Contents lists available at ScienceDirect

Materials and Design





journal homepage: www.elsevier.com/locate/jmad

# Interface stress evolution considering the combined creep–plastic behavior in thermal barrier coatings



### Lin Chen, Li Yueming \*

State Key Laboratory for Strength and Vibration of Mechanical Structures, School of Aerospace Engineering, Xi'an Jiaotong University, Xi'an 710049, China

#### A R T I C L E I N F O

Article history: Received 15 July 2015 Received in revised form 13 September 2015 Accepted 27 September 2015 Available online 3 October 2015

*Keywords:* Thermal barrier coatings (TBC) Interface stresses evolution Combined creep–plastic constitutive

#### ABSTRACT

In this paper, the interface stress evolution in thermal barrier coatings (TBC) is numerically investigated by considering the combined creep–plastic behaviors of thermally grown oxide (TGO) and bond-coat (BC). The return-mapping type algorithm is proposed for the solution of combined creep–plastic constitutive model. The diffusion oxidation-reaction scheme is introduced to describe TGO growth. The numerical results reveal that the TGO creep leads to the relaxation of stress in both top-coat (TC) and BC layers, and the BC creep decreases the stress in BC layer but increases the stress in TC layer, as well as the plastic deformation affects the stress evolution too but its influence is insignificant during oxidation. On cooling, the plasticity rather than the creep affects stress evolution, and the strength properties can affect not only the magnitude but the location of maximum interface stress.

© 2015 Elsevier Ltd. All rights reserved.

#### 1. Introduction

Thermal barrier coatings (TBC), consisting of ceramic top-coat (TC), thermally grown oxide (TGO) scale and metallic bond-coat (BC), plays an important role in aero-engine and land-based gas turbine to improve thermal efficiency and prolong service life [1,2]. However, the interface stress evolution, which induces damage initiation and progression and finally leads to the premature spallation of TBC, seriously restricts the application of TBC [3,4].

Up to now, numerous finite element (FE) strategies have been introduced to evaluate the interface stress development and then probe the failure mechanism of TBC. The accurate prediction of stress mainly depends on the reasonable assumptions for the mechanical properties of TC, TGO and BC. The FE scheme proposed by He et al. [5] has the long history and is widely used, in which TGO and BC are assumed to be the temperature-dependent elasto-plastic materials. As the stress is found to be significantly relaxed by creep at high temperature, creep rather than plastic constitutive theory is mainly applied to the prediction of stress development in the current numerical studies [6–12]. The visco-plastic constitutive model proposed by Chaboche [13] is also employed to reflect the rate dependent deformation behavior of TBC, in which creep is assumed to be indistinguishable from plasticity. The creep and plastic strains are represented in a unified way by one parameter called the visco-plastic strain. In addition, the

\* Corresponding author. *E-mail address:* liyueming@mail.xjtu.edu.cn (L. Yueming). visco-plastic deformation only takes place when stress lies outside the yield surface.

The creep and plastic behaviors are, in fact, governed by different mechanisms [14]. The plasticity is a non-reversible deformation with no time-dependence in response to applied forces, while creep is a time-dependent deformation which might occur under the very low level of stress within the yield limit. Thus, the purpose of the present paper is to develop a numerical approach to the analytical prevision of the interface stress influenced by creep combined with plasticity, and these results could be used as an indication of what combination of properties (elastic modulus, yield stress, creep resistance) should be optimized for improving TBC durability.

The rest of the paper is organized as follows. In Section 2, the combined creep–plastic constitutive relationship is employed to characterize the material behaviors of TGO and BC; the return-mapping type strategy is developed for the solution of the combined creep–plastic model. Furthermore, the diffusion oxidation reaction consideration is proposed to describe TGO growth. In Section 3, a numerical simulation is carried out to investigate the influence of mechanical properties on stress development. In Section 4, the main conclusions are drawn.

#### 2. Theoretical model for the stresses evolution in TBC

#### 2.1. Combined creep-plastic model and its numerical implementation

In this section, the combined creep-plastic constitutive model is employed to characterize the deformation behavior of TGO and BC.



Fig. 1. Creep type return-mapping scheme.



$$\begin{split} \boldsymbol{\epsilon}_{TGO} &= \boldsymbol{\epsilon}_{TGO}^{th} + \boldsymbol{\epsilon}_{TGO}^{e} + \boldsymbol{\epsilon}_{TGO}^{p} + \boldsymbol{\epsilon}_{TGO}^{c} + \boldsymbol{\epsilon}_{TGO}^{g} \\ \boldsymbol{\epsilon}_{BC} &= \boldsymbol{\epsilon}_{BC}^{th} + \boldsymbol{\epsilon}_{BC}^{e} + \boldsymbol{\epsilon}_{BC}^{p} + \boldsymbol{\epsilon}_{BC}^{c} \end{split}$$
 (2.1.1)

where the subscripts TGO and BC, respectively, represent the TGO and BC materials;  $\epsilon^{th}$ ,  $\epsilon^{e}$ ,  $\epsilon^{p}$  and  $\epsilon^{c}$  are, respectively, the thermal, elastic, plastic and creep strains;  $\epsilon^{g}$  is the permanent volumetric swelling strain of TGO, expressed as:

$$\mathbf{\epsilon}_{\mathsf{TGO}}^{\mathsf{g}} = \varepsilon_{\mathsf{v}}^{\mathsf{g}} \mathbf{I} \tag{2.1.2}$$

where  $\varepsilon_v^{g} = 0.08$  is the mean swelling strain derived from Pilling-Bedworth ratio [15];  $\mathbf{I} = [1,1,1,0,0,0]^{T}$  is a vector.

