A physics-based model of temperature-exposure-dependent interfacial fracture toughness of thermal barrier coatings

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Abstract

A physics-based model of temperature-exposure-dependent interfacial fracture toughness of thermal barrier coatings was developed using Arrhenius-type formulæ and experimentally measured interfacial toughness at ambient temperature. The crack delamination occurring at the thermally grown oxide (TGO)/bond coat (BC) interface was assumed in the interfacial fracture toughness evaluation. To evaluate the interfacial toughness at elevated temperatures, the interfacial plastic zone, the interface crack tip opening displacement (ICTOD) and the interface crack density at the thermally grown oxide (TGO)/bond coat interface were specified. The temperature-exposure-dependent Young’s modulus of the topcoat was formulated using the experimentally measured data, and its effect on the interfacial toughness at elevated temperature was investigated. As an application, the proposed interfacial toughness model was then used to study toughness variation versus exposure temperature and time. The trend of interfacial toughness versus temperature and exposure was explained in terms of microstructural changes of topcoat and TGO.

1. Introduction

Thermal barrier coatings (TBCs), with Yttria partially Stabilized Zirconia (YSZ) as topcoat and MCrAlY as bond coat (BC) deposited onto superalloy substrate, have been favourably used as protective coatings for hot section components in advanced gas turbine engines. These high-temperature protective coatings are capable of withstanding high inlet-temperature heat attack, thus increasing engine efficiency and improving the life of the components [1–8].

A general understanding of TBCs failure demonstrates that biaxial compressive stresses are built up on ceramic topcoat/substrate interface during cooling from elevated temperature to ambient due to coefficient of thermal expansion (CTE) mismatch between these two components. The biaxial compressive stresses, however, generate tensile stresses normal to the coating interface due to local non-planar characteristics. The tensile stresses acting on pre-existing flaws and defects promote crack nucleation, propagation and spallation of coatings [9, 10]. Upon the energy release rate of existing interfacial cracks exceeding the interfacial fracture toughness at elevated temperatures and/or during cooling process of the coating, the interfacial cracks then propagate, leading to spallation of the entire TBC system. It was established that failure of TBC systems is largely attributed to the formation and growth of thermally grown oxide (TGO) as large stresses could be generated while TGO thickens upon progressive oxidation of the bond coat [11–20].

Recently much effort has been devoted to measure TBC interfacial fracture toughness at both ambient and elevated temperatures. For instance, Jordan et al [21] carried out a tensile stress–based fracture test using a sandwich-type chevron-notched TBC specimen and obtained TBC interfacial fracture toughness. Yamazaki et al [22] applied a four-point bending interfacial fracture test to measure TBC interfacial fracture toughness exposed at 1273 K. Demarecaux et al [23, 24] estimated TBC interfacial fracture toughness by measuring crack length formed at the tip of the indenter induced by the Vickers indentation test. Evans et al [25, 26] implemented TBC delamination test based on the shear loading formed by indenting the wedge with a tip at 90° angle on the TBC.
surface. In these fracture toughness tests, the mode I type cracks was normally assumed. Xu et al. [27] used three-point bending tests to measure the Young’s modulus of coatings and the complex stress intensity factor of bi-materials interfacial crack. By combining the finite element approach (FEA), the stress field and phase angle in the vicinity of crack were also determined.

Recently, by using the modified four-point bending approach, Zhao et al. [28] studied a single crack growth behaviour of APS-TBC located at the YSZ/NiCrAlY interface. Based on their microstructural model and fracture surface property using scanning electron microscope (SEM), and then combined with FEA, they evaluated the bonding strength and fracture toughness of APS-TBCs at ambient from both analytical solution and numerical simulation. Zhu et al. [29] used a three-point bending test to study the topcoat/bond coat (TC/BC) interfacial cracking behaviour. The displacement and strain fields of the TC/BC cross-section were determined using digital image correlation (DIC) method. The crack length was determined using an inverse FEA based on the crack opening displacement measured by the DIC method. The critical strain energy release rate for crack propagation is determined from a theoretical analysis using compliance methods.

Arai et al. [30] established a mixed-mode interfacial fracture toughness measurement method by using a combination of the compressive and slinging loads enforced to the coating beam, figure 1. They showed that TBC fracture toughness can be measured in a wide range of loading phase angles ahead of the interfacial crack tip. Using this method, they measured the TBC interfacial fracture toughness exposed to high temperatures at 973 K and 1173 K, and examined the influence of high-temperature exposure on interfacial fracture toughness. The measured interfacial fracture toughness is specified in a mode II loading because the TBC spalling damage observed in a gas turbine is normally represented by the mode-II crack nucleation, propagation and spallation.

