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Stability of plasma-sprayed thermal barrier coatings: The role of the waviness of the bond coat and the thickness of the thermally grown oxide layer

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ABSTRACT

In this paper, the effect of the waviness of the bond coat and the thickness of the thermally grown oxide (TGO) layer on the stability of plasma-sprayed thermal barrier coatings is investigated. Large numbers of three-dimensional finite element calculations were performed using a plasma-sprayed *M*CrAlY + YSZ thermal barrier coating as a modeled system and a cosine surface to represent an irregular top-coat/bond-coat interface. Thermal cooling stresses in critical locations (the top coat and the interfaces between the top coat, the TGO, and the bond coat) were evaluated assuming a stress-free initial state and elastic (the substrate, the thermally grown oxide and the top coat) and elastic–ideal plastic (the bond coat) material behavior. The results of this investigation, which have been discussed by taking into account interfacial geometries typical of manufactured coatings, indicate that the waviness could markedly affect the service lifetime and thus should be considered in both theoretical studies and further experimental endeavors.

1. Introduction

Plasma-sprayed thermal barrier coatings (TBCs) are multilayer protection systems used in the power generation and aircraft industries for enhancing operational life of hot-section components [1–6]. TBCs typically consist of an aluminum-rich metallic bond coat (BC) providing protection against hot-corrosion and oxidation and an outer ceramic (usually yttria-stabilized zirconia — YSZ) top coat (TC) providing thermal insulation. As the ceramic layer is permeable to oxygen, an inner oxide layer, the so-called thermally grown oxide (TGO), gradually evolves at the top-coat/bond-coat interface during exposure to high temperatures. One of the key problems related to TBCs is that it is still difficult to understand the full extent of their frequent in-service spallation and thus it is difficult to make sufficiently reliable predictions of expected lifetime of TBCs-protected components even under typical operating conditions. The problem is apparently present because of a large variety of currently used TBCs, all with different compositional, microstructural and geometrical features, and because of a large number of mutually interrelated degradation processes that may be involved in the failure of the coating conforming to applied thermal and mechanical loadings. Such highly system- and application-specific failure renders the comparison of both experimental and numerical results rather difficult and somewhat vague.

Excluding any impact damage and extensive erosion and corrosion conditions, delamination cracks frequently proceed within the top coat in the vicinity of TC/BC interface, starting as subcritical cracks that coalesce with each other, utilizing the pre-existing microstructural defects such as pores or de-bonded splat boundaries as easy-growth crack paths. This type of failure is typical of conventional plasma-sprayed coatings thermally cycled with a short dwell at high temperatures [7,8] but it was reported also for thick dense vertically-cracked coatings [9] or coatings subjected to thermo-mechanical fatigue [10]. In other cases, conditions at the interface are formative and the damage evolves predominantly within the TGO and/or along its either interface. This failure mode seems to be more common when coatings are subjected to prolonged periods at high temperature [7,11–13], but was reported also for thermal cycling at relatively high temperatures with edge-initiated delamination [14]. The formation of damage is generally related to stresses induced by different thermal expansion and contraction of individual layers and to intrinsic volumetric stresses associated with oxidation of the bond coat (TGO growth). These are counteracted by stress relaxation via high-temperature creep and via microcracking and sintering within the top coat, which concurrently leads to changes in its strain tolerance and its thermal resistivity [15–17].

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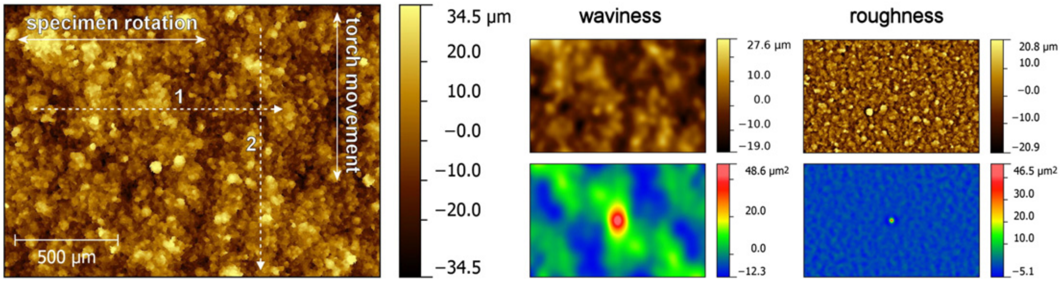

Fig. 1. Air plasma-sprayed CoNiCrAlY bond coat: surface data obtained after subtracting the circular form, its decomposition into the waviness and roughness components by using Gaussian filtering with an arbitrary chosen cut-off wavelength of 125 μm, and their respective autocorrelation functions. The highlighted profiles are shown in Fig. 12.