A return-mapping type algorithm is proposed for the solution of the combined creep-plastic constitutive model. In one time increment  $\Delta t_{n+1} \in [t_n, t_{n+1}]$ , the combined creep-plastic constitutive model



 $\ensuremath{\textit{Fig. 3.}}$  Updated stress derived from the combined creep–plastic return-mapping algorithm.



Fig. 4. Schematic representation of the oxidation front.

is derived in the form:

$$\begin{aligned} \boldsymbol{\sigma}_{\text{TGO}} &= \boldsymbol{\sigma}_{\text{TGO}}^{\text{tr}} \big|_{n+1} - \boldsymbol{D}_{\text{TGO}}^{\text{e}} : \left( \Delta \boldsymbol{\epsilon}_{\text{TGO}}^{\text{p}} \big|_{n+1} + \Delta \boldsymbol{\epsilon}_{\text{TGO}}^{\text{c}} \big|_{n+1} \right) \\ \boldsymbol{\sigma}_{\text{BC}} &= \boldsymbol{\sigma}_{\text{BC}}^{\text{tr}} \big|_{n+1} - \boldsymbol{D}_{\text{BC}}^{\text{e}} : \left( \Delta \boldsymbol{\epsilon}_{\text{BC}}^{\text{p}} \big|_{n+1} + \Delta \boldsymbol{\epsilon}_{\text{BC}}^{\text{c}} \big|_{n+1} \right) \end{aligned}$$
(2.1.3)



Fig. 2. Updated stress derived from the creep-type return-mapping algorithm, which lies (a) within and (b) outside the yield surface.



Fig. 5. (a) SEM image of TBC, (b) geometry of FE mesh and (c) boundary conditions.

where  $\mathbf{D}_{\text{FGO}}^{e}$  and  $\mathbf{D}_{\text{BC}}^{e}$  are, respectively, the elastic isotropic constitutive matrices of TGO and BC;  $\boldsymbol{\sigma}_{\text{TGO}}^{tr}|_{n \ + \ 1}$  and  $\boldsymbol{\sigma}_{\text{BC}}^{tr}|_{n \ + \ 1}$  are, respectively, the elastic trail stresses of TGO and BC, expressed as:

$$\begin{split} \boldsymbol{\sigma}_{TGO}^{tr}\big|_{n+1} &= \boldsymbol{D}_{TGO}^{e}: \left(\boldsymbol{\epsilon}_{TGO}\big|_{n+1} - \boldsymbol{\epsilon}_{TGO}^{th}\big|_{n+1} - \boldsymbol{\epsilon}_{TGO}^{e}\big|_{n+1} - \boldsymbol{\epsilon}_{TGO}^{p}\big|_{n} - \boldsymbol{\epsilon}_{TGO}^{c}\big|_{n}\right) \\ \boldsymbol{\sigma}_{BC}^{tr}\big|_{n+1} &= \boldsymbol{D}_{BC}^{e}: \left(\boldsymbol{\epsilon}_{BC}\big|_{n+1} - \boldsymbol{\epsilon}_{BC}^{th}\big|_{n+1} - \boldsymbol{\epsilon}_{BC}^{p}\big|_{n} - \boldsymbol{\epsilon}_{BC}^{c}\big|_{n}\right). \end{split}$$

$$(2.1.4)$$

If the trail stress lies within the yield limit, i.e.,

$$q(\mathbf{\sigma}_{\text{TGO}}^{\text{tr}})\big|_{n+1} - \sigma_{\text{y},\text{TGO}} \le 0 \text{ (or } q(\mathbf{\sigma}_{\text{BC}}^{\text{tr}})\big|_{n+1} - \sigma_{\text{y},\text{BC}} \le 0 \text{ )}$$

$$(2.1.5)$$

where *q* is the von-Mises equivalent stress;  $\sigma_{y, TGO}$  and  $\sigma_{y, BC}$  are, respectively, the yield strength of TGO and BC.

 Table 1

 Material properties of TC and thermal expansion coefficient of substrate.

| T (°C) | TC [23]               | TC [23]      |  |  |  |
|--------|-----------------------|--------------|--|--|--|
|        | E <sub>TC</sub> (GPa) | $v_{\rm TC}$ | $\alpha_{\rm TC}  (10^{-6}/{\rm ^{o}C})$ | $\alpha_{\rm SUB} (10^{-6}/^{\circ}{\rm C})$ |  |
| 20     | 48                    | 0.1          | 9.7                                      | 14.8   |  |
| 200    | 47                    | 0.1          | 9.8                                      | 15.2   |  |
| 400    | 44                    | 0.1          | 9.9                                      | 15.6   |  |
| 600    | 40                    | 0.11         | 9.9                                      | 16.2   |  |
| 800    | 34                    | 0.11         | 10                                       | 16.9   |  |
| 1000   | 26                    | 0.12         | 10.1                                     | 17.2   |  |
| 1100   | 22                    | 0.12         | 10.1                                     | 17.6   |  |

