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Effects of three-dimensional coating interfaces on thermo-mechanical stresses within plasma spray thermal barrier coatings

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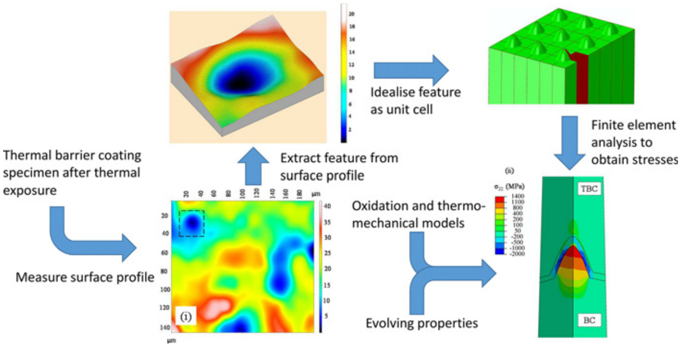
HIGHLIGHTS

- We show that 3D models predict stresses in TBCs around twice those from 2D models.
- We show probable spallation sites caused by out-of-plane tensile stress.
- We predict buckling and decohesion of the oxide layer due to in-plane compressive stress.

GRAPHICAL ABSTRACT



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ABSTRACT

It has been acknowledged that stresses within a thermal barrier coating (TBC) and its durability are significantly affected by the coating interfaces. This paper presents a finite element approach for stress analysis of the plasma sprayed TBC system, using three-dimensional (3D) coating interfaces. 3D co-ordinates of the coating surfaces were measured through 3D reconstruction of scanning electron microscope (SEM) images. These co-ordinates were post processed to reconstruct finite element models for use in stress analyses. A surface profile unit cell approach with appropriate boundary conditions was applied to reduce the problem size and hence computation time. It has been shown that for an identical aspect ratio of the coating interface, interfacial out-of-plane stresses for 3D models are around twice the values predicted using 2D models. Based on predicted stress development within the systems, possible crack development and failure mechanisms of the TBC systems can be predicted.

1. Introduction

Thermal barrier coating (TBC) systems are applied onto various superalloy and metal components e.g. gas turbine blades of an aircraft, diesel engine combustion chambers etc. One of the key functions of a TBC is to create a reduction in the substrate temperature by slowing the rate of thermal conduction of heat from a combustion reaction to the (cooled) substrate. This allows an increase in the combustion temperature which can lead to an increased efficiency. A TBC system typically consists of two applied layers: a metallic bond coat (BC), and a ceramic top-coat (TC). The TC is the outermost layer of the system and provides temperature reduction due to its low thermal conductivity, while the BC provides a structural link with the substrate. Coatings are applied using different methods and here only an air plasma sprayed (APS) system is considered. The method is more commonly used for

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components of land-based gas turbine engines. For this system, the surface roughness of the BC provides a mechanical bond to the TC and also influences its lifetime [1]. The BC is a mixture of β (NiAl), γ′ (Ni_3Al) and γ (Ni) phases in various proportions. At high temperature, the composition of the BC evolves either due to formation of a thermally grown oxide (TGO) at the TC/BC interface from oxygen diffusion [2] or due to interdiffusion at the substrate/BC interface [3,4]. This variation in the BC compositions with service time can affect its mechanical properties significantly [5,6].

Although the rough surface of the BC provides a mechanical bond to the TC, it can also cause out-of-plane stresses within the system as it undergoes thermal cycling. Early efforts to relate BC surface roughness and thermo-mechanical stresses within APS TBC systems have been carried out numerically in Refs. [7–9] where predictions were made using idealised 2D interfaces, based on micrographs of cross-sections of coating layers. Possible reasons for these simple approaches are: inadequate computational power to run FE simulations of actual coating interface and, the difficulty involved with the characterisation of interface profiles from standalone coatings. Idealised interfaces not only fail to give an accurate representation of the actual geometry, but are, therefore, also likely to result in simulated TBC stresses which are insufficiently accurate for predictions of failure of the TBCs. Therefore, it is desirable to construct an FE unit cell to represent the actual surface geometry and hence to predict stress distributions within the TBC system accurately. A recent review [10] explores more generally the use of FE models for predicting TBC thermal behaviour and failure including the use of 3D models.

Nowadays, complex microstructural features can be measured by various advanced methods [11,12]. Furthermore, computational tools (such as object oriented finite element or OOF2 [13]) transform micrograph images into FE meshes to be used for further FE analyses. The application of this method for stress analysis of the TBCs can be found in Ref. [14]. The work not only captures the roughness profile but also porous area within the coatings, which provides useful information to calculate the coating's thermal conductivity. Rezvani Rad et al. [15] and Nayebpashaee et al. [16] used a similar technique to identify the effect of realistic 2D roughness profiles on out-of-plane stresses under thermo-mechanical and thermal fatigue load conditions respectively. Measurements of 3D coating profiles were also used by Gupta et al. [17,18] to construct 3D FE models and the resultant residual stresses were compared against results from 2D FE models. For similar aspect ratio of the interface, out-of-plane stresses predicted from 3D models are around half an order of magnitude higher than those predicted from 2D models under similar loading conditions. The results highlight the importance of 3D interface shape to the estimation of residual stresses within TBC systems. Work by Saucedo-Mora, et al. [19] considered the microstructural roughness and heterogeneity of the coating for damage development within coatings using multi-scale FE model. The work not only demonstrated the effects of surface roughness on stress profiles, but also the influence of microstructural features on Young's modulus and damage within coatings.