2. Interfacial fracture toughness of thermal barrier coatings

The interfacial fracture toughness of a TBC system measures the TBC’s resistance to propagation of delamination cracks along the coating interface. As elucidated in Introduction, attempts were made to measure the interfacial fracture toughness using specific approaches at both ambient and elevated temperatures. However, for TBCs used in aero engines, the coating temperature changes periodically during cyclic oxidation process. This temperature change in a coating and its exposure to high temperature results in sintering of the top coat, and leading to the change of Young’s modulus of the topcoat. Consequently it affects the interfacial fracture toughness, failure and life of TBCs. Therefore, a better understanding of temperature-exposure-dependent interfacial toughness of TBCs can help and facilitate failure analysis and life prediction of TBCs. However, only limited effort and results were reported in the literature. In the present paper, a physics-based model of temperature-exposure-dependent interfacial fracture toughness was developed for TBCs based on the measured interfacial toughness.

For a TBC system, delamination and spallation of a coating could occur along the interface, especially near the region where the TGO forms and grows. It is expected that TGO, topcoat and together with bond coat or substrate affect the interfacial fracture toughness. This synergistic effect can be realized and reflected in the developed interfacial toughness model, in that the TGO growth characteristics, the sintering effect of the topcoat and bond coat yield strength all affect the toughness values.

In this paper, the interfacial fracture toughness measured by Arai et al. [30] at 970 K and 1373 K were used to fit parameters in our proposed physics-based interfacial toughness model at elevated temperatures. In Arai et al. paper [30], the ceramics topcoat is conventional 8 wt % YSZ, the CoNiCrAlY as the bond coat and Co-based superalloys as the substrate. The thickness of the bond coat is 100 μm, and 1.0 mm for the topcoat and 1.0 mm for the substrate. To examine the influence of high-temperature on toughness, atmospheric high-temperature exposure tests were performed isothermally at 973 K and 1173 K for 500 h in the maximum. Based on this
designed test procedure, test samples were removed from a furnace at selected exposure time (<500 h) for SEM examination and toughness evaluation. Before processing toughness evaluation on a sample, a pre-crack was created along the bond coat layer by a diamond cutter with a width of 0.1 mm as depicted in figure 1.

It is noticed that a pre-crack generated by using the diamond cutter with a width of 0.1 mm could cut out the whole component comprising both the bond coat (0.1 mm) and the TGO (∼6 μm). It is necessary to point out that TGO scales were already formed during the initial deposition process of TBC as well as during high temperature oxidation process of coatings isothermally. It was known that a number of failure modes could trigger in a TBC system during oxidation process [6]. Therefore, upon loading on a TBC system, the pre-existing cracks could propagate along several delamination paths such as along the TGO/bond coat (BC) interface, the TGO/topcoat (TC) interface, and could propagate inside the TGO scale or within the TC layer, and could also propagate simultaneously along these paths.

Based on this specifically designed pre-crack distributed in the TBC system of figure 1, the energy release rate for this specific mixed-mode crack tip was derived in [30],

\[
G_0 = \frac{1 - \nu_c}{2\mu_c} p^2 K_0 = \frac{1 - \nu_c}{2\mu_c} \left[ p^2 + 12 \left( \frac{Q h}{h^2} \right) + 4\sqrt{3} \cos \gamma \frac{pQ h}{h} \right] \tag{1}
\]

\[
p = \frac{1 - \beta^2}{1 - \alpha}
\]

\[
\xi = \frac{\xi(a - \xi)(2a - \xi)}{2a^2}
\]

where \(\alpha\) and \(\beta\) are the Dundurs parameters, \(P\) and \(Q\) are the unit width compressive load and slinging load, \(\mu\) is the shear modulus of the coating, \(\gamma\) is the specimen material and geometry dependent characteristic angle. The energy release rate \(G_0\) calculated from equation (1) was used as input to fit the proposed interfacial toughness model parameters at elevated temperatures.