## Table 2Material properties of BC.

| T (°C) | BC [23,                  | 24]          |   |                             |   |                |                            |
|--------|--------------------------|--------------|---|-----------------------------|---|----------------|----------------------------|
|        | E <sub>BC</sub><br>(GPa) | $v_{\rm BC}$ | α <sub>BC</sub><br>(10 <sup>-6</sup> /°C) | σ <sub>y, BC</sub><br>(MPa) | A <sub>BC</sub><br>(MPa <sup>-2.2</sup> s <sup>-1</sup> ) | $ ho_{\rm BC}$ | Q <sub>BC</sub><br>(J/mol) |
| 20     | 200                      | 0.3          | 12.3                                      | 426                         | $\textbf{6.31}\times 10^{-6}$                             | 2.2            | 165,000                    |
| 200    | 190                      | 0.3          | 13.2                                      | 412                         | -   | -              | -                          |
| 400    | 175                      | 0.31         | 14.2                                      | 396                         | -   | -              | -                          |
| 600    | 160                      | 0.31         | 15.2                                      | 362                         | -   | -              | -                          |
| 800    | 145                      | 0.32         | 16.3                                      | 284                         | -   | -              | -                          |
| 1000   | 120                      | 0.33         | 17.2                                      | 202                         | -   | -              | -                          |
| 1100   | 110                      | 0.33         | 17.7                                      | 114                         | -   | -              | -                          |

| Table 3  |            |         |
|----------|------------|---------|
| Material | properties | of TGO. |

| T (°C) | TGO [5,                   | 7,23]         |  |                              |   |                      |                             |
|--------|---------------------------|---------------|--|------------------------------|---|----------------------|-----------------------------|
|        | E <sub>TGO</sub><br>(GPa) | $v_{\rm TGO}$ | α <sub>TGO</sub><br>(10 <sup>-6</sup> /°C) | σ <sub>y, TGO</sub><br>(GPa) | $\begin{array}{c} A_{\rm TGO} \\ ({\rm MPa}^{-2.3}~{\rm s}^{-1}) \end{array}$ | $ ho_{\mathrm{TGO}}$ | Q <sub>rGO</sub><br>(J/mol) |
| 20     | 400                       | 0.23          | 8  | 10                           | $\textbf{6.8}\times 10^3$   | 2.3                  | 424,000                     |
| 200    | 390                       | 0.23          | 8.2  | 10                           | -   | -                    | -                           |
| 400    | 380                       | 0.24          | 8.4  | 10                           | -   | -                    | -                           |
| 600    | 370                       | 0.24          | 8.7  | 10                           | -   | -                    | -                           |
| 800    | 355                       | 0.25          | 9  | 10                           | -   | -                    | -                           |
| 1000   | 325                       | 0.25          | 9.3  | 1                            | -   | -                    | -                           |
| 1100   | 320                       | 0.25          | 9.5  | 1                            | -   | -                    | -                           |

#### Table 4

Diffusion and oxidation parameters.

|   | Parameter                    | Value                 |
|---|------------------------------|-----------------------|
| Diffusion coefficients of oxygen in TC          | $D_{TC}$ (m <sup>2</sup> /s) | 00                    |
| Diffusion coefficients of oxygen in BC [6]      | $D_{BC}$ (m <sup>2</sup> /s) | $3.5 	imes 10^{-14}$  |
| Diffusion coefficients of oxygen in TGO [6]     | $D_{TGO} (m^2/s)$            | $3.5 \times 10^{-14}$ |
| Reference value for the oxidation reaction [25] | $\kappa (\text{mol/m}^3)$    | $0.24\times10^{6}$    |



Fig. 6. Evolution of TGO thickness using the proposed diffusion-oxidation reaction model.



Fig. 7. Contour plots of tensile stress after 300 h oxidation at 1100°C under the (a) elastic, (b) perfect elasto-plastic and (c) combined creep-plastic assumptions of TGO and BC.

In contrast to the general return-mapping scheme [16], the trail stress, in the Eq. (2.1.4), must be relaxed by creep, as shown in Fig. 1, so the general expression of final stress, in the Eq. (2.1.3), is reduced in the form:

$$\begin{aligned} \boldsymbol{\sigma}_{\text{TGO}} &= \boldsymbol{\sigma}_{\text{TGO}}^{\text{tr}} \big|_{n+1} - \boldsymbol{D}_{\text{TGO}}^{e} : \Delta \boldsymbol{\epsilon}_{\text{TGO}}^{c} \big|_{n+1} \\ \boldsymbol{\sigma}_{\text{BC}} &= \boldsymbol{\sigma}_{\text{BC}}^{\text{tr}} \big|_{n+1} - \boldsymbol{D}_{\text{BC}}^{e} : \Delta \boldsymbol{\epsilon}_{\text{BC}}^{c} \big|_{n+1} \end{aligned}$$
 (2.1.6)

where the Norton-type creep [17] strain increment  $\Delta \epsilon_{TGO}^{c}|_{n + 1}$  (or  $\Delta \epsilon_{CGO}^{c}|_{n + 1}$ ) is adopted in the form:

$$\Delta \boldsymbol{\varepsilon}_{\text{TGO}}^{c}\big|_{n+1} = \Delta t_{n+1} \dot{\boldsymbol{\varepsilon}}_{\text{TGO}}^{c}\big|_{n+1} \frac{\partial q(\boldsymbol{\sigma}_{\text{TGO}})}{\partial \boldsymbol{\sigma}_{\text{TGO}}}\Big|_{n+1}$$

