Interfacial Adhesion and Crack Initiation at Metal/Ceramic Interface

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Abstract - Interface crack initiation in layered materials is investigated for mixed mode I and mode II loadings. The dislocation plasticity in the metal layer is considered, and the energy for initial emission of a dislocation is assumed to be attained before the cleavage of the interface crack. Superdislocation modeling is employed to obtain the critical strain energy release rate, for crack initiation and growth. When a stress separation law is satisfied at the interface crack tip, interface debonding occurs. The strong dependence of fracture energy on mixed mode loading is predicted by this model. The role of the metal layer thickness and interfacial strength is also investigated. In addition, interfacial strength measurement for predicting the toughness is touched.

1. INTRODUCTION

Theoretical work on the elastic-plastic interface crack problem by a number of workers [1-6] has given insight into possible explanations for a strong mixed mode effect due to plasticity. Using a finite element analysis, Tvergaard and Hutchinson [7-8] have calculated the mixed mode toughness of an interface joining an elastic-plastic solid and a non-plastic solid. In their work, a potential function, based on the components of the crack face displacement, was used to generate tractions along the interface where the fracture process caused interface separation occur. Recently, Wei and Hutchinson [9-10] studied the relationship between fracture energy at the interface crack tip and the global toughness under mixed mode loading. Using the SSV model proposed by Suo, Shih and Varias [11] and strain gradient plasticity theory for a metal/ceramic layered material, their FEM analysis showed that plasticity in the metal layer plays an important role in interfacial toughness under the mixed mode loading.

Recent work by Mao and Evans [13] has shown that a growing interface crack in an $Al_2O_3 / Au / Al_2O_3$ system does not automatically become sharp. Instead, plastic blunting arises through the activation of slip sources in the metal layer. Using an atomic force microscope (AFM), Mao and Evans also observed that separation still occurs as a result of brittle debonding. In order to model the interface crack growth, a stress criterion (interface separation law) is used in which the interface ruptures when the peak normal stress ahead of the blunt crack exceedes the bond strength at the interface.

This paper develops a stress based approach which predicts mixed mode toughness of an interface joining a solid, which has dislocation plasticity, with another elastic solid that is dislocation-free. We assume that dislocations are emitted from the interface crack tip and that the crack tip will be blunting. The interface ruptures when a nominal stress, which is a function of normal stress and shear stress ahead of the blunted crack, exceeds the strength of the interfacial atomic bonds.

2. ANALYTICAL MODEL

A model of a material with alternating ceramic and metal layers containing a crack on the interface is shown on Fig. 1. The thickness of the metal layer is denoted by h, and

associated materials parameters are: shear modulus μ, Poisson's ratio ν, Burgers vector b and surface energy γ. It is assumed that metal layer has dislocation plasticity and ceramic layers are elastic with no dislocation plasticity. The energy needed for a single dislocation emission from crack tip is assumed to be much smaller than the interface cleavage fracture energy defined by Beltz and Rice [12]. Upon loading, a cluster of dislocations will emit from the crack tip and move along a slip plane in the metal at an angle φ to the interface crack plane, and pile up against the upper interface. The emitted dislocations have two effects on the crack tip. Firstly, if the burgers vector has a component normal to the crack plane, the emitted dislocations blunt the crack tip and a ledge is generated. The blunting reduces the stress concentration at the crack tip such that it is more difficult to reach the cohesive tensile strength. Secondly, the interaction forces between the crack and the emitted dislocations will result in crack tip shielding, giving rise to a crack tip stress intensity lower than the far field applied stress intensity. The detailed relationships are illustrated on Fig. 1.

2.1 Dislocation shielding model

In a layered material, dislocations emitted from the interface crack tip are blocked by the upper interface, sending a back stress to the crack tip which impedes further dislocation emission. For a given applied load and layer thickness, there exists an equilibrium number of dislocations in the pile-ups. Once the equilibrium number is reached, emission of additional dislocations is prevented by the back stress, which hinders further blunting of the crack tip. Considering a group of n dislocations which are blocked by the upper interface as a superdislocation, the total energy of the system, W_T, in the presence of a superdislocation of strength nb is

$$W_T(K_1^{tip'}, K_2^{tip'}, n) = W_d + W_K + W_L \qquad (1)$$

where W_d consists of the dislocation self-energy and the interaction energy between dislocations, W_K is energy of interaction between the crack and the dislocations and W_L is the ledge energy and $W_L = nb\gamma$ (γ is the metal surface energy). $K_1^{tip'}$ and $K_2^{tip'}$ are the mode I and mode II components at crack tip, respectively. The equilibrium condition requires that $\qquad \dfrac{\partial W_T}{\partial n} = 0,$ \qquad\qquad\qquad (2)

