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High temperature stress and its influence on surface rumpling in NiCoCrAlY bond coat



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ABSTRACT

The objective of this work is to develop a methodology to measure the high temperature stress in the bond coat, and investigate its role on the surface rumpling. We first presented an analytical model to evaluate the high temperature stress using X-ray $\sin^2\Psi$ technique coupling with the curvature measurement at room temperature. A typical NiCoCrAlY bond coat with a Hastelloy-X substrate was employed as a model sample. During exposure at 1150 °C, the bond coat was under tension at high temperature, increasing parabolically from 1.05 MPa after 12 h to 3.81 MPa after 120 h. To understand its effect on the surface rumpling, the bond coat surface roughness was recorded as a function of time, and compared with a bulk NiCoCrAlY alloy. A strong correlation between the bond coat stress and the surface roughness was identified. In addition, the origination of the bond coat stress and the rumpling mechanism were discussed. It was revealed that the high temperature stress in the bond coat was caused by the volume shrinkage from β - γ transformation, mainly due to the inter-diffusion. The grain sliding accompanied with diffusional creep in response to the bond coat stress controls the roughening.

1. Introduction

Bond coat is an important part of the thermal barrier coatings (TBCs) used in industrial gas turbines. A dominant failure phenomenon has been found that the crack extends along the interface between the thermally grown oxides (TGO) and the bond coat, which is associated with the progressive surface roughening [1-3]. The roughening also termed as rumpling, ratcheting or undulation. It initiates cracks nucleation and propagation as the TBCs experience thermal cycling. Eventually, the cracks coalesce to cause the TBC to buckle or spall. Extensive works have been carried out to investigate the reasons of the rumpling. However, the mechanisms that govern the surface rumpling of the bond coat are still not fully understood. It has been generally accepted that the stress in the TGO [4-6], either from the growth at high temperature or the thermal mismatch upon cooling, is the primary driving force for the rumpling at the bond coat/TGO interface [7]. However, when thermal cycling in vacuum, the rumpling still occurs [7]. In this case, there is no (or negligible) TGO formation. This implies that the bond coat itself should be a dominant factor for rumpling. Chen and Hemker proposed that the strains caused by the martensitic transformation in the NiPtAl bond coat might be a major factor [8]. However, thermal cycling at a temperature above the martensitic temperature (i.e., 1050-1150 °C, no martensite transformation occurs at this temperature range) the rumpling amplitude does not show significant difference with the thermal cycling at room temperature [7,9]. In addition, the bulk alloy with the same composition exhibits a much smaller propensity to rumple under the same treatment [10]. This demonstrates that the presence of substrate is essential for the surface roughening. At high temperature, inter-diffusion between substrate and bond coat occurs, which could change the bond coat volume. Since the volume change is constrained by the substrate, a stress will be produced in the bond coat at high temperature. The high temperature stress in the bond coat might play a dominant role on the surface rumpling.

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However, due to low yielding strength of the bond coat, the stress in the bond coat (e.g. NiCoCrAlY) at high temperature is only several MPa [11]. Determining such low stress using conventional technique (e.g., X-ray) is extremely difficult, which is beyond the detectable limit of the instruments [10,12]. Nevertheless, the real

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limitation of this approach is that it provides information on only the net elastic strain, and not the plastic deformation associated with the concurrent relaxation process. Therefore, it is necessary to develop an alternative approach to estimate the high temperature stress in the bond coat, which is crucial to understand the rumpling mechanisms.

The objective of this work is to develop a method to measure the high temperature stress in the bond coat, and investigate its role on the surface rumpling. In this study, an alternative approach, based on X-ray $\sin^2 \Psi$ stress and the curvature measurement at the room temperature, was employed to evaluate the stress. The basic idea is to evaluate the net plastic strain (e.g. the bond coat or the substrate) at high temperature, and then the high temperature stress can be derived based on the corresponding creep mechanisms. The paper was organized as follows. First, the methodology to determine the stress was introduced and an analytical model was developed. To validate this, a typical NiCoCrAlY bond coat on superalloy system was used as model specimen. The total strain and the elastic strain were determined using curvature and X-ray techniques, respectively. The surface roughness of the bond coat was recorded as a function of time and compared with that of a bulk alloy with the same composition. To elucidate the role of the bond coat stress, the progressive surface rumpling was correlated with the stress in the bond coat at high temperature. Finally, the origin of the bond coat stress as well as the mechanisms for the rumpling were also discussed.

2. Methodology

In this section, we first presented the methodology to quantitatively evaluate the high temperature stress in the bond coat. It is known that the bond coat system consisted of elastic and non-elastic strain after cooling from high temperature exposure. The elastic strain can be determined from X-ray and the total strain can be measured from the dimension change (e.g., curvature measurement). The non-elastic strain at the room temperature can thus be obtained and equals to the non-elastic strain at high temperature if a fast-cooling is used. Provided that the non-elastic strain at high temperature is known, the stress can be evaluated based on the creep properties of the system.

Fig. 1a is a schematic of an as-deposited bond coat/substrate system, which is slightly curved due to the quenching stress and thermal misfit stress after deposition [13,14]. y = 0 defines as the interface between the bond coat and the substrate. h_{bc} and h_s are the thicknesses of bond coat and substrate, respectively. $y = h_{bc}$ means the surface of the bond coat, and $y = -h_s$ means that of the substrate. Fig. 1b shows a state during heating. Compared with the as-deposited state, the curved shape becomes flatter.