$$\Delta \boldsymbol{\varepsilon}_{\text{BC}}^{c}\big|_{n+1} = \Delta t_{n+1} \dot{\boldsymbol{\varepsilon}}_{\text{BC}}^{c}\big|_{n+1} \frac{\partial q(\boldsymbol{\sigma}_{\text{BC}})}{\partial \boldsymbol{\sigma}_{\text{BC}}}\Big|_{n+1}$$

$$(2.1.7)$$

where  $\Delta t_{n+1}$  is the time increment;  $\dot{\bar{\epsilon}}_{TGO}^c|_{n+1}$  and  $\dot{\bar{\epsilon}}_{BC}^c|_{n+1}$  are, respectively, the equivalent creep strain rates of TGO and BC, expressed as:

$$\dot{\bar{\varepsilon}}_{\text{TGO}}^{c}|_{n+1} = A_{\text{TGO}} \exp\left[-\frac{Q_{\text{TGO}}}{R(T+273)}\right] \left[q(\boldsymbol{\sigma}_{\text{TGO}})|_{n+1}\right]^{\rho_{\text{TGO}}}$$

$$\dot{\bar{\varepsilon}}_{\text{BC}}^{c}|_{n+1} = A_{\text{BC}} \exp\left[-\frac{Q_{\text{BC}}}{R(T+273)}\right] \left[q(\boldsymbol{\sigma}_{\text{BC}})|_{n+1}\right]^{\rho_{\text{BC}}}$$

$$(2.1.8)$$

where A, Q, R, T and  $\rho$  are, respectively, the reference creep strain rate, the creep activation energy, the ideal gas constant, the Celsius temperature and the creep exponent.

When the trail stress, in the Eq. (2.1.4), lies outside the yield surface, i.e.,

$$q(\boldsymbol{\sigma}_{\text{TGO}}^{\text{tr}})\big|_{n+1} - \sigma_{\text{y},\text{TGO}} > 0 \text{ (or } q(\boldsymbol{\sigma}_{\text{BC}}^{\text{tr}})\big|_{n+1} - \sigma_{\text{y},\text{BC}} > 0 \text{ )}$$

$$(2.1.9)$$

the creep-type return-mapping scheme, in the Eq. (2.1.6), is employed to update stress state firstly.

If the updated stress lies within the yield limit, as shown in Fig. 2a, the creep-type return-mapping scheme, in the Eq. (2.1.6), is valid. Otherwise, the combined creep-plastic return-mapping scheme, in the Eq. (2.1.3), is implemented. The final stress must lie on the yield surface (as shown in Fig. 3), so the equivalent creep strain increments of TGO, in the Eq. (2.1.8), become the constants in the form:

$$\dot{\varepsilon}_{\text{TGO}}^{c}|_{n+1} = A_{\text{TGO}} \exp\left[-\frac{Q_{\text{TGO}}}{R(T+273)}\right] (\sigma_{y,\text{TGO}})^{\rho_{\text{TGO}}}$$

$$\dot{\varepsilon}_{\text{BC}}^{c}|_{n+1} = A_{\text{BC}} \exp\left[-\frac{Q_{\text{BC}}}{R(T+273)}\right] (\sigma_{y,\text{BC}})^{\rho_{\text{BC}}}.$$
(2.1.10)

The corresponding plastic strain increments  $\Delta \epsilon_{TGO}^{p}|_{n + 1}$  and  $\Delta \epsilon_{BC}^{p}|_{n + 1}$  are expressed as:

$$\Delta \boldsymbol{\varepsilon}_{\text{TGO}}^{\text{p}} \Big|_{n+1} = \Delta \overline{\boldsymbol{\varepsilon}}_{\text{TGO}}^{\text{p}} \Big|_{n+1} \frac{\partial q(\boldsymbol{\sigma}_{\text{TGO}})}{\partial \boldsymbol{\sigma}_{\text{TGO}}} \Big|_{n+1} \Delta \boldsymbol{\varepsilon}_{\text{BC}}^{\text{p}} \Big|_{n+1} = \Delta \overline{\boldsymbol{\varepsilon}}_{\text{BC}}^{\text{p}} \Big|_{n+1} \frac{\partial q(\boldsymbol{\sigma}_{\text{BC}})}{\partial \boldsymbol{\sigma}_{\text{BC}}} \Big|_{n+1}$$
(2.1.10)



Fig. 8. Evolutions of tensile stress with oxidation time at (a) TC valley and (b) BC peak locations under the elastic, perfect elasto-plastic and combined creep-plastic assumptions of TGO and BC.

| Table 5  |
|--|
| Creep parameters to reflect slow, medium and fast creep rates. |

|              | $A (MPa^{-1} \times s^{-1})$ | ρ | Q (J/mol) |
|--------------|------------------------------|---|-----------|
| Slow creep   | $10^{-6}$                    | 1 | 162,800   |
| Medium creep | $10^{-4}$                    | 1 | 162,800   |
| Fast creep   | $10^{3}$                     | 1 | 162,800   |

where  $\Delta \overline{\epsilon}_{TGO}^p$  and  $\Delta \overline{\epsilon}_{BC}^p$  are, respectively, equivalent plastic strain increments of TGO and BC.

#### 2.2. Diffusion oxidation reaction scheme for TGO growth

In this section, a diffusion oxidation reaction scheme is proposed to simulate TGO growth. The TGO-BC interface is assumed to be a transient oxidation front, in which TGO and BC phases coexist. The dimensionless molar fraction of both phases satisfies:

$$f_{\rm TGO} + f_{\rm BC} = 1.$$
 (2.2.1)

Here,  $f_{\text{TGO}}$  is denoted as  $f_{\text{TGO}} = \xi$ . The schematic representation of the oxidation front is depicted in Fig. 4.

