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Finite element simulation of stresses in a plasma-sprayed thermal barrier coating with an irregular top-coat/bond-coat interface

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ABSTRACT

A three-dimensional finite element model of a conventional plasma-sprayed thermal barrier coating was set up with an irregular top-coat/bond-coat interface that was modelled based on the waviness data of a plasma-sprayed coating surface. The residual stresses upon cooling from a high-temperature stress-free state down to a room-temperature stressed state were studied as a function of thickness of the thermally grown oxide (TGO) layer taking into account the plasticity of the bond coat. The calculations indicate that the delamination cracks at the TGO/bond-coat are more likely to appear with progressive oxidation, and, conversely, the initiation of cracks in the top coat at the interfacial peaks in an intact thermal barrier coating is less probable because the tensile stresses in the top coat initially decrease and the tensile regions gradually become smaller and localized due to the observed stress conversion. Based on the obtained results and experimental evidence from the literature, a role of the interfacial topography in the failure sequence is discussed for oxidized and thermally-cycled coatings.

1. Introduction

Thermal barrier coatings (TBCs) have been used to enhance performance of hot-section components in gas turbines since the early 1980s when their benefits were recognized and successfully tested [1,2]. From a material point of view, the vast majority of current commercially-used TBC systems still consist of the following two applied layers: (i) an aluminide diffusion or *M*CrAlY (where *M* stands either for Co, Ni, or a combination of both) thermally-sprayed bond coat, and (ii) a thermally-sprayed/EB-PVD-deposited (EB-PVD – Electron-Beam Physical Vapour Deposition) yttria stabilized zirconia (YSZ) ceramic top coat, which adheres to the bond coat and serves as a thermal insulator. The ultimate failure mode of the TBCs is buckling or spallation of the YSZ top coat that results from progressive formation of a thin layer of high-temperature oxides and other compounds at the interface (the TGO layer) and accumulation of damage in its vicinity [3,4]. The post-spray thermal treatment of the bond coat aiming to prolong an intermediate oxidation stage dominated by a slowly growing α-Al_2O_3 continuous scale is one of the possibilities to enhance TBCs' lifetime [5]. In plasma-sprayed coatings, spallation is due to propagation and coalescence of YSZ cracks nucleated at microstructural imperfections near the interface, and/or delamination cracks at the interface, being influenced by the relative importance of the misfit stresses experienced upon cooling, volumetric stresses related to high-temperature oxidation and counteracting stress-relaxation processes such as high-temperature creep (especially in the TGO layer) or sintering of the YSZ top coat [4,6].

One of the key features significantly influencing damage development is the initial topography of the bond coat, which in a broad sense includes all geometrical features from the upper large-scale shape down to the small-scale stress-relieving intra-splat microcracks formed when splats (individual molten droplets that have impacted a coated surface) solidify. On this splat/sub-splat microscale, small interfacial irregularities (i.e. roughness) affect local oxidation of the bond coat and also dictate the microstructure of the YSZ top coat near the interface as it is formed during the spraying, most importantly the shape of splats and inter-splat interfaces [7]. On the macroscale, the overall shape of the component controls the macrostresses in the coating and it also influences coating macrostructure, particularly the geometry of individual sprayed layers and appearance of large vertical segmentation macrocracks that increase the strain tolerance of the top coat [7–9]. Nowadays, it is agreed on that the high 'roughness' (regarded still more or less as a vertical surface extent expressed, for instance, in terms of the arithmetic average roughness R_a) is beneficial because the YSZ bonding is primarily mechanical. Based on this premise, the variation of the bond coat surface is being actively studied. For example, Dong et al. [9] used dry-ice blasting, Vaßen et al. [10] and Eriksson et al. [11] used feedstock powders with different size-distribution of

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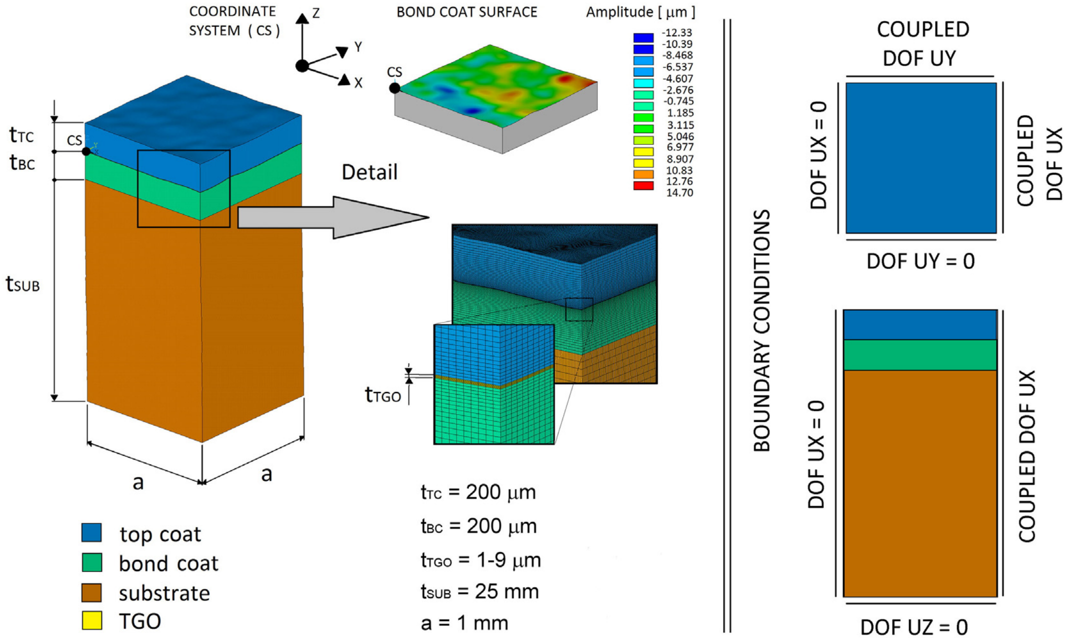