It was known that the failure procedure of TBCs is a dynamic process. The failure locations vary depending on the local stress state, the coating toughness, the composition, the sintering and rumpling behaviour of the coating interface. The cracks of TBCs can nucleate within the top coat, within the TGO and could also be nucleated along the TGO/BC interface. These cracks can propagate individually and/or link together and eventually collapse resulting in final spallation of coatings. In the present paper, as an example case, we assume that the crack delamination occurs along the TGO/BC interface.

In evaluation of energy release rate \(G_0\) of equation (1), only the topcoat and substrate properties are involved although the delamination cracks can propagate along the TGO/BC and TGO/TC interfaces. There are extensive researches [6] demonstrating that delamination along the TGO/BC and/or TGO/topcoat interfaces is the most likely failure modes of a TBC system. Therefore, in the present paper, we assumed that the delamination crack in the APS-TBC system propagate along the TGO/BC interface.

3. Temperature-exposure-dependent interfacial fracture toughness model

Under small scale yielding and plane strain scheme, we developed two types of temperature-dependent fracture toughness models [31, 32] for WC-Co composite coatings deposited on steel systems at micromechanical scale in terms of dislocation mobility and crack density formula. In these two fracture toughness models, the cracks observed in WC-Co based composite coatings are the vertical through-thickness cracks normal to the substrate surface. Using the energy release rate for vertical through-thickness cracks in the coating, a temperature-dependent fracture toughness model \(G_d\) was proposed in terms of strain energy release rate \(G_e\) at ambient [32],

\[
G_d = G_m \exp \left( -\frac{G_e}{\frac{\delta}{n}} \right)
\]  \(\frac{\delta}{m}\) \(\frac{kT}{kT}\)  \(\frac{\delta}{m}\)

Where

\[
G_m = mA \mu_c \frac{kT}{\left( \frac{\delta}{m} \right)^2}
\]  \(\frac{\delta}{m}\)
Where $G_c$ can be calculated using,

$$G_c = -\frac{\Delta U}{t} = \sigma^2 t \left( \frac{\sigma}{3E} + \pi F(\Sigma) \right)$$ (6)

The technical details regarding the calculations of equation (6) can be seen in [32].

To study interfacial fracture toughness of a TBC system, the energy release rate of equation (1) will be changed. For TBCs served at high-temperatures, the sintering of topcoat has a significant effect on TBCs failure modes. Consequently it affects the interfacial fracture toughness. Given these factors involved in the evaluation of interfacial toughness, we proposed a physics-based model of interfacial fracture toughness of TBCs at elevated temperatures,

$$G_{int} = \frac{n}{E_{TC}(T)} \left( \frac{kT}{\delta m} \right)^2 A \delta \exp \left( \frac{\delta m}{k_B T} \right)$$ (7)

Where $T$ is the exposure temperature (K), $k_B$ is the Boltzmann constant, $G_0$ is the interface strain energy release rate at ambient calculated using equation (1), $A$ is the plastic zone area at the interface crack tip, $\rho$ is the interface micro-crack density, $\delta$ is the interface crack tip opening displacement (ICTOD), $E_{TC}(T)$ is the temperature-exposure-dependent topcoat Young’s modulus, $n$ and $m$ are two scaling parameters to be fitted to the measured interfacial toughness at ambient using equation (1).

In this physics-based interfacial toughness model (7), three model parameters, i.e. the plastic zone area $A$ at the interface, the interfacial crack density $\rho$ and the interface crack tip opening displacement $\delta$ need to be specified in their forms. Although these three model parameters ($A$, $\rho$ and $\delta$) were specified for vertical through-thickness cracks in WC-based coatings [32]. For the interfacial cracks in TBCs, these model parameters have difference forms and need re-built. It is necessary to point out that there is no unique approach to specify these three model parameters. Therefore, physics-based method, empirical and semi-empirical formulae are normally applied.

3.1. Plastic zone size $A$ of the interfacial crack
A circled shape plastic zone area $A$ at the interface crack tip was assumed and used as an approximation,

$$A = \pi R_0^2$$ (8)

where $R_0$ is the radius of the circled shape plastic zone. For the mixed-mode toughness at the interface, the stress intensity factor $K_0$, derived by Tvergaard and Hutchinson [33], upon considering the TGO, bond coat contributions, is approximated as,

$$K_0 = \left( \frac{1 - v_{TGO}^2}{E_{TGO}} + \frac{1 - v_{BC}^2}{E_{BC}} \right) \frac{1}{2} \sqrt{ \frac{2G_0}{1 - \beta^2}}$$ (9)

