Effects of interfacial thermal resistance on surface cracking in a coating layer bonded to a substrate

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Abstract

It is known that thermal resistance exists at interfaces in bonded dissimilar materials due to imperfect mechanical and chemical bonding as well as phonon scattering at the interface. This thermal resistance influences the temperature distribution as well as thermal stresses in the bonded material. The purpose of this work is to explore the effect of interfacial thermal resistance on thermal fracture behavior of bonded materials. In particular, we consider an edge crack in the coating layer that is bonded to a substrate. The thermal stress intensity factor for the edge crack considering the thermal resistance at the coating-substrate interface is calculated using an integral transform/integral equation method. The numerical results for an Al$_2$O$_3$ coating on a Si$_3$N$_4$ substrate show that the thermal stress field deviates from that for the coating/substrate system without considering interfacial thermal resistance. The thermal stress intensity factor is increased by the interfacial thermal resistance, which indicates that the thermal shock resistance of the coating/substrate system can be degraded by the presence of thermal resistance at the interface between the coating and substrate.

Key words: Interfacial thermal resistance, Coating, Thermal stress, Thermal stress intensity factor, Thermal shock

1. Introduction

In bonded and composite materials, gaps may develop at the interface between the constituent materials by imperfect mechanical and chemical bonding as well as by thermal expansion mismatch between the constituent materials (Powell et al., 1980). These gaps degrade thermal conductance because the gas trapped in the gap has much lower thermal conductivity than that of the solid constituents. Moreover, phonon scattering at interfaces between dissimilar nanostructured materials also creates a thermal barrier (Hida et al., 2013). The existence of interfacial thermal resistance has a significant impact on the transport properties of bonded materials and heat transfer in the materials. In fact, the effective thermal conductivity of composites is reduced by the thermal resistance at the interfaces between the constituents (Hasselman and Johnson, 1987; Nan et al., 1997).

Most studies on thermal stresses in bonded and composite materials assume perfect thermal contact at the interfaces between the constituents, i.e., both temperature and heat flux are continuous across the interface. While heat flux remains continuous at interfaces with thermal resistance, the temperature undergoes a discontinuity jump across the interface (Hasselman and Johnson, 1987). Although interfacial thermal resistance may play a significant role in understanding thermal stress and fracture in bonded materials, few efforts have been found to address this issue to the best knowledge of the authors although there were some studies that examined the effects of thermal contact resistance on thermal stresses in layered structures that are in contact. Blandford and Tauchert (1985) calculated thermal stresses in a layered structure with interfacial thermal contact resistance using a finite element method. Gundappa et al. (1985, 1987) analyzed the effects of thermal contact resistance on thermal stresses in both flat plate and solid circular cylinder structures. Yang et al. (2008) computed the thermal stress in a gun barrel with interlayer thermal contact resistance.

The present work aims to examine the effect of interfacial thermal resistance on thermal fracture behavior of bonded materials. In particular, we consider edge cracking in a coating layer that is bonded to a substrate. The coating/substrate system is subjected to quenching on the coating surface. Heat conduction thus occurs in the crack direction that is perpendicular to the coating/substrate interface at which thermal resistance exists. In the remainder of the paper, the temperature distribution in the coating/substrate system with interfacial thermal resistance is revisited first. Next, equations for calculating the thermal stress and thermal stress intensity factor are derived. Finally, numerical examples are presented for an Al₂O₃ coating/Si₃N₄ substrate system to examine the effects of interfacial thermal resistance on the temperature, thermal stress and thermal stress intensity factor.

2. Temperature field

Consider a thin coating bonded to a substrate as shown in Fig. 1. The material is initially at a constant temperature $T_0$, and its surfaces $x = 0$ and $x = b$ are suddenly cooled to temperatures $T_a$ and $T_b$, respectively. Denote by $T_1(x, t)$ and $T_2(x, t)$ the temperature distributions in the coating and substrate, respectively. $T_1(x, t)$ and $T_2(x, t)$ satisfy the following basic heat conduction equations:

$$\frac{\partial T_1}{\partial t} = \kappa_1 \frac{\partial^2 T_1}{\partial x^2} = 0, \quad 0 < x < h, \ t > 0$$

