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Numerical investigation of damage protective oxide mechanisms in thermal barrier system for aeronautical turbine blade

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ABSTRACT

The choice of a material for a given application requires insuring a good durability in its conditions of employment, in particular environmental. It is especially true for the systems destined to work in corrosive hot atmospheres. For it, the knowledge and the understanding of the corrosion phenomena, oxidization, ageing and damage are indispensable in order to anticipate the life period of the structures and to propose the adapted protective solutions. The study of the corrosion in high temperature is therefore a greatly interdisciplinary topic, into the interface of the physico-chemistry, metallic and ceramic materials and mechanics.

We propose in this work a finite element method for the simulation of EBPVD TBCs spallation. Our studies concern one of several systems that we call thermal barrier coatings, which are a Composite materials deposited in layers on the hot components to isolate them chemically and thermally at high temperatures. This is the last operational technology adapted on aircraft engines but it is still studied and not fully exploited. This comprehensive article describes the systems currently used and the problem of interaction between mechanical and environment in the turbine.

1 Introduction

When the materials react with their environment, especially at high temperatures, the combined environmental and mechanical stresses degrades the use properties of metallic materials and can lead to premature failure of structures in many industrial sectors such as aeronautics or nuclear. The development of "new" materials at high durability is required. The process is complex and requires a multidisciplinary approach integrating a mechanical, chemical and physical knowledge.

The demands for increased engine efficiency and performance in terms of higher operating temperatures and lower emissions continue to serve as the driving force for the development of a new materials technology. To generate electricity, to take off the aircraft, helicopters and space shuttles, gas turbine engines are widely used, the performance of these gas turbines strongly depends on the operating temperature, several experiments [1-3] shows that an increase of 2% in efficiency involves an increase of 100°C temperature of use (in combustion chamber of turbine blades).

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By against the increasing in temperature involves either to improve the components conception by optimizing the design and cooling systems operation in order to maintain an acceptable temperatures for the metal, or to develop a materials able to resist at high temperatures.

For this reason, the nickel-based superalloys are always used to support the increase in temperature and sustain the most stressed parts of turbine blades. The evolution of these materials in terms of composition and structure in higher temperatures forced the constructors to strengthen the material by multilayer a metal coating who called thermal barrier (TBCs) that gives the best resistances to various environmental sollicitations such as high temperature, corrosion, oxidation...Because of their low thermal conductivity of ceramic layer and thermal diffusivity combined with a good chemical stability at high temperature.

The thermal insulation of TBCs can be advanced by lowering the thermal conductivity of the coating or by increasing the coating thickness. Both ways should be considered when developing new TBC structures. However, when increasing the coating thickness of the TBCs their long-term durability normally deteriorates. For that reason, the coating thickness of a standard TBCs plasma-sprayed (8Y2O3–ZrO2) coating is in most applications limited to 500 μm (see fig.1).