At high temperature, the TGO growth and inter-diffusion will introduce phase transformation in the bond coat, leading to shrinkage or expansion of the bond coat [15]. Assuming no constraint from the substrate, a strain, $\Delta \varepsilon^{\rm T}$, will be generated in bond coat (Fig. 1c), which is a hypothetical state (framed by a dotted box). The symbol with a superscript "T" refers to the high temperature state.

Due to the substrate constraint, both of the bond coat and the substrate will have internal stresses. As shown in Fig. 1d, a tensile stress $\sigma_{\rm bc}^{\rm T}$ will act on the bond coat, and a compressive stress $\sigma_{\rm s}^{\rm T}$ on the substrate. These two opposing stresses are in equilibrium, namely:

$$\sigma_{bc}^{T}h_{bc} = -\sigma_{s}^{T}h_{s} \tag{1}$$

where σ is stress. The subscript "bc" represents the bond coat, and

"s" substrate. Those stresses could lead to the creep deformation in both bond coat and substrate [16–18].

Mechanistically, creep deformation can be achieved by dislocation (i.e., Norton's law), grain-boundary diffusion (i.e., Coble creep), lattice diffusion (i.e., Nabarro-Herring creep), etc [17], which can be written as:

$$\varepsilon^{\mathsf{T}} = \varepsilon^{\mathsf{T}} \Big(\sigma^{\mathsf{T}}, t \Big) \tag{2}$$

where $\varepsilon^{\rm T}$ is the creep strain, $\sigma^{\rm T}$ the creep stress, and t the time. Likely, the creep strains of the bond coat and the substrate at high temperatures can be expressed as $\varepsilon^{\rm T}_{\rm bc}(\sigma^{\rm T}_{\rm bc},t)$ and $\varepsilon^{\rm T}_{\rm S}(\sigma^{\rm T}_{\rm S},t)$, respectively, as shown in Fig. 1e.

Once the system is cooled from high temperature, both elastic and non-elastic strains will be preserved in the system. If the bond coat is free to deform, the elastic strains in bond coat and substrate will be different and that difference is $\Delta\varepsilon$ in a hypothetical schematic (Fig. 1f). If the bond coat is constrained by the substrate (Fig. 1g), the system will have a uniform elastic strain $\overline{\varepsilon}$ (since the displacement compatibility is required) and a pair of equilibrium forces (marked by arrows). To balance the bending moment induced by this pair of forces, bending of the system occurs.

Fig. 1h depicts the final state of the system after cooling. *M* means the bending moment. The total strain of the system at room temperature can be expressed as:

$$\varepsilon = \varepsilon^{\mathsf{e}} + \varepsilon^{\mathsf{ne}} \tag{3}$$

where ε is strain, and the superscripts "e" and "ne" denote elastic and non-elastic, respectively. The elastic strain of the system at room temperature, ε^e , is composed of a uniform component, $\overline{\varepsilon}$, and a bending component, $\overline{\varepsilon}$ (Fig. 1g—h):

$$\varepsilon^{\mathsf{e}} = \overline{\varepsilon} + \widecheck{\varepsilon} = \overline{\varepsilon} + (y - \delta)\kappa^{\mathsf{e}} \tag{4}$$

where $\kappa^{\rm e}$ is the curvature induced by elastic strain. y is the position in the coordinate system ($-h_{\rm s} \le y \le h_{\rm bc}$). δ is the neutral axis (Fig. 1h) [19,20]:

$$\delta = \frac{E_{bc}h_{bc}^2 - E_sh_s^2}{2(E_{bc}h_{bc} + E_sh_s)}$$
 (5)

where E is the elastic modulus.

The elastic strains in the bond coat and the substrate, ε_{bc}^e and ε_{s}^e , are equal to:

$$\varepsilon_{\rm bc}^{\rm e} = \varepsilon^{\rm e} - \Delta \varepsilon \, (0 \le y \le h_{\rm bc})$$
 (6-a)

$$\varepsilon_{\mathsf{s}}^{\mathsf{e}} = \varepsilon^{\mathsf{e}}(-h_{\mathsf{s}} \le y \le 0) \tag{6-b}$$

The variables $\bar{\epsilon}$ and κ^e in Eq. (4) can be determined from three boundary conditions of the model shown in Fig. 1. Firstly, the sum of forces due to the uniform strain component (i.e., the force in Fig. 1g) is zero:

$$E_{\rm bc}h_{\rm bc}(\overline{\varepsilon} - \Delta\varepsilon) + E_{\rm s}h_{\rm s}\overline{\varepsilon} = 0 \tag{7}$$

Secondly, in Fig. 1h, the sum of forces due to the bending strain component is zero:

$$\int_{-h_s}^{\delta} E_s \, \widetilde{\varepsilon} \, dy + \int_{\delta}^{0} E_s \, \widetilde{\varepsilon} \, dy + \int_{0}^{h_{bc}} E_{bc} \, \widetilde{\varepsilon} \, dy = 0$$
 (8)

Thirdly, in Fig. 1h, the sum of bending moments is zero:

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