$$\frac{\partial T_2}{\partial t} = \kappa_2 \frac{\partial^2 T_2}{\partial x^2} = 0, \quad h < x < b, \ t > 0$$

where $h$ is the thickness of the coating layer, $b$ the thickness of the coating/substrate system, and $\kappa_1$ and $\kappa_2$ the thermal diffusivities given by

$$\kappa_1 = k_1/(\rho_1c_1), \quad \kappa_2 = k_2/(\rho_2c_2)$$

in which $k$ is the thermal conductivity, $\rho$ the density, $c$ the specific heat, and subscripts 1 and 2 denote the properties of coating and substrate, respectively.

The initial and boundary conditions of the heat conduction problem of the bonded system are

$$T_1(x, t)\mid_{x=0} = T_0, \quad 0 \leq x \leq h, \quad T_2(x, t)\mid_{x=0} = T_0, \quad h \leq x \leq b$$

$$T_1(x, t)\mid_{x=b} = T_a, \quad T_2(x, t)\mid_{x=b} = T_b, \quad t > 0$$
The conditions at the coating/substrate interface are

\[ \begin{align*}
    k_1 \frac{\partial T_1(x,t)}{\partial x} \bigg|_{x=h} &= k_2 \frac{\partial T_2(x,t)}{\partial x} \bigg|_{x=h} \\
    T_1(x,t) \bigg|_{x=h} - T_2(x,t) \bigg|_{x=h} &= -Rk_1 \frac{\partial T_1(x,t)}{\partial x} \bigg|_{x=h}
\end{align*} \]  

(5a) (5b)

where \( R \) is the so-called interfacial thermal resistance. For perfect thermal contact, \( R = 0 \) and Eq. (5b) reduces to the temperature continuity condition at the interface.

Following Ozisik (1968), the general solutions of the heat conduction problem (1) – (5) can be expressed as follows

\[ T_1(x,t) = T_1^{ss}(x) + \sum_{n=1}^{\infty} A_n \sin (\beta_{1n} x) e^{-\kappa_n t}, \quad 0 \leq x < h, \]

(6a)

\[ T_2(x,t) = T_2^{ss}(x) + \sum_{n=1}^{\infty} A_n C_{2n} \left[ \sin (\beta_{2n} x) - \tan (\beta_{2n} b) \cos (\beta_{2n} x) \right] e^{-\kappa_n t}, \quad h < x \leq b, \]

(6b)

where \( T_1^{ss}(x) \) and \( T_2^{ss}(x) \) represent the steady state solutions given by

\[ T_1^{ss}(x) = T_a - \frac{(T_a - T_b)}{h + R k_1 + (b-h) (k_1 / k_2)} x, \quad 0 \leq x < h, \]

(7a)

\[ T_2^{ss}(x) = T_b + \frac{(T_a - T_b) (k_1 / k_2)}{h + R k_1 + (b-h) (k_1 / k_2)} (b-x), \quad h < x \leq b, \]

(7b)

the constants \( C_{2n} (n = 1, 2, \ldots) \) are

\[ C_{2n} = k_1 \frac{\cos (\beta_{1n} h) \cos (\beta_{2n} b)}{\cos (\beta_{2n} (b-h)) \sqrt{k_1 / k_2}}, \quad n = 1, 2, \ldots \]

(8)

and the eigenvalues \( \beta_{1n} \) and \( \beta_{2n} (n = 1, 2, \ldots) \) satisfy the following characteristic equations

\[ R k_1 (k_1 / k_2) \sqrt{k_1 / k_2} \tan (\beta_{2n} (b-h)) + \tan (\beta_{1n} h) = 0, \quad n = 1, 2, \ldots, \]

(9)

Finally, the constants \( A_n (n = 1, 2, \ldots) \) in Eq. (6) is given by

\[ A_n = \frac{2(T_a - T_b) (1 - \cos (\beta_{1n} h)) + 2(T_b - T_a) \cos (\beta_{1n} h) + 2(T_a - T_b) \cos (\beta_{2n} h) - 1}{(T_a - T_b) \cos (\beta_{2n} (b-h))}, \quad n = 1, 2, \ldots, \]

(10)

We note that there were some typographical errors in the solution in Ozisik (1968) as it does not reduce to the solution for perfect thermal contact in Carslaw and Jaeger (1959) when \( R \to 0 \).