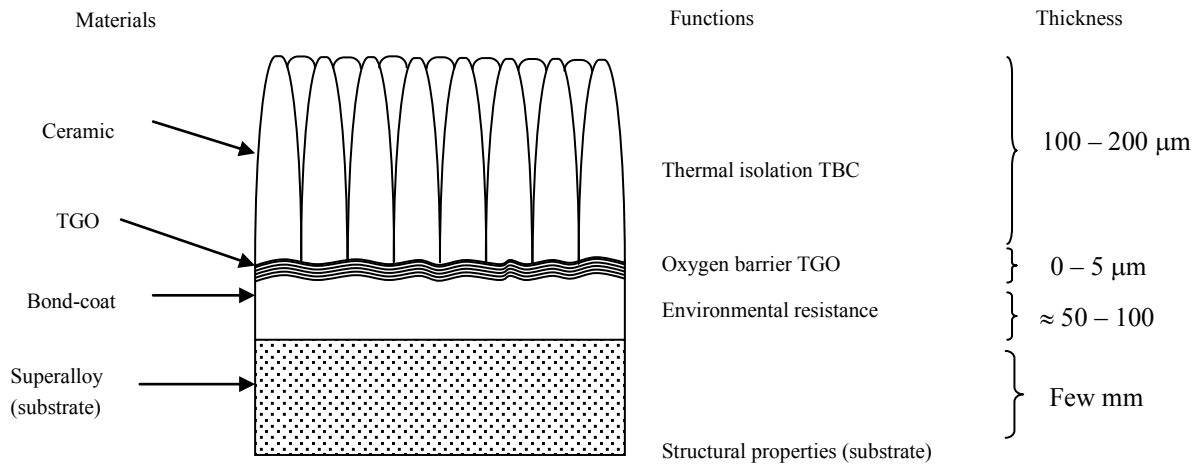


Fig.1- System thermal barrier coating composition

TBCs generally consist of a multilayered structure, as shown in Fig.1. The elaboration process starts by the deposit of a (Ni,Pt)Al bond-coat on the substrate. This layer enables a good adherence of the ceramic on the blade superalloy. The weak thermal conductivity of the ceramic layer makes it possible to increase the admission gas temperature and to decrease the substrate surface temperature. This material is constituted of partially stabilized zirconia ($ZrO_2-8\%Y_2O_3$) and exhibits a columnar microstructure induced by the EBPVD process. A fine coarse alumina ($\alpha-Al_2O_3$) layer is formed between the bond-coat and ceramic layers and grows during high temperature service.

TBCs promise some great advances concerning the engines' efficiency but have the disadvantage of being very brittle. Actually, a spallation of the ceramic is generally observed after a few hundred hours of service. For EBPVD systems subjected to isothermal oxidation, the damage is initiated and mainly localized at the bond-coat/oxide interface [2]. The development of life prediction models became an objective of primary importance for the aeronautic manufacturers.

2 Thermal barrier coatings, materials and functions

The use of thermal barrier coatings system (TBCs) has been generalized in the past few years in aeronautic engines; it becomes a hot topic of research and development recently, although they have been used for thermal protection of hot section components in gas turbines for propulsion and power generation for a long time. The high-pressure turbine blades coatings make possible to improve the engine efficiency by increasing the admission gas temperature and simplifying cooling systems. Moreover, the deposit of a TBC extends the components life by decreasing the superalloy temperature and eliminating transient temperature peaks [3].

The understanding of the mechanisms leading to thermal barrier coating (TBC) spallation is of considerable practical importance. Independent of processing technology (electron beam physical vapor deposition or plasma spraying), failure occurs normally at the bond coat/thermally grown oxide (TGO)/TBC interface region [1, 2] and it has been appreciated in the past by numerous authors, [3–5]

Our systems are designed to fulfill multiple requirements, and they are highly complex. They have four primary constituents as Shown in Fig.1:

1. The thermal barrier coating (TBC) itself;
2. A thermally grown oxide (TGO) that forms between the TBC and the bond coat.
3. Aluminium containing bond coat between the substrate and the TBC;
4. The superalloy substrate.

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This material is constituted of partially stabilized zirconia ($ZrO_2-8\%Y_2O_3$) and exhibits a columnar microstructure induced by the EBPVD process. During the working, a fine coarse alumina ($\alpha-Al_2O_3$) layer is formed between the bond-coat and ceramic layers and grows during high temperature service; this third material constitutes the weak link of the system.

TBCs promise some great advances concerning the engines' efficiency but have the disadvantage of being very brittle. Actually, a spallation of the ceramic is generally observed after a few hundred hours of service [1]. For EBPVD systems subjected to isothermal oxidation, the damage is initiated and mainly localized at the bond-coat/oxide interface [2].

The failure of TBC systems is typically associated with buckling and spalling of ceramic top coat from the thermally grown oxide (TGO) or at TGO/bond-coat interface [4,10,13]. Therefore, the adherence and stress in the TGO layer is important to understand damage mechanism of TBCs. The stress in the TGO is caused by the thermal expansion misfit between the TGO and the substrate, as well as the growth strains in the TGO. The stress in the TGO layer is affected by many factors, such as composition and structure of top coat and bond coat, creep and yielding behavior of bond coat and morphologies of the TGO. The limited research on stress measurement was conducted on the TBC systems with a platinum-aluminide bond-coat [4]. There is little research on a TBC system with CoNiCrAlY bond coat, which will be presented in this paper.

A recent research showed that the failure of the TBC occurred when the TGO attained its critical thickness. If the thickness of the top coat is different and/or the deposition conditions are changed, the existence of such a critical thickness of the TGO is questionable and needs to be evidenced. Furthermore, the stress distribution in the TGO is not uniform although the average value of the stresses in the TGO has been used [4, 7]. To get the stress distribution in the TGO, the stress measurement is conducted on cross section.

