MATERIAŁY CERAMICZNE /CERAMIC MATERIALS/, 62, 3, (2010), 275-279

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Modeling of the Residual Stresses and their Effects on the TBC System After Thermal Cycling Using Finite Element Method

M. Ranjbar-Far[1], J. Absi[1]*, G. Mariaux[2], S. Shahidi[3]

[1] GEMH, Ecole Nationale Supérieure de Céramique Industrielle, Limoges, France
[2] SPCTS, University of Limoges, Limoges, France
[3] LIUPPA, University of Pau, Pau, France
*e-mail: joseph.absi@unilim.fr

Abstract

The main goal of this work is to study the effects of the residual stresses due to the coating process on the final stress distribution within the Thermal Barrier Coatings system (TBC) after thermal cycling. The thermo-mechanical Finite Element Model (FEM) was developed to estimate the stress distribution. This model takes into account several phenomena: residual stress generation during the spraying of coatings, morphology of the top-coat/ bond-coat interface, oxidation at the bond-coat/top-coat interface, plastic deformation of the bond-coat and creep of all layers during thermal cycling. As results, we observed a critical stress after coating spraying, corresponding to a low substrate temperature and high cooling rate during spraying of the top-coat material.
Keywords: Plasma sprayed TBC, Residual stress, Zirconia, Stress distribution, FEM

MODELOWANIE METODĄ ELEMENTÓW SKOŃCZONYCH NAPRĘŻEŃ RESZTKOWYCH I ICH SKUTKÓW DLA UKŁADU TBC PO CYKLICZNEJ ZMIANIE TEMPERATURY

Głównym celem tej pracy są badania nad wpływem naprężeń resztkowych wywołanych procesem pokrywania na ostateczny rozkład naprężenia w układzie powłoki bariery cieplnej (TBC) po cyklicznym ogrzewaniu i studzeniu. Opracowano termo-mechaniczny model elementów skończonych (FEM) w celu oszacowania rozkładu naprężenia. Model ten uwzględnia szereg zjawisk: powstawanie naprężenia resztkowego podczas natryskiwania powłoki, morfologię granicy międzyfazowej pomiędzy powłoką wierzchnią i powłoką wiążącą, utlenianie na granicy międzyfazowej pomiędzy powłoką wierzchnią i powłoką wiążącą, deformację plastyczną powłoki wiążącej i pełzanie wszystkich warstw podczas cyklicznego ogrzewania i studzenia. Jako wynik zaobserwowano naprężenie krytyczne występujące po natryskaniu powłoki, korespondujące z niską temperaturą podłoża i dużą szybkością studzenia podczas natryskiwania wierzchniej powłoki materiału. .
Słowa kluczowe: powłoka bariery cieplnej natryskiwana plazmowo, naprężenie resztkowe, ZrO_2, rozkład naprężeń, metoda elementów skończonych

1. Introduction

Air plasma sprayed (APS) Thermal Barrier Coatings (TBC) protection is widely used to prolong the lifetime of turbine components. Due to the low thermal conductivity of the top-coat layer, the substrate temperature by some hundred degrees can decrease (Fig. 1). The functionality and reliability of plasma spray coatings are strongly related to microstructure, porosity [1] and residual stresses of thin films and coatings [2, 3]. Amongst these parameters, the effect of residual stress is of interest in this study. Residual stresses in the plasma sprayed TBC are generated through four events [4]:

– residual blasting stresses;
– stresses associated with changes in volume at a solid state phase transformation in a typical top-coat;
– stresses originated from rapid contraction of sprayed splats from the deposition temperature to the underlying materials named “quenching stresses”;
– stresses originated from differences in thermal expansion coefficients of the underlying materials and coatings.

The overall magnitude of residual stress in TBC is the summation of quenching stress and thermal stress whereas the contribution of stress due to phase transformation is negligible [3].

The compressive thermal residual stresses can prompt the crack initiation parallel to the interface [5] and cause spalling inside the coatings [6]. These micro-cracks can propagate along the interface and within the ceramic layer during thermal cycling.

It should be noted that the damages in TBCs after several thermal cycles are related to the residual stresses issued from the coatings process, thermal mismatch of the material constituents, oxidation of the bond-coat (BC), complex shape of the ceramic/metal interface, and sintering of the ceramic and redistribution of stresses via creep, plastic deformation and crack resistance.