The plastic zone radius $R_0$ associated with this $K_0$ can be represented as,

$$R_0 = \frac{1}{3\pi} \left( \frac{K_0}{\sigma_Y} \right)^2 = \frac{2}{3\pi} \left( \frac{1 - v_{TGO}^2}{E_{TGO}} + \frac{1 - v_{BC}^2}{E_{BC}} + \frac{1 - v_{TGO}^2}{E_{BC}} \right)^{-1} \left( \frac{1 - \beta^2}{\sigma_Y^2} \right)$$ (10)

Where $\sigma_Y$ is the yield stress of the bond coat, $\beta$ is the second Dundurs’ parameter and is expressed as,

$$\beta = \frac{1}{2} \frac{\mu_{TGO}(1 - 2v_{BC}) - \mu_{BC}(1 - 2v_{TGO})}{\mu_{TGO}(1 - v_{BC}) + \mu_{BC}(1 - v_{TGO})}$$ (11)

where

$$\mu_{TGO} = \frac{E_{TGO}}{2(1 + v_{TGO})}$$ (12)

$$\mu_{BC} = \frac{E_{BC}}{2(1 + v_{BC})}$$ (13)

It is noticed that the evaluation of plastic zone $A$ at the interface not only involves the contribution of TGO elastic properties but also includes the BC properties as well.

3.2. Interfacial crack tip opening displacement (ICTOD)
Like the interface fracture toughness $K_{IC}$, the interfacial crack tip opening displacement (ICTOD) also kindly describes fracture toughness of materials [6]. For the interface comprising two different materials, Yi et al [34] used Dugdale mixed-mode model to study the interface ICTOD by using the continuously distributed edge
dislocation approach, where interface cracks between two semi-infinite materials are described by dislocations. Yi et al. [34] derived analytically an expression of a reference CTOD $\delta_{\text{ref}}$ for homogeneous material associated with its yield stress $\sigma_{\text{YS}}$, Young’s modulus $E_1$, crack length $L$ and external load $\sigma_0$,

$$\delta_{\text{ref}} = \frac{\pi \sigma_0^2 L}{6 \sigma_{\text{YS}} E_1} \left( 1 + \frac{\pi \sigma_0}{2 \sigma_{\text{YS}}} \right)^2$$  \hspace{1cm} (14)

By varying Young’s moduli of two materials, Yi et al derived numerically a formula for ICTOD $\delta_{\text{int}}$ for the interface crack associated with the reference $\delta_{\text{ref}}$ using Young’s moduli of $E_1$ and $E_2$,

$$\delta_{\text{int}} = \delta_{\text{ref}} \left[ 0.42 + 0.58 \left( \frac{E_2}{E_1} \right)^{0.86} \right]$$  \hspace{1cm} (15)

Equation (15) was used in the present paper to calculate the ICTOD at the TGO/BC interface.

### 3.3. Interface crack density

An interface crack density is defined as the number of cracks per unit area distributed at the interface. To the authors’ knowledge, there exists no analytical formula to evaluate the interface crack density versus exposure time at elevated temperatures. Therefore, experimental measurements of the interfacial cracks using SEM approach are essential to help derive empirically an expression for the interface crack density in TBC systems. It is necessary to point out that although the measured interface crack density was for MCrAlY based bond coat, we assumed that the formula derived from MCrAlY alloy can be used for other bond coat alloy such as for CoNiCrAlY alloy, where the interfacial toughness and sintered Young’s modulus were measured and used for establishing temperature-exposure dependent toughness model.

Beck et al. [35] measured the interface crack density between the TGO and BC (MCrAlY) interface in APS-TBC system tested during isothermal oxidation process depicted in figure 2 illustrating the crack density versus exposure time at 1050 °C. Figure 2 also shows the measured TGO growth thickness versus exposure time.

By comparing the trend of interfacial crack density with the TGO grown thickness versus exposure time in figure 2, we proposed a formula that correlates the number $N$ of cracks with the TGO thickness $d_{\text{TGO}}$,

$$N = \left\{ \begin{array}{l} \frac{d_{\text{TGO}}}{\tau_s} + b_1, \\
\chi \\
C \end{array} \right. \hspace{1cm} (16)$$