The different approaches are generally based on the calculation of the macroscopic tensile stress at the bond-coat/oxide interface induced by the blade curvature radius. The life prediction is then driven by a significant parameter that is the maximal admissible stress at this interface, denoted σ_c . Its evolution is often described by a function of the oxide thickness [4]:

$$\sigma = \sigma_{c0} \left(1 - \frac{\delta}{\delta_c}\right) \quad (1)$$

Where δ is the oxide thickness, δ_c is a critical oxide thickness where spallation is supposed to occur and σ_{c0} the initial bond-coat/oxide interface strength.

The difficulty is of course to determine the two parameters σ_{c0} and δ_c . It is now clearly established that these parameters have to be related to a study of the damage initiation at the microscopic scale.

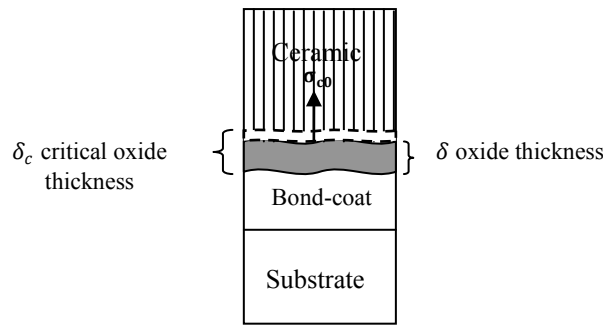


Fig.2- Graphical representation of the oxide thickness function

The thickness of the oxide scale is evaluated using a classical parabolic law:

$$e_{ox} = \sqrt{k_e t_{ox}} + e_{ox}^{init} \tag{2}$$

with e_{ox} the oxide thickness, e_{ox}^{init} the initial oxide thickness formed during the bond-coat deposit process, t_{ox} the oxidation time and k_e the parabolic constant .

Currently, our composite system, such as a brittle coating on a tough substrate, will respond to bending differently. When the strain in the upper fiber of the sample in the coating, reaches the value of crack nucleation, a crack is formed in the coating. The number of cracks will increase with further bending as more crack nuclei become activated [4, 7].

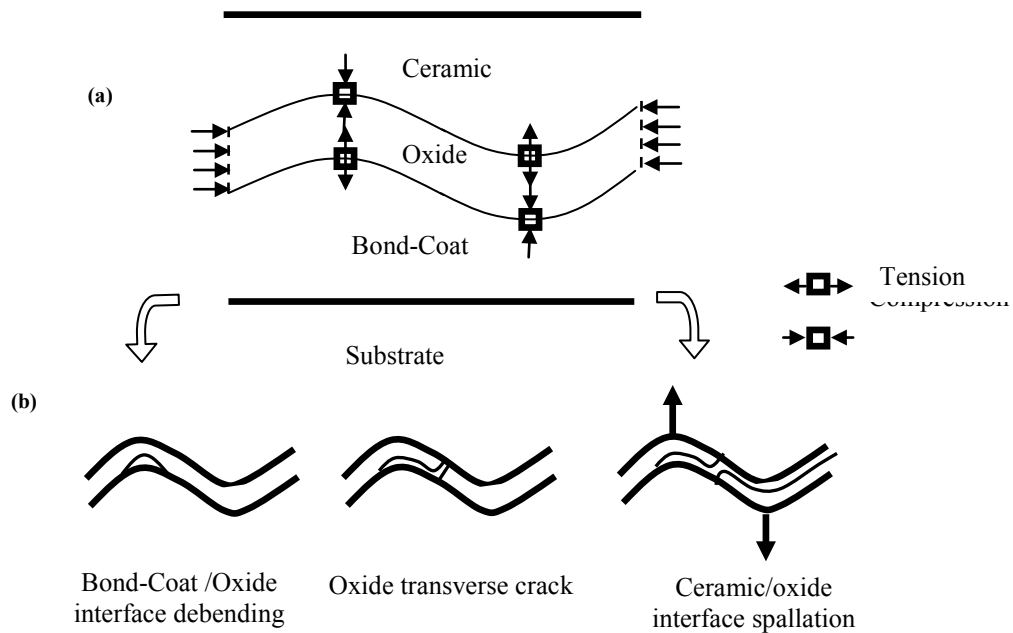


Fig.3 - (a) Schematic stress contours at both the oxide interfaces during cooling and (b) subsequent spallation scenario.