3. Thermal stress in the coating/substrate free of cracks

We use a standard superposition method to solve the thermal crack problem. In the first problem, the thermal stress solution in the coating/substrate system free of cracks is obtained. Next, the crack problem is solved with the crack face tractions equal to the normal and shear stresses in the first problem with opposite signs. The thermal stress intensity factor is finally obtained from this second solution as no stress singularity exists in the first solution. This section presents the thermal stresses in the first problem, i.e., thermal stresses in the coating/substrate system free of cracks.

We assume plain strain deformations in the \( xy \)-plane of the coating/substrate system as shown in Fig. 1. Under the thermal shock conditions described by Eqs. (3) and (4), both shear stress and normal stress in the \( x \)-direction are zero. The thermal stress \( \sigma_{yy}^T \) used in the crack problem has the following general form

\[ \sigma_{yy}^T(x,t) = \frac{E \alpha (T - T_0)}{1 - \nu} + \frac{E}{(1 - \nu^2) A_0} \int_0^b \left[ (A_{12} - \nu A_{11}) \frac{k_1}{k_2} \right] (A_{12} - \nu A_{11}) \frac{E \alpha (T - T_0)}{1 - \nu} x dx \]

(11)

where \( E \) is Young’s modulus, \( \nu \) Poisson’s ratio, \( \alpha \) the coefficient of thermal expansion (CTE), and \( A_{ij} (i, j = 1, 2) \) and \( A_0 \)
given by

\[ A_{11} = \frac{E}{1 - \nu^2} \int_0^b dx, \quad A_{12} = A_{21} = \frac{Ex}{1 - \nu^2} dx, \]
\[ A_{22} = \frac{Ex^2}{1 - \nu^2} dx, \quad A_0 = A_1 A_{22} - A_{12} A_{21} \]

The thermal stress in the coating/substrate system can be further written as

\[ \frac{1 - \nu}{E_i \alpha_i} \sigma_{yy}^r(x, t) = T_0 - T_1 \]
\[ + \frac{4 \tilde{A}_{12} - 6(x/b) \tilde{A}_{11}}{A_i b} \left[ \int_0^b (T_1 - T_0) dx + \delta_x \delta_y \frac{b}{A_i} (T_2 - T_0) dx \right] \]
\[ - \frac{6 \tilde{A}_{12} - 12(x/b) \tilde{A}_{11}}{A_i b^2} \left[ \int_0^b (T_1 - T_0) dx + \delta_x \delta_y \frac{b}{A_i} (T_2 - T_0) dx \right], \quad 0 \leq x < h \]
\[ + \frac{1 - \nu}{E_i \alpha_i} \sigma_{yy}^r (x, t) = \delta_x \delta_y (T_0 - T_2) \]
\[ + \frac{4 \tilde{A}_{22} - 6(x/b) \tilde{A}_{21}}{A_i b} \left[ \int_0^b (T_1 - T_0) dx + \delta_x \delta_y \frac{b}{A_i} (T_2 - T_0) dx \right] \]
\[ - \frac{6 \tilde{A}_{22} - 12(x/b) \tilde{A}_{21}}{A_i b^2} \left[ \int_0^b (T_1 - T_0) dx + \delta_x \delta_y \frac{b}{A_i} (T_2 - T_0) dx \right], \quad h < x \leq b \]

where \( \delta_x \) and \( \delta_y \) are

\[ \delta_x = \frac{E_2}{E_1} \frac{1 - \nu_2^2}{1 - \nu_1^2}, \quad \delta_y = \frac{1 + \nu_2}{1 + \nu_1} \alpha_i \]

and \( \tilde{A}_{ij} \) \( (i, j = 1, 2) \) and \( \tilde{A}_0 \) are given by

\[ \tilde{A}_{11} = \delta_x + (1 - \delta_x) (h/b), \quad \tilde{A}_{12} = \tilde{A}_{21} = \delta_x + (1 - \delta_x) (h/b)^2, \]
\[ \tilde{A}_{22} = \delta_x + (1 - \delta_x) (h/b)^3, \quad \tilde{A}_0 = 4 \tilde{A}_{11} \tilde{A}_{22} - 3 \tilde{A}_{12} \tilde{A}_{21} \]