As dislocations are emitted from the crack tip, a cluster of dislocations piles-up against the upper interface and forms a superdislocation. This superdislocation will reduce the crack tip stress to generate dislocation shielding and the relationship between applied and crack tip stress intensity factors can be expressed by (details are given in [14])

$$\begin{bmatrix} K_1^{tip'} \\ K_2^{tip'} \end{bmatrix} = \begin{bmatrix} K_1^{tip} \\ K_2^{tip} \end{bmatrix} + \begin{bmatrix} k_1 \\ k_2 \end{bmatrix}, \qquad (3)$$

and the stress intensity factor contributed from the superdislocation is

$$\begin{bmatrix} k_1 \\ k_2 \end{bmatrix} = \frac{3n\mu\sqrt{b}}{2\sqrt{2\pi\overline{h}}(1-\nu)} \begin{bmatrix} f_1(\varphi) \\ f_2(\varphi) \end{bmatrix}, \qquad (4)$$

where the subscripts 1 and 2 denote the mode I and mode II load components. K^{tip} and $K^{tip'}$ are the crack tip stress intensity factor and far field applied stress intensity factor.

K^{tip} and $K^{tip'}$ can also be considered as the stress intensity factor at the crack tip before and after dislocation shielding. k is the stress intensity factor contributed by a superdislocation with strength of nb. The functions f_1 and f_2 are given by the expressions $f_1(\varphi) = (1+\alpha)\sin\varphi\cos\frac{\varphi}{2}$ and $f_2(\varphi) = \frac{1}{3}(1+\alpha)(2\cos\varphi\cos\frac{\varphi}{2} - \sin\varphi\sin\frac{\varphi}{2})$, where α is the Dundurs' parameter. The phase angle at the crack tip after dislocation shielding, can be expressed as

$$\tan\Psi^{tip} = K_2^{tip}/K_1^{tip}. \tag{5}$$

Emitted dislocations also create ledges at the crack tip, and the blunting due to these ledges reduces the maximum tensile stress ahead of the crack tip. For simplicity, we approximate the blunted crack tip by a notch with tip radius Δ, as shown on Fig. 1. The slip step Δ (notch tip radius) is formed due to emission of n dislocations from crack. The components of the slip step, Δ_1 and Δ_2, are given by

$$\begin{aligned} \Delta_1 &= \Delta\sin\varphi \\ \Delta_2 &= \Delta\cos\varphi \end{aligned} \tag{6}$$

where $\Delta = nb$. From [14], the crack tip tensile stress σ^{tip} and shear stress τ^{tip} after dislocation emission can be obtained based on Tada *et al.* [15] as

$$\begin{aligned} \sigma^{tip} &= 2\sqrt{2/\pi}\, K_1^{tip}/\sqrt{\Delta_1}, \\ \tau^{tip} &= 2\sqrt{2/\pi}\, K_2^{tip}/\sqrt{\Delta_2}. \end{aligned} \tag{7}$$

2.2. Interface separation law under mixed mode loadings

As mentioned above, upon loading, dislocations will emit from the crack tip and pile-up against the upper interface. This prevents the further emission of dislocations which impedes blunting of the crack tip. Continuous loading will increase the crack tip stress. It is assumed that interface separation will occur when the combination of the tensile and shear stresses at the interface reaches a critical value. This separation law is expressed as

$$\left(\frac{\sigma^{tip}}{\sigma_b}\right)^2 + \left(\frac{\tau^{tip}}{\tau_b}\right)^2 = 1, \tag{8}$$

where, σ_b and τ_b are the tensile strength and shear strength at the interface. We assume that

$$\lambda = \sigma_b/\tau_b, \tag{9}$$

3. CRACK INITIATION TOUGHNESS Γ_i

Based on the analysis presented in section 2, the crack tip stress will be shielded by the superdislocation. Thus, the fracture energy associated with this dislocation shielding will be different from the fracture energy without dislocation emission. In general, the energy release rate at the interface can be expressed by [6]

$$G^{app} = \frac{1-\beta^2}{E*}[K_1^{tip'2} + K_2^{tip'2}] \tag{10}$$

where $\frac{1}{E*} = \frac{1}{2}(\frac{1}{\overline{E_1}} + \frac{1}{\overline{E_2}})$, $\overline{E_i} = E_i/(1-\nu_i^2)$ for plane strain and $\overline{E_i} = E_i$ for plane stress. E_1, E_2 and ν_1, ν_2 are the Young's modulus and Poisson's ratios for the metal and the ceramic layers respectively. From Eqs.(2-9) assuming $\beta = 0$, the energy release rate, G^{app}, after dislocation shielding can be expressed by [14]

$$G^{app} = \frac{1}{E*}\mu^2 b\{[\frac{\sqrt{n\sin\varphi}\,\overline{\sigma}^{tip}}{2\sqrt{2/\pi}} + \frac{3}{2}n\frac{1}{(1-\nu)\sqrt{2\pi\overline{h}}}f_1(\varphi)]^2$$
$$+[\frac{\sqrt{n\cos\varphi}\,\overline{\tau}^{tip}}{2\sqrt{2/\pi}} + \frac{3}{2}n\frac{1}{(1-\nu)\sqrt{2\pi\overline{h}}}f_2(\varphi)]^2\}$$