Due to the large difference in thickness between coating and substrate (typically a few micrometers as compared to a few millimeters) the influence of the coating on the bending resistance of the composite can be neglected in comparison to the influence of the substrate. The strain in the coating along the beam caused by bending is thus approximated by that in the outer fiber of the substrate, ϵ_s , which is calculated using [1]:

$$\epsilon_s = \frac{3F(L_1-L_2)}{2E_s b h^2} \tag{3}$$

Where L_1 and L_2 are the distance between the outer and inner supports, respectively where is proposed previously by M. Caliez, J.-L. Chaboche, F. Feyel and S. Kruch (see fig.4), F is the applied load, E_s is the Young’s modulus of the substrate and b and H are the width and height of the beam, respectively.

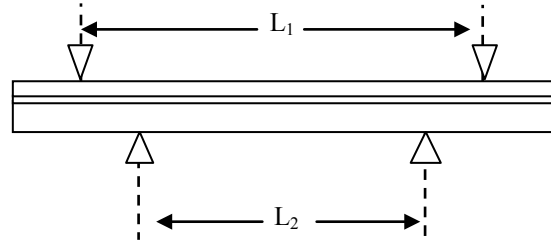


Fig.4- 4points bending

Most coatings produced by EBPVD techniques are in a compressive residual stress state after deposition. One effect of this is that when a coated beam is bent, a certain elongation in the outer fiber is necessary to overcome the coating residual strain. Up to this point, no cracks will form. Further bending will change the condition to a state of tensile stress and cracks will form sooner or later depending on the cracking resistance of the coating. The strain actually experienced by the coating, ϵ_c can thus be expressed as: [1].

$$\epsilon_c = \epsilon_s + \epsilon_{c,res} \quad \epsilon_{c,res} < 0 \tag{4}$$

Where $\epsilon_{c,res}$ is the residual coating strain. The stress in the coating is calculated using Hooke’s law [1] adjusted to the plane stress condition in the coating.

$$\sigma_{c,x} = \frac{E_c}{1-\gamma_c} \left(\epsilon_{c,res} + \frac{1-\gamma_c\gamma_s}{1+\gamma_c} \epsilon_s \right) \tag{5}$$

$$\sigma_{c,x} = \frac{E_c}{1-\gamma_c} \left(\epsilon_{c,res} + \frac{\gamma_c-\gamma_s}{1+\gamma_c} \epsilon_s \right) \tag{6}$$

Where E_c is the Young’s modulus of the coating, and γ_c and γ_s are the poisson’s ratios of the coating and the substrate, respectively. Due to difficulties in determining the elastic constants of coating materials in the form of thin films, such values have to be used with care. To facilitate interpretation, the results in the following are given primarily as coating strain rather than coating stress.

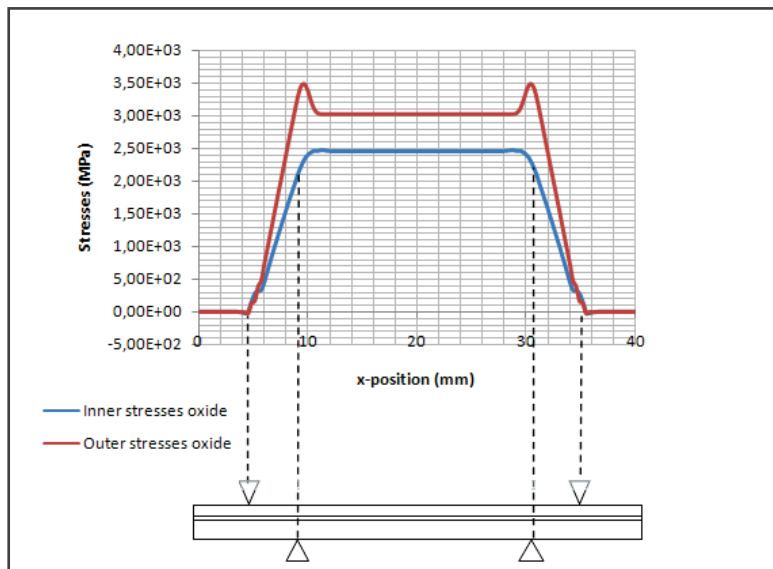


Fig.5 Stress evolution along the layers thicknesses in a four-point bending.