In the oxidation front, the effective strain  $\varepsilon$  and the effective stress  $\sigma$  are derived based on the Voigt's homogenization theory [18], as follows:

$$\begin{split} & \boldsymbol{\epsilon} = \boldsymbol{\epsilon}_{TGO} = \boldsymbol{\epsilon}_{BC} \\ & \boldsymbol{\sigma} = \boldsymbol{\xi} \boldsymbol{\sigma}_{TGO} + (1 {-} \boldsymbol{\xi}) \boldsymbol{\sigma}_{BC}. \end{split}$$

Substituting the Eq. (2.1.1) into the Eq. (2.2.2), the constitutive relationship between effective stresses and effective strains is derived in the form:

$$\begin{split} \boldsymbol{\sigma} &= \boldsymbol{\xi} \boldsymbol{D}_{\text{TGO}}^{e} \left( \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\text{TGO}}^{th} - \boldsymbol{\epsilon}_{\text{TGO}}^{p} - \boldsymbol{\epsilon}_{\text{TGO}}^{c} - \boldsymbol{\epsilon}_{\text{TGO}}^{g} \right) \\ &+ (1 - \boldsymbol{\xi}) \boldsymbol{D}_{\text{BC}}^{e} \left( \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\text{BC}}^{th} - \boldsymbol{\epsilon}_{\text{BC}}^{p} - \boldsymbol{\epsilon}_{\text{BC}}^{c} \right). \end{split} \tag{2.2.3}$$

During oxidation,  $\xi$  varies from 0 to 1. The rate of evolution of  $\xi$  is assumed to be controlled by the concentration of oxygen anion and available BC material:

$$\xi = \gamma (1 - \xi) c_{0^{2-}} \tag{2.2.4}$$

where  $\gamma$  is a constant. In general, the distribution of concentration of oxygen anion  $c_{O^{2-}}$ , in the Eq. (2.2.4), is determined by Fick's law, as follows:

$$\dot{c}_{0^{2-}} = D \operatorname{div}(\nabla c_{0^{2-}})$$
 (2.2.5)



**Fig. 10.** Displacements  $u_2$  of TGO–TC interface, after 300 h oxidation at 1100 at 1100 °C, under the combined creep–plastic assumption of TGO with three types of creep rates.

where div and  $\nabla$  are, respectively, the divergence operator and gradient operator; *D* is oxygen diffusion coefficient, expressed as follows:

$$D = \xi D_{\rm TGO} + (1 - \xi) D_{\rm BC} \tag{2.2.6}$$

where  $D_{\text{TGO}}$  and  $D_{\text{BC}}$  are, respectively, the oxygen diffusion coefficients of TGO and BC. Note that during oxidation, TGO formation consumes oxygen. Therefore, with the reference of alkali-silica reaction model proposed by [19], Fick's law, i.e., Eq. (2.2.5), is modified by adding an oxidation term  $-\kappa \dot{\xi}$ , as follows:

$$\dot{c}_{\Omega^{2-}} = D \operatorname{div}(\nabla c_{\Omega^{2-}}) - \kappa \dot{\xi}$$
 (2.2.7)

where  $\kappa$  is the amount of oxygen consumed per unit reference volume during oxidation.

#### 3. Numerical analysis and its results

Based on the proposed combined creep–plasticity constitutive model, a numerical simulation is carried out in ABAQUS/Standard via a self-development user-defend-element (UEL) subroutine [20].

The FE mesh, consisting of 14,114 two dimensional four-node generalized plane strain elements, is adopted in the simulation. Its geometry is illustrated in Fig. 5(b), in which the morphology of TC-BC interfaces is extracted from the scanning electron microscope (SEM) image [21] as shown in Fig. 5a and idealized as the sinusoidal shape with the amplitude of 18  $\mu$ m and half-wavelength of 30  $\mu$ m.



Fig. 9. Evolutions of tensile stresses with oxidation time in (a) TC valley and (b) BC peak locations under the combined creep-plastic assumption of TGO with three types of creep rates.



Fig. 11. Evolutions of tensile stresses with oxidation time in (a) TC valley and (b) BC peak locations under the combined creep-plastic assumptions of BC with three types of creep rates.

In the simulation, TBC is assumed to be exposed at 1100 °C for 300 h, and then cooled down to 20 °C within 120 s. The homogeneous temperature distribution in TBC is assumed. Concerning the extremely short cooling time, the diffusion oxidation reaction only takes place at high temperature. Since the TC layer is commonly regarded to be fully transparent to oxygen and the oxidation reaction does not occur in TC layer, the TC top surface is assumed to be equal to the TC–BC interface in the concentration of oxygen anion. Based on the relationship between oxygen anion concentration and partial oxygen pressure  $p_{O_2}$  [22], the value of oxygen anion concentration can be estimated as 1.5 mol/m<sup>3</sup> when  $p_{O_2} = 0.021$  MPa.

