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A diffusion-based oxide layer growth model using real interface roughness in thermal barrier coatings for lifetime assessment

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ABSTRACT

The development of thermo-mechanical stresses during thermal cycling can lead to the formation of detrimental cracks in Atmospheric Plasma Sprayed (APS) Thermal Barrier Coatings systems (TBCs). These stresses are significantly increased by the formation of a Thermally Grown Oxide (TGO) layer that forms through the oxidation of mainly aluminium in the bondcoat layer of the TBC. As shown in previous work done by the authors, the topcoat–bondcoat interface roughness plays a major role in the development of the stress profile in the topcoat and significantly affects the lifetime of TBCs. This roughness profile varies as the TGO layer grows and changes the stress profile in the topcoat leading to crack propagation and thus failure.

In this work, a two-dimensional TGO growth model is presented, based on oxygen and aluminium diffusion–reaction equations, using real interface profiles extracted from cross-section micrographs. The model was first validated by comparing the TGO profiles artificially created by the model to thermally cycled specimens with varying interface roughness. Thereafter, stress profiles in the TBC system, before and after the TGO layer growth, were estimated using a finite element modelling model described in previous work done by the authors. Three experimental specimens consisting of the same chemistry but with different topcoat–bondcoat interface roughness were studied by the models and the stress state was compared to the lifetimes measured experimentally. The combination of the two models described in this work was shown to be an effective approach to assess the stress behaviour and lifetime of TBCs in a comparative way.

1. Introduction

Thermal Barrier Coatings systems (TBCs) are widely used in modern gas turbines to serve the purpose of protecting gas turbine components from the severe thermal environment, thus improving the efficiency and lifetime of the gas turbines [1,2]. Typical TBCs consist of an insulating ceramic topcoat layer and an intermetallic bondcoat layer applied over a substrate. The major functions of the bondcoat layer are to provide substrate oxidation protection and improve adherence of the topcoat. Atmospheric Plasma Spraying (APS) is one of the common methods to deposit TBC topcoats.

Failure in APS TBCs during thermal cyclic loading is associated with the thermo-mechanical stresses developing due to the formation of a Thermally Grown Oxide (TGO) layer and thermal expansion mismatch between different layers during thermal cycling. These thermo-mechanical stresses induce crack growth and eventually coalescence which leads to failure due to the spallation of the topcoat [3–5]. The failure is often observed to occur close to the topcoat–bondcoat interface where the TGO layer is built up. The topcoat–bondcoat interface roughness, although essential for effective adherence of the topcoat provided by the mechanical interlocking, plays a key role in the development of thermo-mechanical stresses as it creates locations of high stress concentrations [6].

A crack propagation mechanism theory for APS TBCs has been proposed in earlier works, namely 'stress inversion' theory [7–9]. According to the proposed theory, in the initial state without a TGO layer, tensile stresses exist in the hills while compressive stresses exist in the valleys within the topcoat as shown in Fig. 1a. This stress state is inverted as the TGO layer grows during thermal cyclic loading, as shown in Fig. 1b. Thus, a crack starts from the hill and propagates to the adjacent valley as the TGO is formed joining the corresponding crack from the other side eventually leading to the spallation of the topcoat. The thickness of the TGO when the stress inversion takes place depends on several factors such as the thermal cyclic loading times, geometry, and material parameters [6,10].

The stress inversion theory has been observed to follow the trend in earlier works when the time to stress inversion was compared to the experimental lifetime of TBCs. A two-dimensional (2D) sinusoidal profile representing the topcoat–bondcoat interface roughness was used in finite element models by Vassen et al. to evaluate the residual stresses developed in TBCs and it was observed that the time to stress inversion

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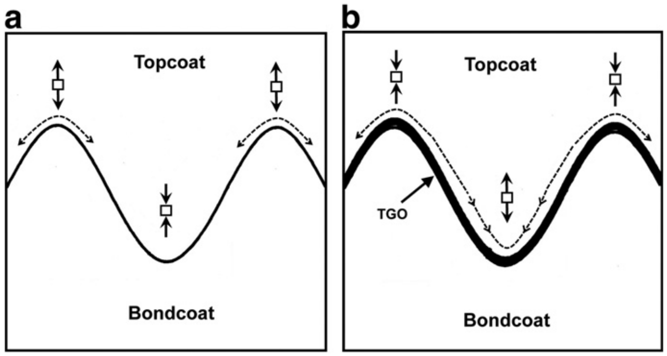

Fig. 1. Schematic illustration of the stress behaviour in the topcoat near the bondcoat surface (a) in as-sprayed condition, and (b) after TGO growth.

was shorter for samples which failed earlier in experiments [8]. In a recent work done by Gupta et al., real 2D and three-dimensional (3D) surface topographies were used in finite element models to compare different samples and it was again observed that the time to stress inversion was shorter for samples which failed earlier in experiments [11]. Based on the conclusion from these works, it can be assumed that the time to stress inversion according to the stress inversion theory could be implemented to compare coating lifetimes using both simplified as well as real topcoat–bondcoat interface topographies in a finite element model.