Despite current abilities to incorporate complex coating interfaces into FE analyses, there are still many shortcomings among the models presented in the previous paragraph. The models in Refs. [15,18] ignore oxidation of the BC completely, yet this is very important due to the non-planar nature of the interface shape. When a BC oxidises, directional oxide growth strains and subsequent stresses build up within the system in a manner dependent on interface geometry. Nayebpashaee, et al. [16] considered oxidation by applying an empirical swelling strain to an initial oxide later without taking account of continuous consumption of the BC due to oxidation. Gupta et al. [17] calculated the oxide layer thickness based on the diffusion at the BC interfaces. However, the simulation only used a linear elastic material model to investigate the mismatch stress due to change in temperature. The model also ignored the stress build up and redistribution due to creep of coatings during the steady state. To address the aforementioned shortcomings, this paper reports an FE model that has been produced which describes the effect of stresses within a coating system of 3D microscopic features, extracted from 3D analysis of real coating interfaces. Appropriate boundary conditions presented by Li et al. [20] were applied to reduce the size of the surface profile unit cell and hence its computation time. Changes in material properties of the coating due to oxidation and sintering have also been incorporated to fully describe the changes taking place during service. A simple case study has been carried out using simplified 2D and 3D TGO interface idealisations with identical aspect ratios (ratio of amplitude to wavelength). Subsequently, two FE unit cells based on 3D microscopic features of the BC were built to carry out analysis of stress distribution and relate them to the failure of the TBC.

This work fits into the present Journal's priority area [21] of the analysis, structure, morphology and role of interfaces in the context of multi-physics phenomena, specifically by describing the influences of manufacturing-related interface geometry on the development of stresses and cracks due to thermo-mechanical and oxidation effects. This paper documents the development of a theoretical model of interface stress with the use of experimental data of interface geometry which can be used in the design of future turbine blade coatings.

2. Roughness modelling

2.1. Capturing and post processing of TGO surface profiles

Cross-sections of TBC systems are traditionally imaged using a scanning electron microscope (SEM). Nevertheless, as these interfaces are often view in cross-section, their interface roughness and surface profile data measured using this method might not always represent the actual aspect ratio. The concept can be appreciated through the examination of Fig. 1 where three different sectioning paths of an idealised surface with identical aspect ratio throughout its surface could form radically different cross-section profiles. To avoid this, 3D images of the coating interface were captured for the current work.

The specimen used for the capture of the TGO surface profile was composed of a Ni22Co17Cr12Al0.6Y (wt%) BC with an APS TBC which was isothermally heated to a temperature of 940 °C for 500 h. In order to view the TGO/BC interface, the BC was dissolved in hydrochloric acid (36%) for 36 h at ambient temperature to reveal the surface of the oxide interface as used by Sohn et al. [22]. To produce a 3D representation of the TGO/BC interface, secondary electron images were collected using a Cambridge 360 Stereoscan SEM at a number of tilt angles and analysed using Alicona Mex 3D. The x-y-z coordinates of the measured surface profile were then saved in ASCII format and post-processed using 'Fogale Nanotech Profilometry Software' (FNPS) [23]. In order to approximate a TGO layer of constant thickness within the FE model, it was assumed that both TGO interfaces (i.e. TBC/TGO and TGO/BC) follow identical geometries.

The measured TGO surface coordinates in ASCII format were imported into FNPS, and the roughness profile (short wavelength undulations) and waviness (longer wavelength than the roughness profile) of the interface were separated using a standardised Gaussian filtering method (ISO 11562) [24]. The weight function of the filter ($S(x)$) is given by Eq. (1) [25]. The mean line of the raw data was obtained by convolving it with the weighting function. The roughness and waviness profiles were separated by subtracting the mean line from the raw profile. The transfer function was obtained by performing a Fourier transform of the continuous function $S(x)$ as shown in Eq. (2) [26].

$$S(x) = \frac{1}{\alpha\lambda_c}\ \exp\left(-\pi\left(\frac{x}{\alpha\lambda_c}\right)^2\right) \tag{1}$$

$$Sf(\lambda) = \int_{-\infty}^{\infty} S(x)\ \exp(i\lambda x)\,\mathrm{d}x = \ \exp\left(-\pi\left(\frac{\alpha\lambda_c}{\lambda}\right)^2\right) \tag{2}$$