4. Thermal stress intensity factor

In this work, we focus on the effect of thermal resistance at the coating/substrate interface on thermally induced cracking in the coating layer. We thus assume that the coating and substrate have the same elastic modulus and Poisson’s ratio so that the standard inverse square root stress singularity still exists for a crack terminating at the coating/substrate interface and the effect of interfacial thermal resistance can be quantified by the stress intensity factor as a finite \( K \)-dominance zone exists near the crack tip. We use an integral transform/integral equation technique to solve the thermal crack problem of the coating/substrate system. The final singular integral equation has the following form

\[ \int_{-1}^{1} \left[ \frac{1}{r - r'} + K(r, r') \right] \psi(r', t) dr' = \frac{2 \pi (1 - \nu_i^2)}{E_i} \sigma_{yy}^r (r, t), \quad -1 \leq r \leq 1 \]

where \( K(r, s) \) is a known kernel, \( r = 2x/a - 1 \), \( a \) the crack length, \( \psi \) a continuous function related to the displacement discontinuity along the crack surface

\[ \psi(r, t) = \sqrt{1 - r^2} \varphi(r, t), \quad \varphi = \frac{\partial \psi(x, 0^+) - \partial \psi(x, 0^-)}{\partial x} \]

in which \( \psi(x, y) \) is the displacement in the \( y \)-direction.

Once the solution of the above integral equation is obtained, the nondimensional thermal stress intensity factor (TSIF), \( K^* \), at the edge crack tip can be computed from
\[
K^* = \frac{(1-\nu_1)K_1}{E_1\alpha_1(T_0 - T_a)\sqrt{\pi b}} = -\frac{1}{2} \sqrt{\frac{a}{b}} \psi(1, t)
\]

where \(K_1\) denotes the TSIF.

5. Numerical results and discussion

In this section we present numerical results for an Al\textsubscript{2}O\textsubscript{3} coating/Si\textsubscript{3}N\textsubscript{4} substrate system to examine the effects of interfacial thermal stress on the thermal stress and thermal stress intensity factor (TSIF). Al\textsubscript{2}O\textsubscript{3} and Si\textsubscript{3}N\textsubscript{4} are advanced ceramics in a number of applications including cutting tools. Si\textsubscript{3}N\textsubscript{4} has good high temperature deformation resistance and Al\textsubscript{2}O\textsubscript{3} coating layer can minimize chemical reactions of Si\textsubscript{3}N\textsubscript{4} with steels (Komanduri, 1994). Because the elastic moduli of Al\textsubscript{2}O\textsubscript{3} and Si\textsubscript{3}N\textsubscript{4} are similar and Poisson’s ratio plays a minor role in thermal fracture, it can be assumed that the coating/substrate system has constant modulus and Poisson’s ratio. Thus the normalized thermal stress and TSIF will become independent of Young’s modulus and Poisson’s ratio. The thermal properties of the two ceramics are as follows: \(k_1 = 20\) W/(m-K), \(\rho_1 = 3.8\) g/cm\(^3\), \(c_1 = 0.9\) J/(g-K), \(\alpha_1 = 8 \times 10^{-6} /\)K for Al\textsubscript{2}O\textsubscript{3}, and \(k_2 = 35\) W/(m-K), \(\rho_2 = 3.2\) g/cm\(^3\), \(c_2 = 0.7\) J/(g-K), \(\alpha_2 = 3 \times 10^{-6} /\)K for Si\textsubscript{3}N\textsubscript{4}. In the numerical calculations, we only consider the quenching case of \(T_b = T_0\), which means that only the coating surface \(x = 0\) is subjected to quenching. Moreover, the thickness of Al\textsubscript{2}O\textsubscript{3} coating is chosen as \(h/b = 0.1\).