At the beginning, TBC is regarded as stress-free. The upper surface is assumed to be unconstrained, while the other surfaces are constrained by the frictionless movable hinge support. On cooling, the generalized plane strain boundary condition is applied to reflect the influence of thermal contraction of substrate, i.e., the left TBC surface is allowed to move in  $x_1$  direction with the same displacement  $u_1$  as:

$$u_1 = \alpha_{\rm SUB} (T - T_{\rm ref}) W \tag{3.1}$$

where  $T_{\rm ref} = 1100$  °C is the reference temperature,  $\alpha_{\rm SUB}$  is the thermal expansion coefficient of substrate and  $W = 30 \ \mu m$  is the width of FE mesh (as shown in Fig. 5b). In addition, an equal thermal strain is applied to all nodes of TBC in the direction normal to the  $x_1$ - $x_2$  plane (as shown in Fig. 5c) as follows:

$$\varepsilon_{33} = \alpha_{\rm SUB}(T - T_{\rm ref}). \tag{3.2}$$

In simulation, TC is assumed to be isotropic elastic material deposited by APS technique. The sintering behavior of TC is not considered. The temperature-dependent elastic parameters from [23] are listed in Table 1. The mechanical parameters of BC are summarized in Table 2, including elasto-plastic properties from [23] and creep properties from [24]. The material properties of TGO are listed in Table 3, in which elastic parameters are taken from [23], yield strength are derived from [5] and the creep properties are obtained from [7]. The diffusion and oxidation parameters from [6,25] are listed in Table 4. In addition, the thermal expansion coefficient of substrate from [23] is listed in Table 1.

The parameter  $\gamma$ , in Eq. (2.2.4), is calibrated by the experiment data [26] of TGO thickness. When  $\gamma$  is chosen to be  $1.25 \times 10^{-4} \text{ m}^3/(\text{mol} \times \text{s})$ , the predicted TGO thickness agrees well with the experiment data, as shown in Fig. 6.

#### 3.1. Interface stress evolution during oxidation

In this section, the influence of mechanical properties of TGO and BC on interface tensile stress development, during oxidation, is investigated. The contour plots of tensile stress  $\sigma_{22}$ , after 300 h oxidation at 1100 °C, are illustrated in Fig. 7. Here, TGO and BC are, respectively, assumed to be elastic (in Fig. 7a), perfect elasto-plastic (in Fig. 7b) and combined creep–plastic (in Fig. 7c) materials.

It's observed that the maximum tensile stresses along TC-TGO and TGO-BC interfaces are, respectively, at the TC valley and the BC peak locations. These locations are consistent with the crack initiation locations from experimental observation [1], so tensile stress developments, at the TC valley and the BC peak, need to be investigated carefully. The evolutions of tensile stress  $\sigma_{22}$  at TC valley and BC peak locations are, respectively, plotted in Fig. 8a and b.

When TGO and BC are assumed to be elastic and perfect elastoplastic materials, the considerable compressive growth stress, induced by oxidation, generates in TGO and leads to the out-of-plane displacement of TGO layer. Such an out-of-plane displacement results in the tractions at TC valley and BC peak, so the extremely large tensile stresses accumulate with oxidation time at these locations, as shown in Fig. 8.

When the TGO and BC are considered as the combined creep-plastic materials, the growth stress is relaxed rapidly by the sizable creep deformation, which weakens the out-of-plane displacement and then suppresses the accumulation of tensile stress at TC valley and BC peak. Finally, the approximate zero-stress state is observed throughout



**Fig. 12.** Displacements  $u_2$  of TGO-TC interface, after 300 h oxidation at 1100 at 1100 °C, under the combined creep–plastic assumptions of BC with three types of creep rates.



Fig. 13. Evolutions of tensile stresses with oxidation time at (a) TC valley and (b) BC peak locations under the creep and the combined creep-plastic assumptions of TGO.

oxidation as shown in Fig. 8. It means that the creep properties of TGO and BC can significantly affect the interface stress evolution during oxidation. However, the creep properties of TGO and BC are expected to vary for different particle size or ratio of components. For example, the range of reference creep strain rate can span several orders of magnitude due to the variation in particle size or ratio of components [27,28]. In order to reflect the differences in creep rate, three types of creep parameters, listed in Table 5, are adopted. The magnitudes of parameters in Table 5 are kept within the reasonable bounds, although they are not derived from the actual experimental data.

Two different cases are considered:

In the case I, TGO is assumed to exhibit the combined creep–plastic behavior with the three types of creep parameters, while BC is considered to be perfect elasto-plastic material. The evolutions of tensile stress  $\sigma_{22}$ , at TC valley and BC peak, are plotted in Fig. 9.

The displacement  $u_2$  of TGO–TC interface, after 300 h oxidation at 1100 °C, is illustrated in Fig. 10. It's observed that the creep of TGO can suppress the out-of-plane displacement. When TGO manifests slow creep rate, the accumulation of growth stress by oxidation rather than the relaxation of growth stress by creep mainly affects the out-ofplane displacement of TGO, which leads to the increases of tensile stress at TC valley and BC peak. When TGO exhibits medium creep rate, the interface stress evolution is considered as the consequence of competition between the accumulation of growth stress by oxidation and the relaxation of growth stress by creep. As the oxidation rate decreases with oxidation time, the accumulation of growth stress tends to slow down and the relaxation of growth stress by creep effectively suppresses the out-of-plane displacement of TGO. Finally, the tensile stresses, at TC valley and BC peak, increase first and decrease afterwards with oxidation time, as shown in Fig. 9. When TGO shows fast creep rate, the relaxation of growth stress by creep significantly weaken out-of-plane displacement of TGO. The tensile stress states, at TC valley and BC peak, are kept at the very low level throughout oxidation, as shown in Fig. 9.

