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Numerical study of residual stress and crack nucleation in thermal barrier coating system with plane model

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ABSTRACT

The residual stresses could cause extensive damage to thermal barrier coatings and even failure. A finite element model of thermal barrier coating system had been designed to simulate the residual stresses and then to analyze the crack nucleation behavior. The distribution of normal and tangential stress components along top coat (TC) / thermally grown oxide (TGO) and TGO / bond coat (BC) interfaces are shown in this work. It is found that the maximum tensile stress along TC/TGO interface occurs in the peak region during heating-up, and that along TGO/BC interface is also located in the peak region, but during the process of cooling-down. A parameter correlating the normal stress component with corresponding tangential one was used to evaluate the interfacial cracks, indicating that cracks will initiate at the peak-off region of TC/TGO interface in the heating-up phase, but for TGO/BC interface, cracks will initiate at the peak position in the cooling-down phase.

1. Introduction

Air plasma sprayed(APS) thermal barrier coatings(TBCs) have been widely used to protect turbine parts from high temperature, resulting in the improvement of the performance and efficiency of engines [1–8]. From the perspective of material engineering, a complete thermal barrier coating system consists of four layers: a ceramic top coat(TC), a thermally grown oxide(TGO), a metallic bond coat(BC), and a metal substrate [9–11]. TBCs have to be subjected to the residual stresses and possible crack propagation due to severe operating environments and their own complexity [12]. The residual stresses will, in turn, affect the lifetime of TBCs.

The residual stresses in TBC system are basically attributed to two aspects: 1) thermal mismatch between all the constituents; and 2) thermal growth of TGO layer [13–16]. Regarding the residual stresses, lots of work has been done using finite element technique. The thermo-mechanical finite element model was developed to estimate the stress distribution within TBC system [17]. By performing the parametric studies of creep strengths of TC and TGO, it was shown that a single parameter, called creep strength parameter, can be used to calculate the resulting stresses in the high-temperature steady state [18]. The effect of the interface geometry and amplitude on the stress distribution was examined to study the cause of the subsequent delamination of the TBC system [19]. The cooling stress in the TBC system is determined by the thermal mismatch between layers, while TGO and BC have an opposite effect on the stress in TC [20]. In addition, the crack propagation has also been studied by some researchers. Marcin Białas used cohesive elements to model the development of the interfacial micro-crack [16]. Martin Bäker investigated the crack initiation and propagation in the TBC system for different values of the creep strength of the materials [21]. M. Ranjbar-Far simulated the crack propagation along interfaces using the contact tool "*Debond*" in ABAQUS finite element code [22,23]. However, there is something in their work that should be noticed. The growth rate of TGO was kept as constant throughout the calculation of the residual stresses or possible cracks. Actually, it decreases gradually with TGO thickness increasing [4,24]. In this regard, the oxidation process was simulated based on CREEP subroutine interface provided in ABAQUS [23]. Furthermore, much of these work did not involve the normal and tangential components of the residual stress along interfaces, but they play an important role in determining the initiation and propagation of the interfacial cracks.

In order to understand the failure mechanisms of the TBC system further, the following issues will be addressed in our work: 1) evolution of the residual stresses in TC and TGO; 2) distribution of the normal and tangential stresses along the TC/TGO and TGO/BC interfaces; and 3) evaluation of the interfacial cracks by constructing a scalar parameter that can reflect the corresponding interface stress states.

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Nomenclature

α	coefficient of thermal expansion [°C^{-1}]
E	Young's modulus[GPa]
ν	Poisson's ratio
$\dot{\bar{\varepsilon}}^{cr}$	uniaxial equivalent creep strain rate[s^{-1}]
B	creep pre-factor[s^{-1}MPa^{-n}]
n	creep exponent
σ	von Mises equivalent stress[MPa]
h_{ox}	the TGO thickness forming due to the oxidation of the BC[μm]
k	parabolic growth rate constant[μm^{2}s^{-1}]
t_{ox}	oxidation time[s]
h_0	initial TGO thickness[μm]
t_0	the time shift corresponding to the initial thickness h_0 [s]
ε_{ox}	the oxidation strain in the thickness direction
σ_N	stress normal to interface[MPa]
σ_T	stress tangential to interface[MPa]
$[\sigma_N]$	interface toughness in the purely normal mode[MPa]
$[\sigma_T]$	interface toughness in the purely tangential mode[MPa]
β	interface stress state parameter
β_c	the critical value of β

2. TBC system model

2.1. Modeled unit and boundary conditions

The current TBC system is composed of an air-plasma-sprayed(APS) TC, a TGO produced from BC, a NiCrAlY-BC and an Inconel 617 substrate. Fig. 1 shows the TBC system with plane structure and the corresponding plane strain model. The thicknesses of the TC, BC and Substrate layers are 250, 100, 1600 μm, respectively [19,25,26]. The initial thickness of TGO layer was assumed to be 1 μm here.