The simulation of the local mechanisms of damage or the initiation of the damage in a material is not piloted by average values of stresses or strains, In our case, the finite element analyses are also reveals that the central part of the

beam develops a stress, and strain, that is virtually strong and constant (see fig.5).Near each of the inner supports however, an increase in stress occurs due to the inevitable deformation of the beam sections contacting the supports. These stress peaks will affect the radius of curvature and hence the coating strain along the beam and have to be kept in mind when searching for coating cracks, as they limit the maximum length of investigation.

A finite element method analysis (FEMA) of a bent beam shows the large influence of the friction strength between the beam and the supports on the radius of curvature. Four theoretical cases have been considered representing different degrees of freedom for the beam to slide at the supports. values of experimental deflection for an identical beam are also indicated in the figure, strongly suggesting that the no-friction case is most appropriate in describing the deflection, this in turn indicates that the beam experiences the desired deformation state, in which the stress in the outer fiber is a result of pure bending instead of a combination of bending and tension.

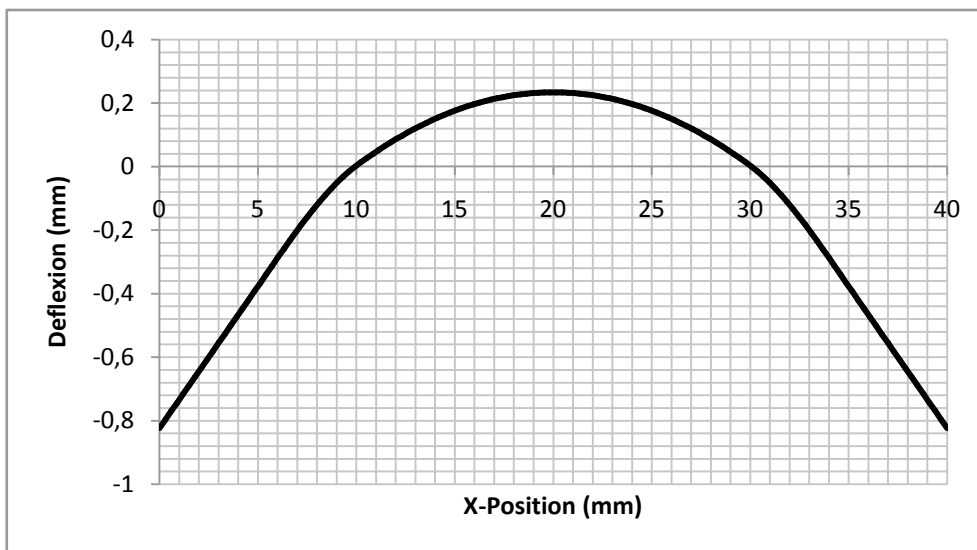


Fig.6 - Deflection in the external fiber

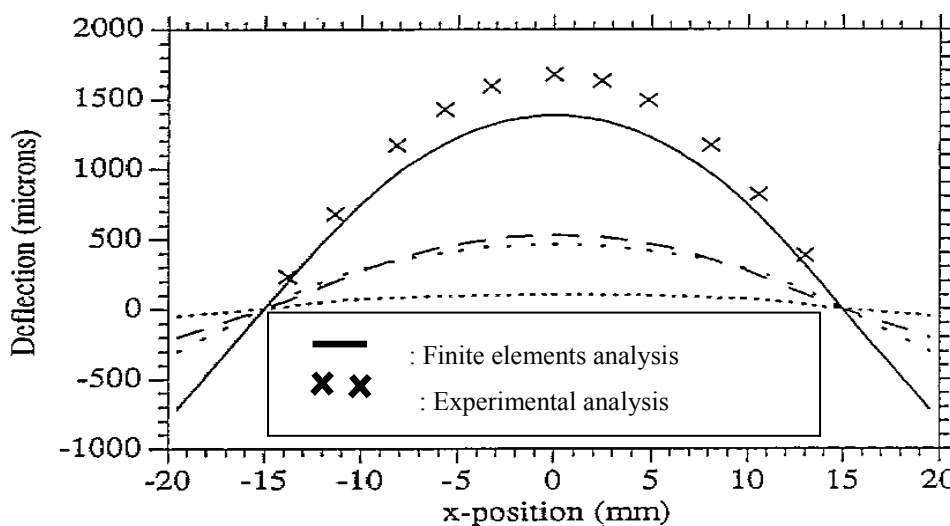


fig .7- Researches works: Urban wiklund (surface and coating technology 1997 P59)

The results obtained from the simulation show the difference in stress values between the two interfaces oxide (Al₂O₃), the external interface (between the ceramic and oxide) and the inside interface (between the oxide and basis metal (Ni)).Currently and in Figure 6 we see that the stresses in the external interface is strongly than the inside interface, it means that the thermal barrier system spallation, starts with the pull of the outer layer (ceramic).

