test specimen. The proportions of the layers in the figure do not resemble their actual dimensions

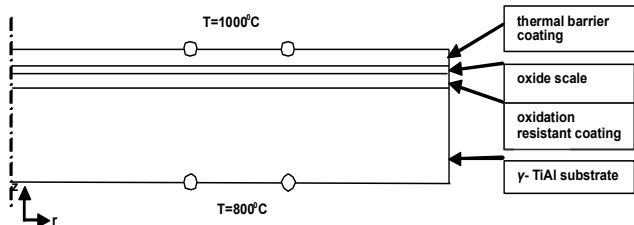


Fig. 6 – The model of the circular plate specimen for testing. The proportions of the layers in the figure do not resemble their actual dimensions

and a ratcheting part accumulated during cycling.

Redistribution of the temperature in transient state over the specimen wall can be found considering Fourier's law for heat transfer. Boundary conditions at the inner and outer surfaces of the specimens in a form of the temperature profile given in Fig. 7 should be considered too. Here $T_1 = 1000^\circ\text{C}$ at the outer surface of TBC, and $T_1 = 800^\circ\text{C}$ at the inner surface of the substrate.

Chemically induced strains that occur in TGO during oxidation are connected with oxygen concentration δ [35], i.e.

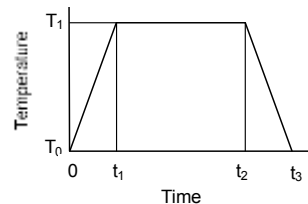


Fig. 7 – Temperature profile during a single loading cycle

$$\varepsilon_{ij}^{ch} = B(\delta - \delta_0)\delta_{ij} \quad (2)$$

where δ_0 is the magnitude of oxygen concentration at the reference state, δ_{kl} is the Kronecker's symbol, and B is the material parameter. Oxygen concentration can be described by the second Fick's law:

$$\frac{\partial \delta}{\partial t} = D\nabla^2 \delta \quad (3)$$

where t is the time, and D is the diffusion coefficient of oxygen.

The creep strain rates are related to the stresses under multiaxial loading as follows [36]:

$$\frac{d\varepsilon_{kl}^c}{dt} = \frac{\sigma_e^n}{(1-\phi)^m} \left(\frac{3}{2} \frac{A s_{kl}}{\sigma_i} + C \delta_{kl} \right) \quad (4)$$

where $\sigma_e = A\sigma + C\sigma_k \delta_{kl}$, $\sigma_i = \sqrt{\frac{3}{2} s_{kl} s_{kl}}$, s_{kl} is the stress deviator, σ_{kl} is the stress tensor, and A , C , n , m are material parameters. A continuum damage parameter by Kachanov-Rabotnov ϕ has been introduced into the creep law given by Eq. (4) with the formulation of the following creep damage growth equation

$$\frac{d\phi}{dt} = \frac{\Sigma_e^k}{(1-\phi)^l} \quad (5)$$

where $\Sigma_e = A_0\sigma + C_0\sigma_k \delta_{kl}$, A_0 , C_0 , k and l are material parameters. Equations (4) and (5) reflect the tension/compression asymmetry of creep and creep damage of the materials under study.

Description of ratcheting and fatigue is considered too. In this regard, the components of the ratcheting strain tensor can be defined as follows:

$$\varepsilon_{kl}^r = \frac{N}{(1-\phi)^f} \left(\frac{3}{2} \kappa_{kl} \tau_{kl} \right) \quad (6)$$

where N is a number of cycles, $\tau_e = a\tau + c\tau_k \delta_{kl}$, $\tau_i = \sqrt{\frac{3}{2} \kappa_{kl} \tau_{kl}}$, κ_{kl} is the stress amplitude deviator during cycling, τ_{kl} is the tensor of the mean stresses during cycling, dot above the symbol denotes the derivative with respect to the number of cycles, and a , c , p , q and f are material parameters. Fatigue damage parameter ϕ can be described by the following kinetic equation

$$\frac{d\phi}{dt} = \frac{\rho_e [(\dot{\varepsilon} - \nu)(\sigma - \sigma_0)]}{(1-\phi)^v} \quad (7)$$

where $\rho_e = d\tau + e\tau_k \delta_{kl}$, d , e , x , b and v are material parameters. Equations (6) and

(7) reflect the tension/compression asymmetry of ratcheting and fatigue damage of the materials under study.