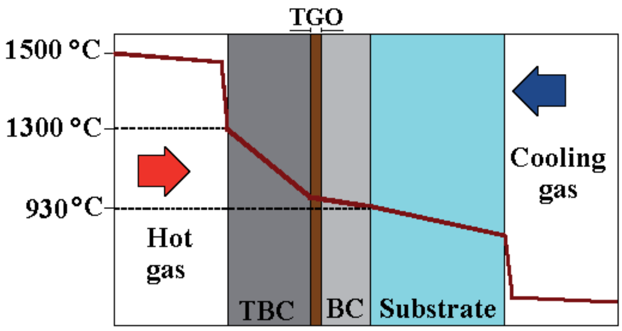

Fig. 1. Qualitative temperature distribution across the TBC system.

The objective of this paper is to describe the development of residual stresses during spraying of zirconia-based thermal barrier coatings and their effects on the crack formation in the top-coat and final stress distribution in the system after having been in service. The calculation of these stresses as a function of the different preheating underlying materials and different cooling rates at the first step of elaboration of the TBCs has been taken into account. A numerical model has been proposed to study the thermo-mechanical behavior using the finite element code ABAQUS.

2. Finite element model

2.1. TBCs composition

The TBC system is composed of an Inconel 617 substrate, a NiCoCrAlY bond-coat and an APS Yttria Partially Stabilized Zirconia top-coat. The thickness of each layer is considered to be 1.6 mm, 0.1 mm, and 0.25 mm, respectively. A Thermally Grown Oxide (TGO) layer of 1 μm in thickness is considered between the top-coat and the bond-coat.

Due to the manufacturing process (blasting step) the TBC/BC interface is very rough. Through the irregular ceramic/metal interface, the asperity can be convex or concave with a different amplitude and wavelength (Fig. 2) [7]. Reproducing a real interface shape in the model would considerably increase the effort required to generate a suitable mesh and the size of the calculation domain needed to represent different rugosity shapes. Consequently, long calculation times would be requested. For these reasons, the geometries associated to the numerical simulations were ideally considered as a perfect sinusoidal or semicircular shape. Consequently, the TBC/BC rough interface is modelled by a sinusoidal wavy interface with a wavelength, λ, of 60 μm and an amplitude equal to 15 μm. These values are commonly obtained through observations of coating micrographs (Fig. 2) and usually used in literature [8, 9].

Due to its symmetry, the calculation domain is reduced to a half period, $\lambda/2$. The symmetrical boundary condition is imposed on the left side and the periodicity boundary condition is imposed on the right side of the model by Multi-Point Constraint (MPC) (see Fig. 3).

For this representative region, a 2D mesh is generated with generalized plane strain elements. To improve the result accuracy, the interface layer has been discretized with a small element size in the order of 0.25 μm.

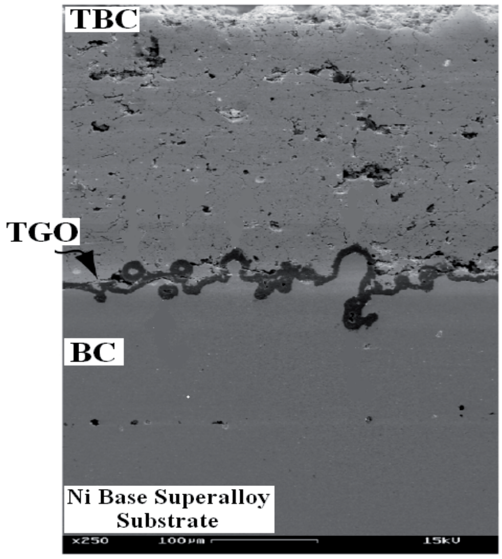

Fig. 2. Micrograph of plasma sprayed thermal barrier coating system [7].

2.2. Materials behavior and properties

In this model, the thermally grown oxide, ceramic and substrate layer are treated as elastic and viscous materials whereas the BC is an elastic and visco-plastic material. The material properties are temperature dependent [3, 9]. Rösler *et al.* [10] described the creep behavior for all layers.

The growth of the alumina layer at high temperature is modelled by anisotropic swelling of the elements in the TGO layer. This phenomenon was described in literature [10]. We have considered the normal growth as well as the lateral TGO growth in the system.