(11)

where $\overline{\sigma}^{tip} = \sigma^{tip}/\mu$ and $\overline{\tau}^{tip} = \tau^{tip}/\mu$. n also can be considered as a measure of crack tip opening. With the separation condition expressed by (8), the crack initiation toughness under mixed mode is

$$\Gamma_i(\Psi^{tip},\overline{h},\overline{\sigma}_b,\lambda) = \frac{1}{E*}\mu^2 b\{[\frac{\sqrt{n'}\overline{\sigma}_b}{2\sqrt{2/\pi}f} + \frac{3}{2}n'\frac{1}{(1-\nu)\sqrt{2\pi\overline{h}}}f_1(\varphi)]^2$$
$$+[\frac{\sqrt{n'}\overline{\sigma}_b\tan\Psi^{tip}}{2\sqrt{2/\pi}f} + \frac{3}{2}n'\frac{1}{(1-\nu)\sqrt{2\pi\overline{h}}}f_2(\varphi)]^2\}$$

(12)

where $n'(\overline{\sigma}_b,\Psi^{tip},\overline{h},\overline{\gamma})$ is a critical dislocation number at crack initiation and can be derived from equations (2, 7-8).

5. RESULTS AND DISCUSSION

In order to demonstrate the theoretical model developed above, an $Al_2O_3 / Au / Al_2O_3$ system was selected with experimental results obtained by Mao and Evans [13]. With FCC Au as the middle layer[14], the interface crack is on the plane (100) and (111) is the slip plane. The angle between these two planes is 70.5^o, which means that dislocations will emit from the interface crack tip with an angle $\varphi = 70.5^o$. Different values of normalized layer thickness $\overline{h}$ and theoretical tensile stress at the interface crack tip $\overline{\sigma}_b$ are employed to compare the toughness of the material. As also done by Mao and Evans [13], the Burgers vector b is set to $0.286\,nm$ (for Au), h is on the order of a few microns, $\lambda = 1$, $\nu = 0.44$ and $\alpha = 0.58$

A pure mode I loading is obtained if $\Psi^{tip} = 0$. This case was analyzed in detail by Mao and Evans [13], and one important result is shown on Fig. 2. For a fixed layer thickness, the fracture energy needed for the interface crack to initiate cleavage increases when the interfacial tensile strength of the layered material is increased. For fixed interfacial tensile strength, the thicker layer needs more energy to encourage crack cleavage. For $\Psi^{tip} \neq 0$, fracture energy curves for crack initiation are plotted on Fig. 3 as a function of Ψ^{tip} at fixed values of $\overline{\sigma}_b$. Generally, the transition from mode I to mode II increases the difficulty for the interface crack to propagate. Variation of the interfacial tensile strength showed that the stronger the interfacial strength, the metal layer, the more energy that is needed for crack propagation. Fig. 3 shows that there is a large increase in fracture energy when the loading phase is above 60°. Using Eq (12, interfacial toughness can be predicted if we know the interfacial strength. The interfacial strength σ_b measurement is being developed by Mao recently. Fig. 4 shows an example of the interfacial adhesion force measurement of Au/Al₂O₃ interface by indenting Au coated tip on Al₂O₃ (0001) single crystal substrate.

6. CONCLUSION

In summary, the strong dependence of interface toughness on the relative proportion of mode II to mode I loading, seen in experimental data, is predicted by a dislocation model with an embedded traction separation law that characterizes the fracture process on the interface. The increase in toughness with increasing proportion of mode II to mode I loading is predicted to be a consequence of dislocation shielding outside of the fracture process zone. The dependence of the interfacial fracture toughness on the thickness of metal layer and interfacial strength have been found.

7. REFERENCE

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Figure Caption

Fig. 1. Layered material mode with an interface crack.

Fig. 2. Crack initiation fracture toughness energy.

Fig. 3. Interfacial strength effect on crack initiation energy versus phase angle Ψ^{tip}.

Fig. 4 Example of Interfacial adhesion force measurement by atomic force microscope.