In the case II, BC is considered to be the combined creep–plastic material, while TGO is the elasto-plastic material. The evolutions of tensile stress  $\sigma_{22}$ , at TC valley and BC peak, are plotted in Fig. 11.

The creep of BC, on one hand, significantly suppresses the accumulation of tensile stress at BC peak, as shown in Fig. 11a. On the other hand, such a creep weakens the deformation resistance of BC and leads to the increase of out-of-plane displacement of TGO (as shown in Fig. 12), so the tension, at TC valley, is enhanced with the rise of creep rate of BC, as shown in Fig. 11b.

When creep rate is slow, the plastic deformation, during oxidation, can affect the stress evolution too. Both the tensile stresses, at TC valley and BC peak, are reduced by the plastic deformation of TGO (as shown in Fig. 13), but only the tensile stress, at BC peak, is decreased by the plastic deformation of BC (as shown in Fig. 14).

#### 3.2. Interface stresses evolution during cooling stage

In this section, the influence of mechanical properties of TGO and BC on interface tensile stress development, on cooling, is explored. Here,



Fig. 14. Evolutions of tensile stresses with oxidation time at (a) TC valley and (b) BC peak locations under the creep and the combined creep-plastic assumptions of BC.



Fig. 15. Contour plots of tensile stress, after 300 h oxidation at 20 °C, under the (a) elastic, (b) creep, (c) perfect elasto-plastic and (d) combined creep-plastic assumptions of TGO and BC.



Fig. 16. Contour plots of equivalence plastic strain, after 300 h oxidation at 20 °C, with different value of pre-factor k.



Fig. 17. Contour plots of tensile stress, after 300 h oxidation at 20 °C, with different value of pre-factor k.

TGO and BC are, respectively, assumed to exhibit elastic, creep, perfect elasto-plastic and combined creep–plastic behaviors. The contour plots of tensile stresses, after 300 h oxidation at 20 °C, are illustrated in Fig. 15.

As shown in Fig. 15, there are no obvious differences in stress distribution between the perfect elasto-plastic and combined creep-plastic assumptions, but the creep and the combined creep-plastic assumptions exhibit significant differences in stress distribution. It suggests that on cooling plastic rather than creep behavior mainly affects stress development.

As the yield strength of TGO rises rapidly from 1 GPa to 10 GPa on cooling, the plastic deformation mainly occurs in BC layer. The influence of BC plastic behavior on stress evolution should be investigated by the variation of yield strength  $k\sigma_{y, BC}$  or  $\sigma_{y, BC}$  is the yield strength of BC, listed in Table 2, and k is a pre-factor.

As shown in Fig. 16, the area of plastic zone, at BC valley, is significantly reduced with the increase of BC yield strength, which enhances the deformation resistance of BC at valley location and suppresses out-of-plane displacement of TGO. As a consequence, the movement of maximum tensile stress along TC–TGO interface takes place, as shown in Fig. 17. The corresponding tensile stresses along TC–TGO interface, after 300 h oxidation at 20 °C with pre-factor k = 0.5/1/2.5, are also illustrated in Fig. 18.

#### 4. Conclusion

In this paper, the combined creep-plastic constitutive relationship is considered to characterize the mechanical properties of TGO and BC. The return-mapping type algorithm is proposed for the solution of combined creep-plastic constitutive model. In addition, the diffusion oxidation-reaction scheme is introduced to describe the TGO growth. Based on these approaches, the numerical simulation is implemented to investigate the influence of mechanical properties of TGO and BC on the interface stress development.

#### 4.1. During oxidation

The creep of TGO can effectively relax the growth stress induced by oxidation and then suppress the out-of-plane displacement of TGO, which leads to the significant reductions of tensile stress in both TC and BC layers. The creep of BC also affects the stress development: on one hand, it suppresses the accumulation of tensile stress in BC layer; on the other hand, it weakens the deformation resistance of BC that leads to the increase of out-of-plane displacement of TGO and the rise of tensile stress in TC layer. In addition, when creep rate is slow, the plastic deformation can affect the stress evolution too, but its influence is insignificant.

#### 4.2. On cooling

The plasticity rather than creep affects the interface stresses evolution. In present simulation, the plastic deformation mainly occurs in BC layer. The out-of-plane displacement of TGO is suppressed with the increase of BC strength, which leads to a movement of maximum tensile stress along TC–TGO interface.



**Fig. 18.** Tensile stress along TC-TGO interface, after 300 h oxidation at 20 °C, with pre-factor k = 0.5/1/2.5.

#### Acknowledgments

This work is supported by the National Basic Research Program of China (No. 2013CB035704) and the National Nature Science Foundation of China (No. 11472206).