Where $N$ is the total number of cracks, $d_{\text{TGO}}$ is the TGO thickness, $\chi$ is related to crack nucleation coefficient, $b_1$ represents the cracks formed before thermal exposure or during coating fabricating and/or spraying processes, but it is assumed to be zero here for simplicity. $C$ is the crack number when the specimen tends to stay at steady state and cracks stop nucleating, $\tau_s$ represents the effective shear yield stress and is represented by,

$$\tau_s = \left( \frac{1 - v_{\text{BC}}}{\tau_{\text{BC}}} \right)^{-1} = \frac{\tau_{\text{BC}}}{1 - v_{\text{BC}}}$$  \hspace{1cm} (18)
The TGO grows follows \[35\],

\[d_{TGO} = k(t_{\text{max}})^n\]

Where \(t_{\text{max}}\) is the exposure time under the maximum exposure temperature \(T_{\text{max}}\), \(k\) and \(n_0\) are both oxidation coefficients fitted to the measured TGO thickness versus exposure time. Since the interface crack density represents the number of cracks per unit interface area, we proposed that the interface crack density follows,

\[\rho = \begin{cases} 
\varsigma (t_{\text{max}})^n \left( \frac{1 - v_{\text{BC}}}{\tau_{\text{BC}}} \right) & 100 > t \geq 0 \\
C_i & t \geq 100
\end{cases}\]

Where \(\varsigma\) is also a crack nucleation coefficient. The growth exponent coefficient \(n_0\) of the TGO is taken as 0.25 [35]. In summary, although our failure mode only involves the delamination at the TGO/BC interface, in an evaluation of \(\rho\), the properties of TGO, BC and TC are all involved.

3.4. The effect of the top coat sintering on Young’s modulus of top coat

During high temperature exposure of TBC systems (\(\sim 1000 \degree C\)), the ceramic YSZ topcoat experiences significant sintering, leading to an increase of topcoat Young’s modulus \(E\). This increase in Young’s modulus affects considerably fracture toughness, failure behavior and the life of TBCs. Arai \textit{et al} [30] evaluate experimentally the change of Young’s moduli \(E\) due to the top coat sintering at both 973 K and 1073 K, and obtained curves of Young’s moduli \(E\) versus exposure time depicted in figure 3. It is observed that \(E\) initially drops within the first 100 h exposure, and then increases gradually. The trend of \(E\) at these two exposure periods can be described by empirical formulae. Within the first 100 h exposure period, the decreasing Young’s modulus \(E_{\text{TC}}\) of ceramic topcoat can be fitted to an exponential expression versus exposure time,

\[E = a \exp(-bt)\]

Where \(t\) is exposure time. The two fitting parameters \(a\) and \(b\) will be fitted to the measured Young’s modulus in figure 3. After 100 h exposure, the measured \(E\) increases, and the curve can be well described by an existing formula [36],

\[E_{\text{BBC}}(t) = \frac{\omega E_{\text{BBC}}^0 E_{\text{TC}}^\infty}{\omega E_{\text{BBC}}^0 + E_{\text{TC}}^\infty - E_{\text{TC}}^0}\]

Where the Young’s modulus \(E_{\text{BBC}}^0\) and \(E_{\text{TC}}^\infty\) represent the starting and the bulk moduli, and in this paper, they are taken as the specimen’s Young’s modulus at 100 h and 500 h under thermal exposure, respectively. \(\omega\) is given by,

\[\omega = 1 + A_{\text{sin}} \exp\left(\frac{E_{\text{sin}} t}{k_B T}\right)^{n_{\text{sin}}}\]

Where \(t\) is thermal exposure time, \(A_{\text{sin}}, E_{\text{sin}}, n_{\text{sin}}\) are the sintering kinetics parameters. The values of \(a, b, A_{\text{sin}}, E_{\text{sin}}\) and \(n_{\text{sin}}\) were fitted to the test data of Arai \textit{et al} [30] and then results are listed in table 1.
Table 1. The used parameters in interfacial fracture model.

| Parameters | 973 K   | 1173 K  |
|------------|---------|---------|
| a          | 0.0231  | 0.0230  |
| b          | 0.00243 | 0.00195 |
| $A_{\text{min}}$ | $2.67 \times 10^{-15} \text{ s}^n$ | $6.17 \times 10^{-13} \text{ s}^n$ |
| $E_{\text{int}}$ | 0.24 eV | 2.58 eV |
| $n_{\text{min}}$ | 6.45   | 8.46    |
| $E_{\text{TGO}}^0$ | 32.46 MPa [30] | 35.1 MPa [30] |
| $E_{\text{TBC}}^0$ | 52.76 MPa [30] | 60.1 MPa [30] |