The shape of the deflection curve which is presented here clearly shows that our finite element model is very well defined and that it complies well with the literature (see the experimental curve fig.7).

3 Samples and microstructures

From the perspective of metallographic, the proper preparation of a composite material can be a challenging, and the presence of a thermal barrier coating further complicates the work of sample preparation.

Our test sample comes from a military aircraft engine having spent undergoing an explosion in their engine (see fig.8). This is a turbine blade damaged (by breaking a few areas on the surface outside, and corrosion or creep).

In our studies, we have established some basic operations on the sample (cutting, polishing,...) to see their microstructure (thermal barrier layers, formation of oxide Al_2O_3 , ...) before they are compared with the literature.



Fig.8-Turbine blades damaged samples.

The micrograph extracted by the optical microscope is achieved with expansions of 5, 10, 20, 50, 100x motorized given in the figure below.

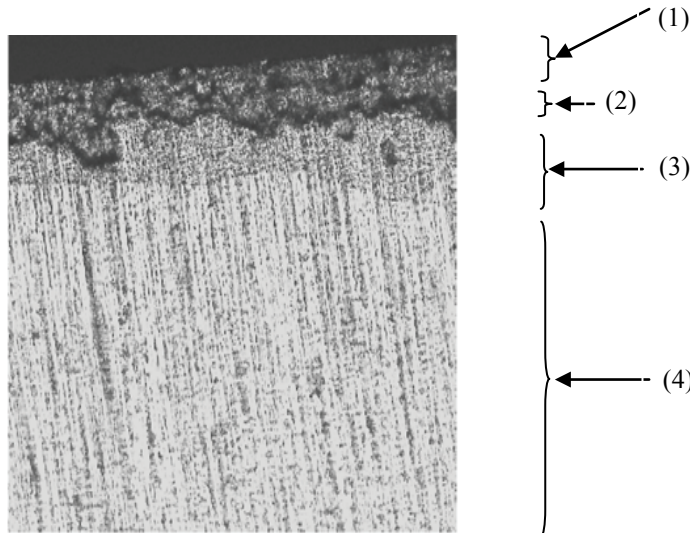


Fig 9-thermal barrier system: (1) ceramic layer, (2) oxide layer, (3) bonding layer, (4) Base metal.

4 Influence of the oxide layer on the stability of the TBC system.

The execute calculations concern our system are in isotherm conditions with more and more an ambient temperature to predict the evolution of the stresses states according to the TBC thickness and to know the influence of the oxide layer on the stability of this system.

On the fig.6, the results are extracted to the level of the central line of the specimens, we can note that the growth of the oxide layer (currently after some hours of working) change the behavior of the thermal barrier system, however, what implies that this layer, between the zircon and the bond-coat, constitute the weak link of this system.

The layer oxide serve in ones to the enhancement of the deposit ceramic adherence on the under layer (bond-coat), but also a barrier that prevents the oxygen diffuse toward the bond-coat or the substrate, in order to reduce the oxidation maximally. The alumina must be in its form α , who is dense and present a weak diffusion coefficient, serving to prevent the diffusion of oxygen from the external environment to the substrate.

We note a beginning crack in the interfaces after a few hundred hours of service that can generate a scaling of this system. This damage is essentially due to the presence of extortion stresses in the interfaces that are born by the setting in strong compression of the oxide during the phases of cooling.