The interfaces are either convex or concave for the following reasons: 1) asperities formed during the manufacturing process [12,19]; 2) progressive roughening of the interfaces due to the cyclic creep of BC layer, often called "ratcheting" phenomenon [4,11]; and 3) the interface displacement, which has a connection with volumetric changes caused by aluminum depletion in BC [9]. It was assumed that the interface morphology is of cosine shape. The interface roughness can obviously affect the residual stresses and has been studied in much work [18,27–29]. It is shown that smaller wavelength and larger amplitude lead to greater residual stresses. The wavelength and amplitude of the interfaces were set to 60 and 15 μm, respectively [25,26,30]. In fact, the interface roughness not only increases the initial adhesion between the coating layers through mechanical interlocking, but also accelerates their delamination [29,31].

As shown in Fig. 1, the area between the two vertical dashed lines can be taken out of the TBC system model and be regarded as a separate modeled unit due to the periodicity and symmetry. Fig. 2a shows the unit model and its boundary conditions. The symmetry boundary conditions were imposed on the left side of the unit model. The couple constraint [23] was applied to the right side of the unit model, so that all the points on the right side maintained the same horizontal displacement all the time.

A two-dimensional mesh was generated on the unit model. There were 25,349 elements in total for the computation. And the element type for each of the elements was a 4-node bilinear plane strain quadrilateral(CPE4). Fig. 3 shows the part of the mesh surrounding the interfaces.

2.2. Thermal loading

A homogeneous temperature field was implemented on the whole unit model. The unit model is heated up from 25 to 1100 °C in 300 s, kept at 1100 °C for 100 h, and cooled down to 25 °C in 300 s, as shown in Fig. 3. The coating failure is expected to be concerned with not only stresses developed upon heating to high temperatures but also those developed upon cooling to ambient temperature [5]. Four different time points A, B, C, and D were chosen to check the stress states in current system. They refer to the endpoint of the heating-up phase, the midpoint of the dwelling phase, the endpoint of the dwelling phase, and the endpoint of the cooling-down phase, respectively, as depicted in Fig. 3.

2.3. Material parameters

The materials for all the layers were assumed to be isotropic and homogeneous. In general, the materials for the TC, TGO and Substrate layers are regarded as viscous-elastic, with the material for the BC layer elastic and viscous-plastic [19,32]. The temperature-dependent data for Coefficients of thermal expansion α, Young's moduli E and Poisson's ratios ν are listed in Table 1 [19,26]. And the temperature-dependent data for plasticity of the BC layer are listed in Table 2 [30,33].

Norton's law was used for the creep behaviors of all the constituents. That is,

$$\dot{\bar{\varepsilon}}^{cr} = B\sigma^n \tag{1}$$

Where $\dot{\bar{\varepsilon}}^{cr}$ is an uniaxial equivalent creep strain rate, and σ is von Mises equivalent stress when materials are isotropic. The parameters B and n are also temperature-dependent, listed in Table 3 [18,30,34]. According to the report of Rösler et al. [18], values were chosen for creep prefactors of TC and TGO.

2.4. Growth of TGO

The oxidation process was replaced with TGO growth. The correlation between TGO thickness and oxidation time has been experimentally studied by A. G. Evans et al., showing that TGO growth is essentially parabolic until spalling occurs [1,4].

The simulation of growth of TGO with time can be achieved using CREEP subroutine in ABAQUS [23]. It was assumed that: 1) The initial value of TGO thickness is 1 μm; 2) TGO growth only takes place in the dwelling-time phase. Since the swelling strain rate decreases gradually with increasing of TGO thickness [35], the equation of TGO growth provided by A. G. Evans et al. was modified as follows

$$h_{TGO}^2 = 2k(t_{ox} + t_0) \tag{2}$$

where h_{TGO} is TGO thickness, k a parabolic growth rate constant, t_{ox} the

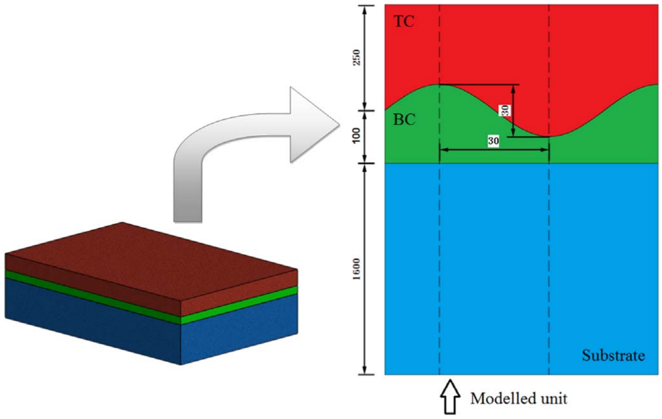

Fig. 1. Illustration of the TBC system with plane structure and the corresponding plane strain model.