2.3. Thermal loading

To calculate the stresses generated during spraying, the top-coat layer was set to the material melting temperature of 2680°C [11]. This layer was tied to the underlying materials (substrate +BC +TGO) with different initial temperatures 25, 400 or 627°C that we call “substrate pre-heating” in the first step of elaboration of the TBCs (Step-1 in the Fig. 4). To study the effect of different cooling rates on the residual stress distribution within coating, the convection coefficients, *h*, to the environment were taken to be 10 W/m^{2}K, 25 W/m^{2}K or 100 W/m^{2}K, respectively. The convection to the surrounding environment was used as a thermal boundary condition in step-1 (Fig. 3).

The thermal loading affecting the top-coat surface is presented in Fig. 4. It consists of two steps. Step-1 is cooling from coating deposition temperature 2680°C to ambient temperature 25°C during 12000 seconds. After that, Step-2 has three stages during service: the heating stage from 25°C to 1300°C in 300 s, followed by a dwell-time of 100 hours at 1300°C and finally, a cooling stage from 1300°C to 25°C in 300 s.

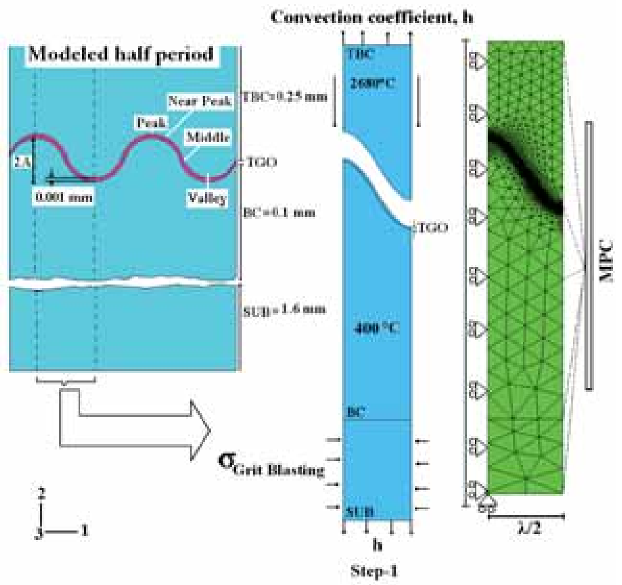

Fig. 3. TBC system model, finite element mesh and boundary conditions.

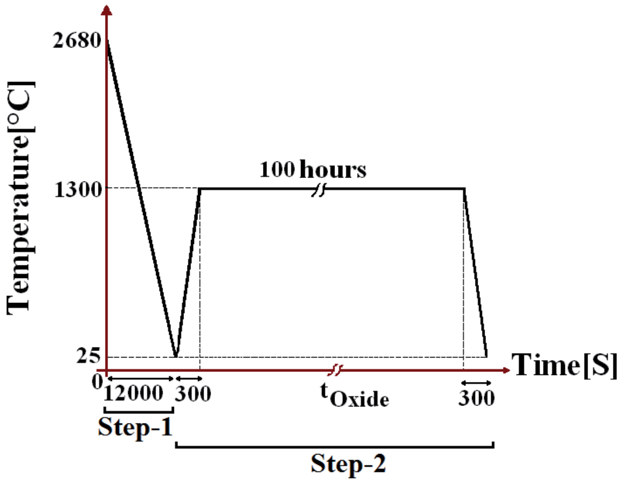

Fig. 4. Thermal cycle used in FEM simulation.

3. Results

The coating qualities are influenced by a number of factors such as the cooling rates and substrate preheating process. We will focus on the contribution of the residual stresses formed during cooling from deposition temperature to room temperature on the stress state in TBCs. These results quantities are used as the initial conditions to calculate the stress distribution in the top-coat at the end of the thermal loading cycle.

3.1. Formation of the residual stresses in a plasma sprayed

During spraying, the thermal model predicts a rapid decrease in temperature of the deposited material, from melting temperature (2680°C) to the temperature of the underlying materials (25, 400 or 627°C). By heat conduction, all layers reach a steady-state temperature leading to the quenching stress. Simultaneously but with a higher time constant, the thermal transfer of the whole system proceeds by convection with the environment leading to a decrease of the TBCs temperature until 25°C, which creates a thermal stress.

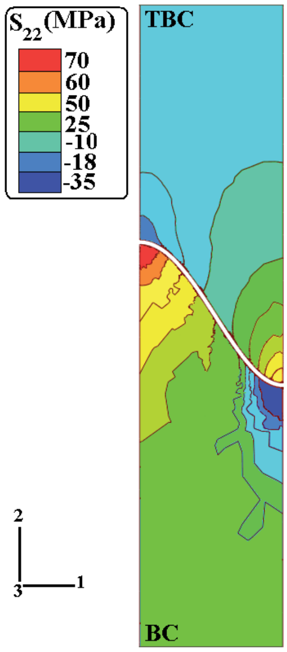

Fig. 5. S_{22} residual stress generated during spraying process after 400°C substrate pre-heating and 25 W/m²K convection rate.