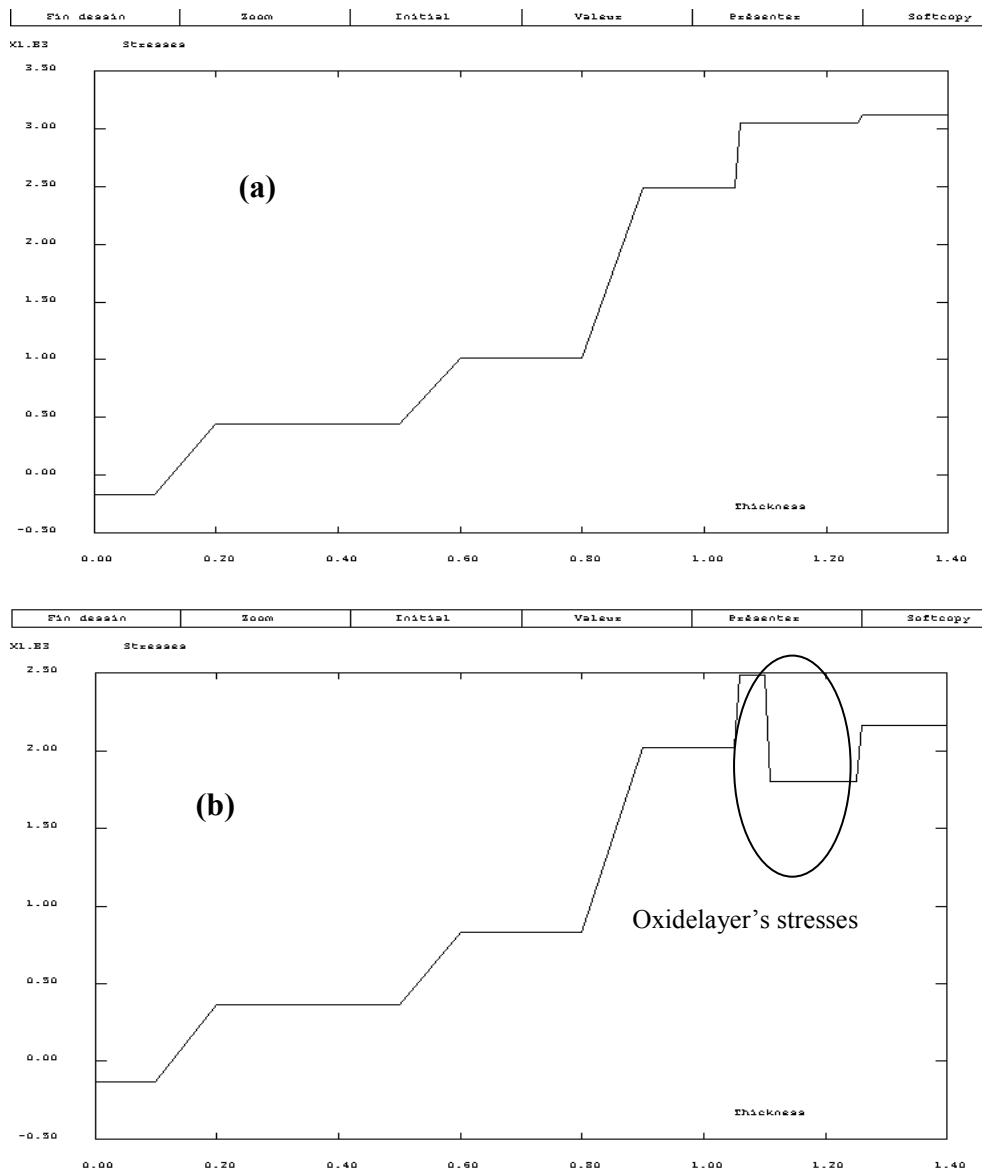


Fig 10- influence of the oxide layer on the TBC system stability by finite element method.(a): TBC system before the creation of the oxide layer, (b): TBC system after the creation of the oxide layer.

4.1 wave form of the oxide layer

If our system is simulated as in reality, (the oxide layer with a curved wave) which is shown in the fig.11, the oxide layer receives the set of all the forces on the TBC system, this implies that there are two stresses forms: a tension stresses (which make the spallation of ceramic) and compressive stresses (which continues to stabilize the system).