Table 2. The model parameters used in interfacial fracture toughness evaluations.

| Parameter name                                      | Parameter symbol | Value under 973 K | Value under 1173 K |
|----------------------------------------------------|------------------|-------------------|--------------------|
| Young’s modulus of TGO                              | $E_{\text{TGO}}$ | 375 GPa [6]       |                    |
| Young’s modulus of bond coat                         | $E_s$            | 200 GPa [6]       |                    |
| Poisson’s ratio of top coat                          | $v_{\text{ts}}$  | 0.20 [6]          |                    |
| Poisson’s ratio of TGO                               | $v_{\text{TGO}}$ | 0.25 [11]         |                    |
| Poisson’s ratio of bond coat                         | $v_{\text{bs}}$  | 0.3 [11]          |                    |
| First scale-linking parameter                       | $m$              | 4388              |                    |
| Second scale-linking parameter                      | $n$              | $9.5 \times 10^{15}$ | $1.5 \times 10^{14}$ |
| Shear yield stress of bond coat                      | $\tau_{\text{ys}}$ | 460 MPa [6]      |                    |
| Yield stress of bond coat                            | $\sigma_y$       | 800 MPa [6]       |                    |
| Strain energy release rate at room temperature       | $G_0$            | 38 /m² [30]       |                    |
| Pre-crack length                                    | $L$              | 17.88 mm [30]     |                    |
| Applied mode II load                                | $\sigma_p$       | 64,719 MPa [40]   |                    |
| Plastic zone size                                   | $A$              | $9.91 \times 10^{-12}$ m² | |
| Crack tip opening displacement                       | $\delta_{\text{int}}$ | 1.11 \times 10^{-6} m | |

3.5. Determination of two-scaling parameters $n$, $m$

The parameter $n$ in equation (7) is a temperature-dependent scaling variable. It links the energy release rate $G_0$ of the crack tip of equation (1) at ambient to the micromechanical scale to those by dislocation motion of atoms at the atomic-scale. The main function of this parameter $n$ is to ensure that the energy release rate calculated from equation (7) matches the value of $G_0$ at ambient, whereupon $n$ is obtained by fitting to the test data from Arai et al [30].

Another model parameter $m$ links the ICTOD $\delta$ with Burgers vector $b$ of dislocations appearing along the interface consisting of TGO (Al₂O₃) and CoNiCrAlY bond coat by,

$$mb = \delta$$  \hspace{1cm} (24)

As the bond coat alloy comprises multi-phases, it is impossible to define a specific Burgers vector for CoNiCrAlY bond coat alloys. Instead, a Burgers vector of Co-base alloys was used as an approximation. FCC Co–Co phase, it consists of both screw and edge dislocations under indentation loading. The Burgers vector of 1/2[110] on the slip plane {111} could point to either edge dislocation or screw dislocation [37], and one of its partial dislocations, the Burgers vector of 1/6[112], which corresponds to the edge dislocation [38]. Therefore, the Burgers vector for CoNiAlY is approximated as 2.379 Å [37] and for Al₂O₃ at [39] direction as 2.7125 Å. The average interfacial Burgers $b$ can be calculated from these two Burgers vectors of Al₂O₃ (TGO) and CoNiCrAlY bond coat phases. Accordingly, the interfacial ICTOD $\delta$ is calculated as 1.1177 μm. Thus the parameter $m$ is determined as 4388 using equation (24).

3.6. Results and discussions

Table 2 lists elastic properties of TGO, bond coat and topcoat used in interfacial toughness evaluations using equation (7). Table 2 also lists the loading $\sigma_p$, the geometry size $L$ of mixed-mode testing system of figure 1 used in energy release rate calculation of equation (1) at ambient. The calculated three model parameters of plastic zone size $A$, ICTOD $\delta_{\text{int}}$ and the strain energy release rate $G_0$ are also listed at ambient in table 2.

Figure 3 illustrates the sintered Young’s moduli of topcoat exposed at 1173 K and 973 K respectively. The figure also shows the fitted Young’s moduli using equations (21) and (22) in two exposure periods. In the exposure period before 100 h, the equation (21) was applied, while after 100 h, the equation (22) was used. The two different trends of Young’s moduli due to sintering changes topcoat mechanical properties, and thus affect the interfacial fracture toughness accordingly.
Figure 4 shows the measured interfacial toughness along with the prediction using the proposed toughness model (7) at 1173 K versus the exposure time. It is observed that the proposed model well describes the measured toughness in both prior to 100 h and also beyond 100 h. Comparing figures 3 and 4 regarding the sintered Young’s moduli and measured toughness, it is evident that the interfacial toughness follows an opposed trend of the Young’s moduli versus exposure time.