Fig. 1. Finite element model (not in scale).

particles, and Nowak et al. [12] varied spraying parameters of a thin *M*CrAlY plasma-sprayed flash-coat demonstrating that the manipulation of the bond coat makes it feasible to control the durability of the coatings.

Given the complexity of TBCs and their operational regimes, numerical methods have become important tools for design and in-service life estimation. Present models, e.g. [13–21], allow the inclusion of many aspects of the degradation process, such as the creep deformation of individual constituents, the actual growth of the TGO layer, or sintering of the YSZ top coat, but they are usually restricted to two-dimensional problems and the continuum representation of the top coat as the realistic modelling of any intricate irregular topography or multiple material microstructural defects can impose enormous computational costs. Roughness of the YSZ/bond-coat interface in such studies is thus mostly modelled by an elementary two-dimensional functions, e.g. sine or semi-ellipse. The recent numerical calculations that incorporated geometrically realistic YSZ/bond-coat interfaces [22–24], nevertheless, have shown that the relevant bond coat topography is 3D in nature and although, for example, a conversion of stresses in the YSZ top coat (i.e. progressive conversion of residual cooling stresses, from tensile to compressive near the interfacial peaks and vice-versa near the valleys [10]) occurs, the surface is still too complex to be reduced to a simple two-dimensional approximation. At the same time, the irregular 3D interface significantly increases the computational demands and so the models were either fully elastic [22,23] or involved a regular periodic interface as in our previous paper [24]. The objective of this work was to evaluate, for the first time, the residual cooling stresses in the full TBC system with the low-spatial frequency (waviness) data of a real plasma-sprayed coating, which were obtained via the optical profilometry, employed to model the geometry of the top-coat/bond-coat interface. Unlike the previous similar studies, the evolution of the stress state of the YSZ layer (a stress-conversion pattern) was calculated by taking the plasticity of the bond coat into account. Based on the calculation results, the role of the bond coat topography in the failure process was discussed and compared with available experimental observations.

2. Methodology

2.1. Numerical model

The three-dimensional finite element model was composed of a thick infinite-plate substrate and a thermal barrier coating consisting of (i) a *M*CrAlY bond coat, (ii) a single TGO layer, and (iii) an YSZ top coat, Fig. 1. The thickness of the substrate was 25 mm. The thickness of the bond coat and the YSZ was 200 μm. The thickness of the TGO layer was 3, 6, and 9 μm. All materials were modelled using 3D

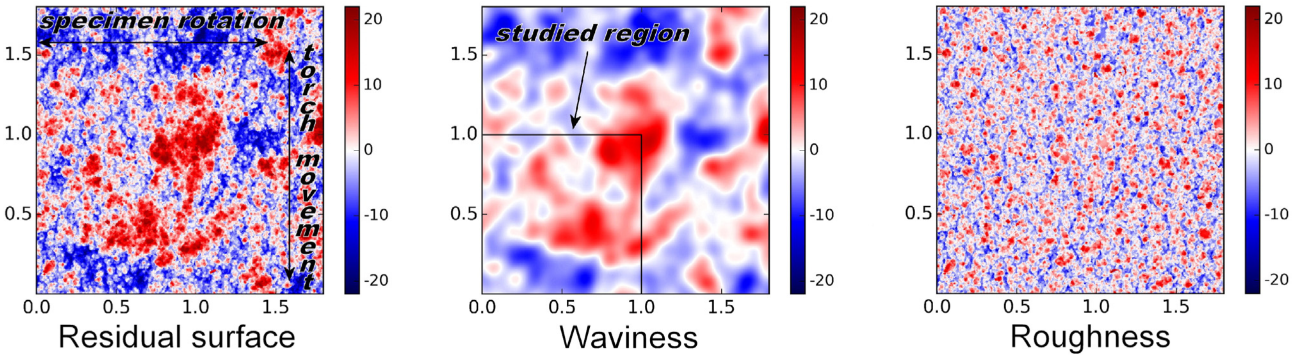

Fig. 2. The residual surface of the as-sprayed YSZ and its decomposition into the waviness and roughness components (Gaussian filtering with cut-off wavelength $\lambda_c = 200\,\mu\mathrm{m}$). The size of the shown area is 1.8 × 1.8 mm. The colour bar encodes the height coordinate measured in microns. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)