The development of TGO in-situ during thermal cyclic loading conditions needs to be implemented in the finite element model used for stress calculations for evaluating the time to stress inversion as the TGO formation occurs. Visualisation of TGO growth in-situ by experimental methods is highly non-trivial, so a modelling approach was undertaken in this work. A few studies have been performed earlier to model the TGO layer formation. A multi-scale continuum mechanics approach based on a coupled diffusion-constitutive framework was implemented by Busso et al. to study the local stresses induced in TBCs using a parametric unit cell finite element model [12]. A numerical model describing the TGO growth by an oxygen diffusion–reaction model was developed by Hille et al. to perform an analysis of a representative TBC system subjected to a thermal cycling process and to make a parametric study for different fracture strengths of the topcoat to determine its influence on the durability of a TBC system [13]. A one-dimensional oxidation–diffusion model considering both surface oxidation and coating–substrate interdiffusion as well as aluminium depletion during operating conditions was developed by Yuan et al. to predict the lifetime of TBCs [14]. A diffusion–reaction of aluminium and oxygen to form TGO in TBCs was studied through an analytical model by Osorio et al. and the results were compared to experiments to evaluate the TGO growth rate [15]. However, all of the models discussed above did not incorporate the TBC microstructure or the topcoat–bondcoat interface topography.

In this work, a 2D diffusion-based TGO growth model was developed using a Computational Fluid Dynamics (CFD) approach consisting of real topcoat–bondcoat interface topography extracted from cross-sectional micrographs. The model was first validated by comparing the TGO profiles artificially created by the model to thermally cycled specimens with varying interface roughness. Thereafter, the TGO profiles at different stages of TGO growth were extracted to the finite element model for stress analysis and the time to stress inversion was evaluated. Three experimental specimens consisting of the same chemistry but with different topcoat–bondcoat interface roughness were studied by the models and the time to stress inversion was compared to the lifetimes measured experimentally. The objective of this work was to make a tentative evaluation of the capability of the combination of the TGO growth and stress analysis models to assess the lifetime of TBCs in a comparative way.

2. Experimental

2.1. Material

A set of three specimens with varying bondcoat roughness were used as basis for the study. The TBC system consisted of a 200 µm thick Ni–25Cr–5Al–2.6Si–1Ta–0.6Y (wt.%) bondcoat and a 350 µm thick 7 wt.%-Yttria partially-Stabilized Zirconia (YSZ) topcoat layer. The bondcoat was sprayed using Vacuum Plasma Spraying (VPS) and the topcoat using APS. The TBC system was deposited on 30 × 50 mm rectangular coupons cut from 5 mm thick Haynes 230 sheet material.

The variation in topcoat–bondcoat interface roughness was achieved mainly by varying the powder size during spraying of the bondcoat. The interface roughness was measured on micrographs of cross-sectioned specimens after thermal cycling using a previously developed image analysis routine as described in previous work [16]. The image analysis routine was calibrated against profilometer results and all roughness parameters were implemented in accordance with ISO standards. The measurements on the micrographs were conducted to agree with profilometer results with the following parameters: 5 µm stylus tip radius, cut-off wavelengths $\lambda s = 10$ µm and $\lambda c = 800$ µm. Data were collected from ~50 mm of the cross-section. The specimens, here referred to as A, B, and C, had Ra values 6.6, 8.1 and 9.7 µm respectively. The cross-section images taken with a Light-Optic Microscopy (LOM) of the three thermally cycled specimens A, B and C are shown in Fig. 2a, b and c respectively.

2.2. Thermal cycling and microscopy

The specimens were cycled to failure in a cyclic furnace which, automatically, moved the specimens in and out of a resistance furnace. One thermal cycle consisted of 1 h dwell time at 1100 °C followed by ~10 min of forced airflow cooling until the substrates of the specimens reached 100 °C. When the specimens had suffered 20% visible topcoat damage, the specimens were considered to have failed and the test was interrupted.

Prior to cross-sectioning for microscopy, the samples were infiltrated in vacuum by epoxy to avoid damage during the subsequent cutting and grinding steps. Microscopy was performed using a Hitachi SU-70 field emission gun scanning electron microscope (SEM) as well as LOM. Energy Dispersive X-ray spectroscopy (EDX) was performed using a detector from Oxford Instruments which was calibrated against standards.

3. Modelling

3.1. TGO growth model

3.1.1. Oxidation mechanism

As soon as the TBC is put into operating conditions, the bondcoat starts to undergo oxidation due to the exposure to high temperatures. Alumina is the primary and most stable oxide formed for a NiCoCrAlY

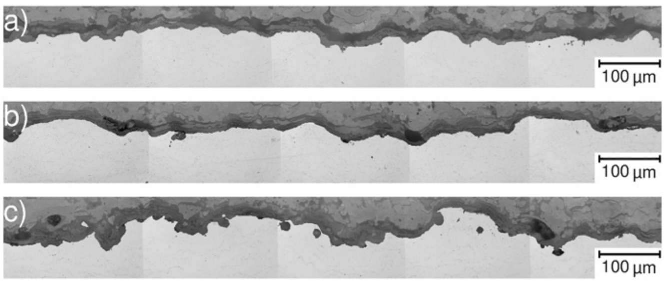

Fig. 2. Overview of the interfaces of the four thermally cycled specimens: a)–c) in order of increasing roughness (*Ra*).