Figure 5 shows the measured interfacial toughness along with the prediction using the toughness model (7) at 973 K. It is observed that the proposed model well describes the measured toughness before the exposure 100 h. However, the toughness model (7) illustrates some discrepancy after 200 h exposure, particularly around the toughness exposed at 500 h. It is not yet clear if this discrepancy origins from the measured results or it is due to the proposed model, because there are no measured toughness available around 500 h as a further validation. It may indicate that the failure mode at 973 K may differ from that at 1173 K, as a result, further research is needed to explore the interfacial toughness models at this temperature.

Arial et al [30] provided a possible explanation on what they observed regarding the interfacial toughness depicted in figures 4 and 5. They suggested that for interfacial toughness tested at 1173 K, a high-temperature exposure process could result in stronger cohesion of YSZ topcoat splat boundaries and interface. However, at 973 K, the exposure temperature is not high enough to enhance the interface cohesion, and this could lead to a considerable drop in toughness values [30].

Using the proposed interfacial toughness model of equation (7), figure 6 shows the predictions of interfacial toughness versus exposure temperature at specific exposed hours. It was found that for the toughness examined at the 100-exposure hour at different temperatures, the toughness values will increase versus temperature, and this calculated toughness illustrates the maximum values compared with other toughness examined at 50, 200
and 500 h. This trend can be understood by comparing figures 4 and 5. It is noticed that although the toughness increases versus exposure temperature, the toughness exposed at 500 h reaches the minimum. The reason for this result indicates that after 100 h thermal exposure, the material could turn soft, and the sintering effect is still relatively weak, thus the corresponding low topcoat Young’s modulus results in large interfacial fracture toughness.

In addition, it shows that the scale parameter $n$ illustrates a temperature-dependent characteristics upon fitting to two measured toughness data, and a linearized relationship for $n$ versus exposure temperature $T$ is obtained,

$$n(T) = 2.83 \times 10^{11} \cdot T - 1.8 \times 10^{14}$$  \hspace{1cm} (25)$$

It indicates that a non-linearized scaling parameter $n$ versus exposure temperature could result if there are tested toughness available at two more different temperatures. The scale parameter $m$, linking Burges vector $b$ and ICTOD $\delta$, is considered as a constant. Its value equals to 4388 by fitting to the averaged Burgers vectors of TGO and CoNiCrAlY bond coat alloy. This fitted parameter $m$ was used to predict the interfacial toughness at selected temperatures shown in figure 6.

It is necessary to point out that the interfacial toughness formula (7) we proposed is used to model the experimentally measured apparent fracture toughness, figures 4 and 5. To model the intrinsic interfacial fracture toughness (figure 12 of [30]), we need to develop a residual stress model of TBC shown in figure 9 of [30]. Such stress model should show the following behaviour: (1) the residual stress varies as a function of both temperature and exposure time, (2) the stress model illustrates tensile stress state at the early exposure period and then shows a compressive stress state beyond a certain exposure period (100 h). Therefore, a further study is needed to build up such residual stress model in order to investigate the intrinsic interfacial fracture toughness of APS-TBCs.

4. Conclusions

A physics-based interfacial fracture toughness model of TBC systems was developed. The temperature-exposure-dependent effect was described by using Arrhenius-type equation, and the toughness model parameters were fitted to the experimentally measured toughness at ambient. In this proposed model, the existing interfacial plastic zone size and the interface crack tip opening displacement (ICTOD) were used. The crack delamination occurring at the thermally grown oxide (TGO)/bond coat (BC) interface was assumed in the interfacial fracture toughness evaluation. The interface crack density measured at the TGO/BC interface was employed to specify an empirical crack density formula that correlates the TGO thickness, the yield stress of the bond coat and exposure time. The effect of Young’s moduli due to the top coat sintering on interfacial toughness was investigated. Increasing the topcoat Young’s moduli due to sintering was found to decreases the toughness. The discrepancy that the proposed toughness model shows compared with the measured toughness values at 973 K could result from the failure modes involved upon evaluating the interfacial toughness, and therefore further investigation is needed to clarify such toughness-temperature-exposure correlation.
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