The quenching stresses cause the substrate to expand and the deposit to shrink, which produces tensile stress in the coating layer.

During cooling to room temperature, the difference in thermal expansion coefficient between the deposit and the substrate causes the compressive stresses, which were superimposed on the top coating quenching stresses. It can be found that the final generated stresses in the top-coat after spraying are compressive (~ -18 MPa), except a limited tensile zone (~ 50 MPa) at the valley region (see Fig. 5). This is due to larger thermal stresses with respect to the quenching stresses in the TBC.

In the bond-coat, the residual stresses are found to be tensile (70 MPa) except a small zone at the valley region.

The types and magnitudes of our predicted stresses in the top-coat layer are in accord with the experimental data reported by Bengtsson and Persson [2], Widjaja *et al.* [3] and Matejicek and Sampath [12], which have been measured in the interval values limited by -14 MPa and -92 MPa. In view of these results, our numerical approach is justified despite its phenomenological aspect and lack of fundamental theory.

3.2. Effect of substrate pre-heating

The effect of the initial temperature of underlying materials (25, 400 or 627°C) prior to deposition process on the residual stress distribution with a constant cooling rate in order of 25 W/m²K is summarized in Fig. 6. The stress repartition along the TBC/TGO interface in the horizontal position (from peak x = 0 to valley x = 30 μm) is presented. As expected, the pre-heating temperature of the substrate at 400 or 627°C significantly reduced the maximum value of the stresses generated during the spraying process in comparison to 25°C.

Briefly, it can be stated that higher values of stresses are found when using the lower underlying temperatures during spraying of the top-coat material.

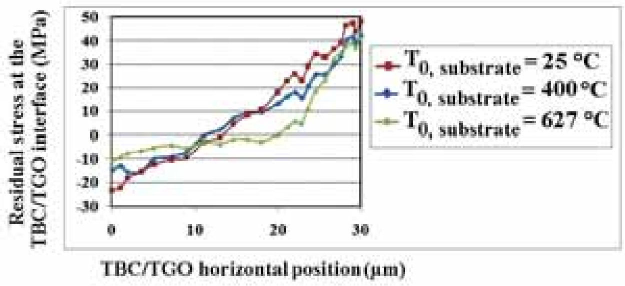

Fig. 6. Effect of substrate pre-heating on the residual stress generated after spraying process in the TBC/TGO horizontal position.

3.3. Effect of cooling rate

To understand the influence of the cooling rate on our system, we consider different convection coefficient values (10 W/m^{2}K, 25 W/m^{2}K, and 100 W/m^{2}K) with a constant substrate pre-heating temperature of 400°C. Fig. 7 shows the effect of different cooling rates. The residual stress S_{22} distribution at the TBC/TGO interface in the horizontal position shows that the residual stresses are slightly higher for high convection. As more heat is dissipated toward the environment for the higher convection coefficient, it results in less heat being transferred by thermal conduction toward the underlying levels. Thus, the following layers would be colder. As sprayed coatings loose their heat rapidly, it leads to high quenching stresses and their effect would dominate the overall magnitude of residual stresses.

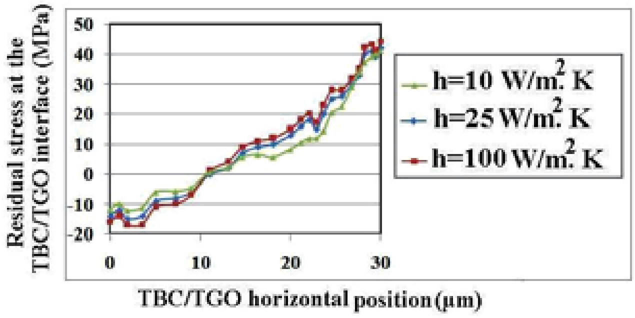

Fig. 7. Effect of cooling rates on the residual stress generated after spraying in the TBC/TGO horizontal position.

3.4. Estimation of the crack propagation path

Zhang *et al.* [13] have shown that the tensile quenching stress is responsible for cracks in the individual splats normal to the interface. However, residual compressive stress can make a buckling of the coating and can prompt the crack initiation parallel to the interface and eventual spallation of it. Teixeira [14] summarized the nucleation of these different damages.