Taking into account that TBCs are vulnerable to erosion and spalling from high speed particle impact damage on the leading edge of high pressure turbine blades, the effect of the TBC geometry upon the contact radius, the indentation load, the average indentation pressure and the bending stresses within each column should be examined. Finite element simulations will be considered for spherical indentation of an elastoplastic columnar TBC. In this way, plastic damage mechanisms, as well as, and elastodynamic mechanisms are involved.

Analysis of stress distributions in multilayer thin films on the γ -TiAl alloys and coating system degradation over time as well as life-prediction studies in this research are related to the consideration of the physically nonlinear initial/three-dimensional boundary value multiphysics problem. Therefore, various commercial software packages can be used for structural analysis, computational modeling and simulation, when the integrated constitutive model proposed in the project will be implemented into its codes. The ABAQUS codes [37, 38] as well as software CFD-Fluent and equation solver software gProms are accepted in the present research. This computer-based structural modeling tool (ABAQUS, CFD-Fluent and gProms) was used for analyzing operation-induced stress distributions in a coating system and system degradation with time, for durability analysis and lifetime predictions, and for improving the performance and safety of multilayer thin films on the γ -TiAl alloys. The results of this analysis were obtained by analogy with TBCs on the Ni-based superalloys [39, 40], and they will be discussed in the future paper.

Conclusion. If the modeling tool proposed in this paper will demonstrate the ability to predict experimental results obtained on systems tested in Germany, then it can be used to optimize protective coatings, to explore new configurations, and, finally, to form a conception and design platform for multilayer thin films on the γ -TiAl alloys. This gives the possibility to work in the Ukraine in the area of protective coatings without need of expensive experiments.

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Damage accumulation in multilayer thin films on gamma titanium aluminides / **A. Zolochovsky, L. Parkhomenko, V. Gnitko, A. Kühhorn, M. Kober** // *Вісник НТУ «ХПІ»*. Серія: Машинознавство та САПР. – Х. : НТУ «ХПІ», 2014. – № 29 (1072). – С. 182-195. – Бібліогр.: 40 назв. *ISSN 2079-0075*.

Настоящая статья включает в себя всеобъемлющие исследования, направленные на понимание то-

го, как агрессивные среды, высокие температуры и время цикла нагружения влияют на рост повреждаемости и сокращение долговечности различных компонентов автомобильных двигателей внутреннего сгорания и авиационных двигателей, изготовленных из гамма алюминидов титана с защитными покрытиями. В результате этих исследований установлено, как рост поврежденности при высоких температурах в многослойных тонких пленках на основе гамма алюминидов титана в условиях теплового циклического нагружения и многоосного напряженного состояния можно контролировать с целью снижения деградации под влиянием окружающей среды, оптимизации защитного покрытия и увеличения срока службы элементов конструкций для автомобильной, энергетической и аэрокосмической промышленности.

Ключевые слова: гамма алюминид титана; ползучесть; усталость; повреждаемость; многослойная тонкая пленка; напряжение

Дана стаття включає в себе всеосяжні дослідження, спрямовані на розуміння того, як агресивні середовища, високі температури і час циклу навантажування впливають на зростання пошкоджуваності і скорочення довговічності різних компонентів автомобільних двигунів внутрішнього згоряння та авіаційних двигунів, виготовлених з гамма алюмінідів титану з захисними покриттями. У результаті цих досліджень встановлено, як зростання пошкодженості при високих температурах в багатослойних тонких плівках на основі гамма алюмінідів титану в умовах теплового циклічного навантаження і багатослойного напруженого стану можна контролювати з метою зниження деградації під впливом навколишнього середовища, оптимізації захисного покриття і збільшення терміну служби елементів конструкцій для автомобільної, енергетичної та аерокосмічної промисловості.

Ключові слова: гамма алюмінід титану, повзучість, втома, пошкоджуваність, багатослойна тонка плівка, напруга