Figure 2a shows the normalized temperature variation, \((T - T_a)/(T_0 - T_a)\), in the coating/substrate at a nondimensional time of \(\tilde{t} = \kappa_1 t/b^2 = 0.01\). The nondimensional interfacial thermal resistance is chosen as \(R^* = R k_1/b = 0.2\) which corresponds to a dimensional value of \(R = 5 \times 10^{-5}\) m\(^2\)K/W for \(b = 0.5\) cm. Here we assume that the thermal resistance is constant following Hasselman and Johnson (1987) and Nan et al. (1997). The temperature for perfect thermal contact \((R^* = 0)\) is also included. The normalized temperature varies from zero at the substrate boundary \((x/b = 1)\) to -1 at the coating surface \((x = 0)\). For the case of nonzero interfacial thermal resistance, the temperature undergoes a discontinuity jump at the interface between the coating and substrate. The temperature is higher than that for the perfect thermal contact case in the substrate, and becomes lower in the coating layer. Fig. 2b shows the steady state temperature field. In the steady state case, the temperature distribution is linear in both substrate and coating layers.

Figure 3 shows the normalized thermal stress \(\sigma_{yy}\) (normalized by \(E_1\alpha_1(T_0 - T_a)/(1-\nu_1)\)) in the coating/substrate at a nondimensional time of \(\tilde{t} = 0.01\). Again, we consider both cases of \(R^* = 0\) and \(R^* = 0.2\). Tensile stress prevails in the coating layer and near the outer boundary of the substrate, and compressive stress develops in the substrate adjacent to the interface. The thermal stress undergoes a discontinuity at the interface even for the perfect thermal contact case because of thermal expansion mismatch. This stress discontinuity is intensified by the thermal resistance at the coating/substrate interface.

![Fig. 2a Normalized temperature distributions in the coating/substrate at \(\tilde{t} = \kappa_1 t/b^2 = 0.01\).](image-url)
Figure 4a shows the normalized TSIF versus nondimensional time $\tilde{t}$ for a crack length of $a/h = 0.5$. The TSIF first rapidly increases with time, reaches a peak value, and then gradually decreases to its steady state value with further increase of time. The peak TSIF, the driving force of crack propagation, is increased by the presence of thermal resistance at the coating/substrate interface. Fig. 4b shows the normalized TSIF versus nondimensional time $\tilde{t}$ for $a/h = 1$, i.e., the crack terminates at the coating/substrate interface. Because we assume that the coating and substrate have the same Young’s modulus and Poisson’s ratio, the inverse square root stress singularity still prevails and the SIF can be well-defined. The behavior of TSIF is similar to the case of $a/h = 0.5$ although the peak TSIF becomes higher.

Figure 5 shows the normalized peak TSIF versus the nondimensional crack length $a/h$. Now a nondimensional interfacial thermal resistance of $R^* = 0.05$ is also considered. The peak TSIF increases with an increase in the crack length in all cases. For crack lengths shorter than $a/h = 0.3$, the peak TSIF remains almost unaffected by the interfacial thermal resistance. The peak TSIF becomes higher for higher interfacial thermal resistance for cracks longer than $a/h = 0.3$. For $a/h = 1.0$, the peak TSIF for $R^* = 0.2$ is 30% higher than that without considering the interfacial thermal resistance.

6. Concluding remarks
Thermal fracture behavior of bonded materials may be significantly influenced by the thermal resistance at interfaces in the materials. This work aims to shed some light on the effect of interfacial thermal resistance on thermal fracture of bonded materials. We consider an edge crack in the coating layer in a coating/substrate system. The temperature and thermal stress are determined in the system with thermal resistance at the coating-substrate interface. The thermal stress intensity factor for the edge crack is calculated using an integral transform/integral equation method. We present the numerical results for an Al$_2$O$_3$ coating on a Si$_3$N$_4$ substrate and show that the thermal stress field deviates from that for the coating/substrate system with perfect thermal contact. The thermal stress intensity factor is increased by the interfacial thermal resistance, which indicates that the thermal shock resistance of the coating/substrate system can be degraded by the presence of thermal resistance at the interface between the coating and substrate. To improve the thermal shock resistance the interfacial thermal resistance should be minimized.

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Fig. 5 Normalized peak thermal stress intensity factor versus nondimensional crack length $a/h$

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