The coating failure modes by cracking and spalling are both dependent on the sign/magnitude of residual stress with respect to the relative yield strengths of coating. It is postulated that the interface strength is close to that of the material having the lowest mechanical resistance, that is to say, the ceramic at the TBC/TGO interface and bond-coat for TGO/BC interface. The yield strength of ceramic varies from 10 MPa to 100 MPa [15, 16] and for the bond-coat layer is about 270 MPa [3]. Considering the yield strengths of the top-coat, Fig. 5 predicts that a micro-crack probably can be formed near the peak of the TBC/TGO interface due to coating buckling. Additionally, the horizontal micro-cracks between the lamellar may appear. Under tensile stresses in the valley asperity, the vertical micro-cracks inside the lamellar may be developed. These micro-cracks can propagate along the interface and within the ceramic layer during thermal cycling.

On the bond coat, the level of the residual stress is lower than the yield strength value. Thus, the analysis of the effect of the coating process on the integrity of the bond-coat is omitted.

For the sake of good agreement between the experimental data and the results of the FEM analysis, let us consider the coating residual stress value as an initial condition of the numerical simulation at the beginning of the step-2 called thermal cycle.

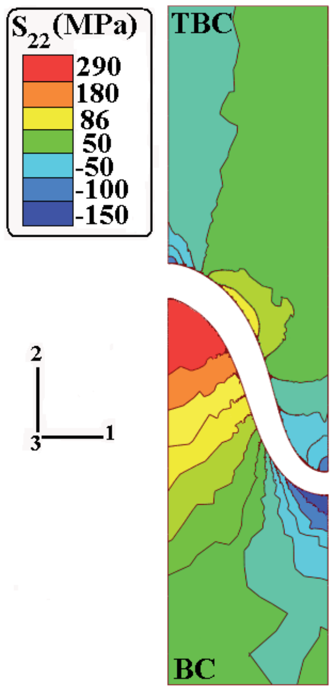

Fig. 8. S_{22} stress distribution at the TBC and BC layers, after cooling.

3.5. Stress distribution on the system after thermal loading cycles

In this study, the stress distribution is also calculated while the coating is in service. As viewed in the previous sections, we know that residual stresses can increase the failure probability. The stress state depends crucially on the ratio of the loading rate caused by growth and swelling of the oxide layer, the thermal mismatch between all layers and the unloading rate by creep and plastic relaxation during thermal cycle loading.

The numerical results show that after 100 h at high temperature and after cooling, the compressive stresses zone increases in the "peak" of the TBC layer and goes from –18 MPa (Fig. 5) to –120 MPa (Fig. 8). At the same time, the tensile zone existing initially, after spraying process, in the “valley” region moves to the “middle” region and reaches a value of 86 MPa. Finally, in the valley asperity, the stress distribution becomes a compressive state with a level of -100 MPa.

Concerning the bond-coat layer (see Fig. 8), an important zone of tensile stresses takes place at the peak (295 MPa) and a zone of compressive stresses at the valley asperity (−150 MPa). These important values, larger than yielding thresholds, make us not omit their effects on the damage state at the end of the Step-2.

4. Conclusions

Among the many factors affecting the durability and failure mechanisms of thermal spray coatings in service, the residual stresses play an especially important role. A numerical study using finite element analysis (FEA) was used to study the build up of stresses during coating solidification, and to understand the effect of deposition conditions on crack formation during plasma spraying deposition and to evaluate the stresses induced during thermal cycling in typical plasma sprayed TBCs.

Numerical results showed that after coating spraying, there is a concentration of residual stresses at the ceramic/metal interface, which can be slightly reduced by adopting a low cooling rate of the deposit (10 W/m^2K) and greatly reduced by substrate preheating (627°C). These stresses can induce micro-cracks at the interface that can propagate in the system after several thermal cycles.

After service, at the top-coat layer, we observed an increasing of compressive level of initially zones (after deposition) and an emergence of new zones in a compressive state in the valley. Another phenomena is observed concerning the migration of initial area in tensile state towards the middle of the sinusoidal asperity with an increasing of their values. These changes favorite the degradation of the top-coat and lead, finally, to the delamination of the ceramic layer.

Acknowledgement

Maryam Ranjbar-Far would like to express her gratitude towards the Limousin Region and the European Social Fund for the financial support to the present work.

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Received 13 April 2010; accepted 5 May 2010