#### References

- N.P. Padture, M. Gell, E.H. Jordan, Thermal barrier coatings for gas-turbine engine applications, Science 296 (2002) 280–284.
- [2] V. Viswanathan, G. Dwivedi, S. Sampath, Engineered multilayer thermal barrier coatings for enhanced durability and functional performance, J. Am. Ceram. Soc. 97 (2014) 2770–2778.
- [3] L. Saucedo-Mora, K. Slámečka, U. Thandavamoorthy, T.J. Marrow, Multi-scale modeling of damage development in a thermal barrier coating, Surf. Coat. Technol. 276 (2015) 399–407.
- [4] L. Zhou, S. Mukherjee, K. Huang, Y.W. Park, Y. Sohn, Failure characteristics and mechanisms of EB-PVD TBCs with Pt-modified NiAl bond coats, Mater. Sci. Eng. A 637 (2015) 98–106.
- [5] M.Y. He, J.W. Hutchinson, A.G. Evans, Simulation of stresses and delamination in a plasma-sprayed thermal barrier system upon thermal cycling, Mater. Sci. Eng. A 345 (2003) 172–178.
- [6] J. Rösler, M. Bäker, M. Volgmann, Stress state and failure mechanisms of thermal barrier coatings: role of creep in thermally grown oxide, Acta Mater. 49 (2001) 3659–3670.
- [7] E.P. Busso, Z.Q. Qian, M.P. Taylor, H.E. Evans, The influence of bondcoat and topcoat mechanical properties on stress development in thermal barrier coating systems, Acta Mater. 57 (2009) 2349–2361.
- [8] M. Ranjbar-Far, J. Absi, G. Mariaux, F. Dubois, Simulation of the effect of material properties and interface roughness on the stress distribution in thermal barrier coatings using finite element method, Mater. Des. 31 (2010) 772–781.
- [9] P. Seiler, M. Bäker, J. Rösler, Multi-scale failure mechanisms of thermal barrier coating systems, Comput. Mater. Sci. 80 (2013) 27–34.
- [10] S. Kyaw, A. Jones, T. Hyde, Predicting failure within TBC system: finite element simulation of stress within TBC system as affected by sintering of APS TBC, geometry of substrate and creep of TGO, Eng. Fail. Anal. 27 (2013) 150–164.
- [11] C.V. Di Leo, J. Luk-Cyr, H. Liu, K. Loeffel, K. Al-Athel, L. Anand, A new methodology for characterizing traction-separation relations for interfacial delamination of thermal barrier coatings, Acta Mater. 71 (2014) 306–318.

- [12] A. Cocks, N. Fleck, S. Lampenscherf, A brick model for asperity sintering and creep of APS TBCs, J. Mech. Phys. Solids 63 (2014) 412–431.
- [13] M. Caliez, F. Feyel, S. Kruch, J.L. Chaboche, Oxidation induced stress fields in an EB-PVD thermal barrier coating, Surf. Coat. Technol. 157 (2002) 103–110.
- [14] H.J. Frost, M.F. Ashby, Deformation Mechanism Maps: The Plasticity and Creep of Metals and Ceramics, Pergamon Press Ltd., 1982
   [15] H.E. Evans. Stress effects in high-temperature oxidation of metals. Int. Mater. Rev. 40
- [19] The brans, successing and the perturbed attraction of metals, the water for even of (1995) 1–40.
   [16] E.A. De Souza Neto, D. Peric, D.R.J. Owen, Computational Methods for Plasticity:
- Theory and Applications, John Wiley & Sons, 2008.
- [17] J. Skrzypek, Plasticity and Creep. Theory, Examples and Problems, CRC Press Inc., 1993
- [18] L. Dormieux, D. Kondo, F.J. Ulm, Microporomechanics, John Wiley & Sons, 2006.
- [19] F.J. Ulm, O. Coussy, L. Kefei, C. Larive, Thermo-chemo-mechanics of ASR expansion in concrete structures, J. Eng. Mech. 126 (2000) 233–242.
- [20] H. Hibbitt, B. Karlsson, P. Sorensen, Abaqus User Subroutine Reference Manual Version 6.10, Dassault Systèmes Simulia Corp., 2011
- [21] S. Wei, F. Qun-bo, W. Fu-chi, M. Zhuang, Modeling of micro-crack growth during thermal shock based on microstructural images of thermal barrier coatings, Comput. Mater. Sci. 46 (2009) 600–602.
- [22] P.W. Atkins, J. De Paula, Atkins' Physical Chemistry, Oxford University Press, 2010.
- [23] J. Cheng, E.H. Jordan, B. Barber, M. Gell, Thermal/residual stress in an electron beam physical vapor deposited thermal barrier coating system, Acta Mater. 46 (1998) 5839–5850.
- [24] A.A. Wereszczak, J.G. Hemrick, T.P. Kirkland, J.A. Haynes, T.J. Fitzgerald, J.E. Junkin, Stress relaxation of MCrAlY bond coat alloys as a function of temperature and strain, ASME 1998 International Gas Turbine and Aeroengine Congress and Exhibition, 5, 1998.
- [25] P.N. Quested, R.F. Brooks, L. Chapman, R. Morrell, Y. Youssef, K.C. Mills, Measurement and estimation of thermophysical properties of nickel based superalloys, Mater. Sci. Technol. 25 (2009) 154–162.
- [26] M. Martena, D. Botto, P. Fino, S. Sabbadini, M.M. Gola, C. Badini, Modelling of TBC system failure: stress distribution as a function of TGO thickness and thermal expansion mismatch, Eng. Fail. Anal. 13 (2006) 409–426.
- [27] D. Pan, M.W. Chen, P.K. Wright, K.J. Hemker, Evolution of a diffusion aluminide bond coat for thermal barrier coatings during thermal cycling, Acta Mater. 51 (2003) 2205–2217.
- [28] M.P. Taylor, H.E. Evans, E.P. Busso, Z.Q. Qian, Creep properties of a Pt-aluminide coating, Acta Mater. 54 (2006) 3241–3252.