Table1 - Thermal barrier layers

Materials	Thicknesses μm	νE (MPa)	
Layer 01 (Ni-based superalloy)	1000 – 1500 μm	0.20	250000
layer 02 : CoCrAlY	$\approx 50 - 100$	0.30	192000
Layer 03: $\alpha\text{-Al}_2\text{O}_3$	0 – 5 μm	0.20	380000
layer 04: ceramic	100 – 200 μm	0.25	180000

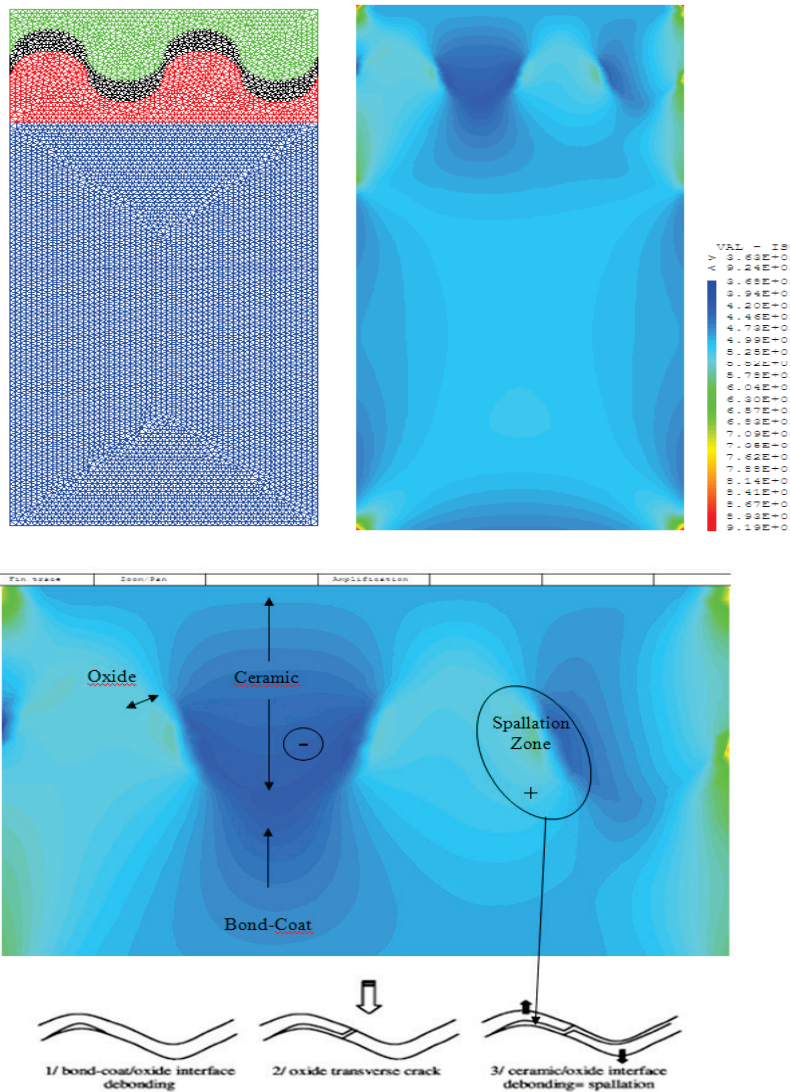


Fig.11- Finite element simulation of an adulatory system

The mesh generation done automatically with two forms of nodes, the quadratic nodes and the other is triangular, with a density of 0.02. The results show that the precision with triangular nodes is almost ideal.

The oxide layer is receiving more and more an environmental stresses form (such as temperature, oxidation...), or a mechanical stresses form (traction and compression) that develop in training of this layer, else a centrifugal forces is translated by tensile forces (see fig .11) that is experiencing the oxide layer is the lowest in the system thermal barrier.

5 Conclusion

To improve the performances of each protector system, TBCs for example, it is necessary to understand the mechanisms of damage or deterioration which take place during their use. All the layers constituting these systems, such as the ceramic, the oxide and the Nickel based super alloys, are subjected to mechanical and thermal cyclic loadings. The materials used are nickel base superalloys, because their mechanical properties enable them to resist the mechanical loadings. However, they do not enable them to resist the thermal loadings; this is why these materials are covered with an alloy system which aluminum is one of these compounds (NiPtAl). These coatings have weak kinetics of oxidation at high temperature and form a protective and adherent oxide layer, to characterize the behavior of these materials and to compare their performances.

We were interested here in the numerical simulation of the TBCs behavior based. A model can makes it possible to determine in an automatic way the stresses and strains evolution kinetics and the probability of chipping to each cycle starting from the experimental curves. By comparing the numerical and experimental results obtained on an alloy models.

Finally, the friction forces play an important role in characterizing the numerical behavior of thermal barriers systems, because the stresses are increased to the support compared to actual cases, so it must betaken into account.

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