One of the key features influencing the failure mode and the lifetime of TBCs is the roughness of the bond coat [8,12,18–21]. The interfacial geometry affects the initial microstructure of the top coat, especially the geometry of splat boundaries near the interface, dictates expansion of the TGO and governs the nature and evolution of residual stresses induced in the system during cooling down to low temperatures. The experiments have shown that the modification of interfacial roughness could be beneficial to coating lifetime [8,18,19]. It is agreed on that a certain level of bond coat roughness is needed, as the top coat bonding is provided primarily via mechanical interlocking, and that very rough coatings would fail prematurely because of an extensive TGO growth. In engineering and surface sciences, it is convenient to consider 'roughness' to be composed of three parts: (i) the form — an overall shape, (ii) the waviness — low-spatial frequencies, and (iii) the roughness — high-spatial frequencies [22]. These are generally of different origins and affect surface behavior in different ways. In plasma spraying, the roughness component should be related to the size of individual splats or small splat clusters and thus is affected by properties of powder feedstock and by parameters that control the distribution of temperatures and velocities of particles in the plasma jet and solidification of liquid droplets. The waviness component, on the other hand, stems from spraying parameters, such as the surface speed, torch traverse speed or the number of gun passes, and consequently would exhibit some periodicity. Rationality of this assertion is demonstrated in Fig. 1 that shows the surface data of the CoNiCrAlY bond-coat obtained after subtracting the circular form, and its decomposition into the waviness and roughness components. The respective autocorrelation functions (ACF) are also shown, bearing evidence of isotropic surface roughness and anisotropic surface waviness.

The TC/BC interface, when studied numerically, is typically modeled as a periodic sinusoidal profile/surface with wavelengths and amplitudes in the range of about 5–20 μm and 20–80 μm, respectively [19]. Derived life-time prediction models correspondingly adopt a macroscopically flat interface modulated with roughness ripples, or if necessary a curved one to include the form. As much as the early formation of the damage is undoubtedly controlled by the local features, the omission of the waviness from calculations still causes some discrepancy in predicting actual stresses within the coating. This becomes even more important in the next stage, when propagation and linking of delamination cracks at interface or in YSZ (across undulations and parallel to the interface) are addressed and it can cause difficulties in comparing calculations with experiments on coatings with an inconsiderable waviness. The intention of this paper is to assess the cooling stresses in a typical plasma-sprayed TBC coating as affected by the waviness of the bond coat (wavelengths in the range of 125 to 500 μm) and by the thickness of the TGO, and to make suggestions for further scientific undertakings aiming to achieve improvements of service lifetime and its prediction. The findings of this study are particularly relevant for thermally cycled plasma-sprayed coatings in which the propagation of cracks within the ceramic layer is expected to dominate the total lifetime.

Table 1
Geometrical parameters.

t_s [mm]	t_b [mm]	t_t [mm]	t_{TGO} [μm]	λ [μm]	A [μm]
25	0.2	0.2	$0 \div 9$ $\Delta t_{TGO} = 3$	$125 \div 500$ $\Delta\lambda = 62.5$	$10 \div 30$ $\Delta A = 10$

2. The numerical model

Finite element (FE) calculations were carried out on a nickel-base superalloy substrate with a thermal barrier coating consisting of (i) a *M*CrAlY bond coat, (ii) a single α-alumina TGO layer and (iii) an YSZ top coat. The system has been modeled as an infinite plate with geometry of the TC/BC interface generated by the following function:

$$z = A \cdot \cos\left(\frac{2\pi}{\lambda}x\right) \cdot \cos\left(\frac{2\pi}{\lambda}y\right), \tag{1}$$

where A is the amplitude and λ is the wavelength. These parameters were varied in the range of 10–30 μm and 125–500 μm, respectively, corresponding to waviness of manufactured plasma-sprayed coatings, such as, for example, the one shown in Fig. 1, or those presented in micrographs in references [8,12,19,23]. Based on preliminary calculations, the thickness of the substrate, t_S, was set to 25 mm so as to exclude its influence on the stress distribution in the coating. The thicknesses of the bond coat and the top coat were set equally to $t_b = t_t = 200$ μm. The thickness of the TGO, t_{TGO}, was varied in the range of 0–9 μm, Table 1. Note that in the as-deposited state, the thickness of the TGO is in fact already on the order of tenths of micron as a result of partial oxidation during deposition [17]. All materials were modeled by using 3D structural elements with quadratic base functions and full integration; multi-point constraint (MPC) algorithm was used to define the coupling between individual layers. The discretization was the same in all studied cases as the model is being developed to be ultimately utilized for mapping the stresses to local roughness descriptors of the real bond-coat surfaces. Boundary conditions were chosen based on symmetry and periodicity that allowed for the reduction of the model to one quarter part, Fig. 2.

The substrate, the TGO and the top coat were treated as isotropic homogeneous materials with ideally elastic behavior. The material data used in calculations corresponded to Inconel 713LC nickel-base superalloy (substrate), α-alumina (the TGO layer) and the porous plasma-sprayed YSZ (the top coat), and were obtained from references [25,26]. The bond coat was modeled as an elastic-ideally plastic isotropic homogeneous material with properties taken from the reference [26] and the in-house database. All material properties are summarized in Table 2; temperature-dependent data were fitted to piecewise linear functions when used in FE calculations.

The thermal loading consisted of a single isothermal cooling step starting at temperature of 1020 °C at which a stress-free state was assumed in all materials. The system was isothermally cooled down to the room temperature and the stresses at critical locations (YSZ and interfaces between YSZ, TGO, and BC) were studied. Thermal cycling