COHESIVE MODEL FOR THIN FILM/SUBSTRATE INTERFACIAL CLEAVAGE FRACTURE

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ABSTRACT Film/substrate structure is a basic structure widely used in microelectronic and materials science and technology. A modified three-parameter (Γ_0,σ/σ_y,t) cohesive model was used to investigate the cleavage fracture under plastic atmosphere. The model was also used to discuss the whole process of the initialization and extension of interface crack between uniform and functional graded metal thin film and ceramic substrate under residual stresses. This model was also used to analyze the interfacial crack extension between enhanced functional graded thin film and substrate. The characteristic of the interfacial crack in graded film/substrate was emphasized.

KEYWORDS embedded elastic zone, cohesive model, thin film/substrate structure, interfacial fracture

COHESIVE MODEL FOR CLEAVAGE FRACTURE UNDER PLASTIC ATMOSPHERE

Film/Substrate structure is a basic structure widely used in microelectronic and materials science and technology.. Liplin *et al.* [1] observed that the maximum separation stress can reach a high level, which was about 10 times of the yield stress. Tvergaard & Hutchinson [2][3] proved the results by using conventional plastic theory and EPZ model. At the same time, Hutchinson [4] pointed that for general metal/ceramic interface, the cleavage fracture toughness is about 1Jm^{-2},the macroscopic fracture toughness is about 400 Jm^{-2} to1000 Jm^{-2} and the crack tip keeps atomic scale keenness. There is great difference between these two fracture toughness.

It was considered that the fracture mechanism is atom separation. On the basis of this idea, SSV model has been proposed by Suo et al. [5], who assumed a dislocation-free strip present near crack tip. The SSV model was used by Wei et al. [6] Wei et al. [7] introduced a cohesive model in cleavage fracture process. This method was adopted and developed in this paper.

In EPZ and SSV model, two parameter were introduced to describe the fracture process zone. In EPZ model, the parameters are fracture toughness Γ_0 and maximum separation stress $\hat{\sigma}$,In SSV model, they are Γ_0 and the thickness of elastic strip, t. In cohesive model introduced by Wei [7] and used in this paper, SSV model and EPZ model were combined and three parameters, Γ_0, $\hat{\sigma}$ and t, were introduced to discuss the fracture process, which was shown in Fig.1.

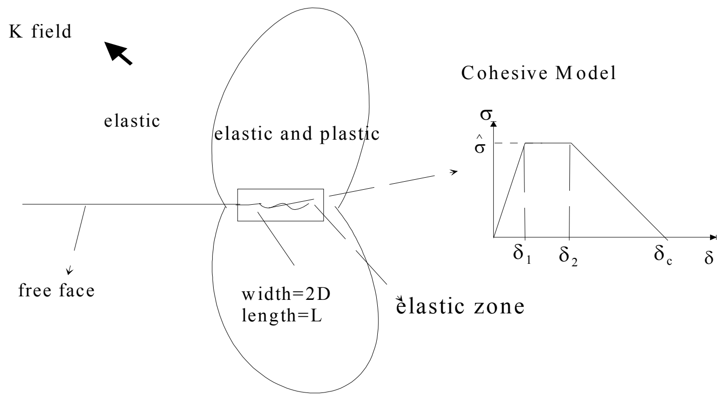


Fig. 1 Cohesive model for embedded elastic zone

INTERFACIAL FRACTURE OF UNIFORM FILM/SUBSTRATE STRUCTURE

Model for the residual stress induced interfacial fracture

In the machining process of film/substrate, the residual stress is often produced for the change of the temperature. The temperature of the film and the substrate is t_0 either. Aparently , there are residual stresses in the film, and the stress can induce the interface crack to initiate and propagate. It was assumed the film keeps plane strain restriction in x-y plane. Taking $T＝t_1-t_0$, the residual stress can be express as

$$\sigma_R = \sigma_x = \sigma_z = \alpha E T/(1-\nu) \tag{1.}$$

Energy release ratio can be expressed as

$$G = \frac{1-\nu^2}{2E}\sigma_R{}^2 h \tag{2.}$$

Taking $\delta_1/\delta_c=0.15$, $\delta_2/\delta_c=0.5$, $E/\sigma_y=300$, $k=\hat{\sigma}/\sigma_y$ and N=0.1, we can got the initial residual stress and initial temperature difference of crack propagation as below

$$\sigma_R{}^0 = E\sqrt{\frac{4.5*10^{-3}}{(1-\nu^2)}}\sqrt{\frac{k\delta_c}{h}},\quad T^0 = \frac{1}{\alpha}\sqrt{\frac{4.5*10^{-3}(1-\nu)}{1+\nu}}\sqrt{\frac{k\delta_c}{h}} \tag{3.}$$

In brief, the module mismatch of film and substrate was ignored and we take E_m= E_c and $\nu_m=\nu_c=0.3$. In the computation, we introduce nondimensional method for fracture process. When the results were changed to dimensional value with Γ_0=1Jm^{-2} and E=6×10^{10}Pa, we can acquire δ_c=7.407Å, R_0=0.1749μm, t=8.74nm and h=0.3498um.

Resistance curve of crack propagation and the influence of the parameter on crack propagation

With $t/R_0=0.05$, $\hat{\sigma}/\sigma_y=10$ and $h/R_0=2$, the resistance curve can be calculated from the curve that Γ_s/Γ_0 approximately equals to 88.36. Compared with the results of infinite medium in which Γ_s/Γ_0 approximately equals to 400~1000, the plastic zone was restricted and can't develop completely for the scale of the thin film and the free upper surface.

The slopes of the two curves only have minor difference. The main differences are the critical $\sigma_R{}^c$ and the critical length of crack propagation. The values of $h/R_0=4$ are much larger than that of $h/R_0=2$ because the plastic zone can more fully develop when the thickness of the film is larger. It can be concluded that when $h>>R_0$, the value of Γ_s will reach to the macroscopic fracture toughness of the interface between metal film and ceramic substrate.

INTERFACIAL FRACTURE OF GRADED FILM/SUBSTRATE STRUCRURE

Functionally graded structure is an important structure widely used in microelectronic and materials science and technology. The continuous changes of materials' nature can greatly decrease the thermal and mechanical mismatch between different materials. In this paper, the enhanced thin graded film on ceramic substrate and the weakened graded film on metal substrate were discussed. The main purpose is to investigate the character of the propagation of interfacial crack under the drive force of residual stress and to make sure the effect of decreasing the mismatch. And the cohesive model and embedded elastic zone were used in the computation.

Enhanced graded film on ceramic substrate

The similar model showing above was introduced in this section. The process that residual stress induced crack to propagate was simulated. First we assume that the value E_m equals to E_c and v_m equals to v_c. T was taken as drive force for crack propagation. The T_0 was taken as the initial resistance force.

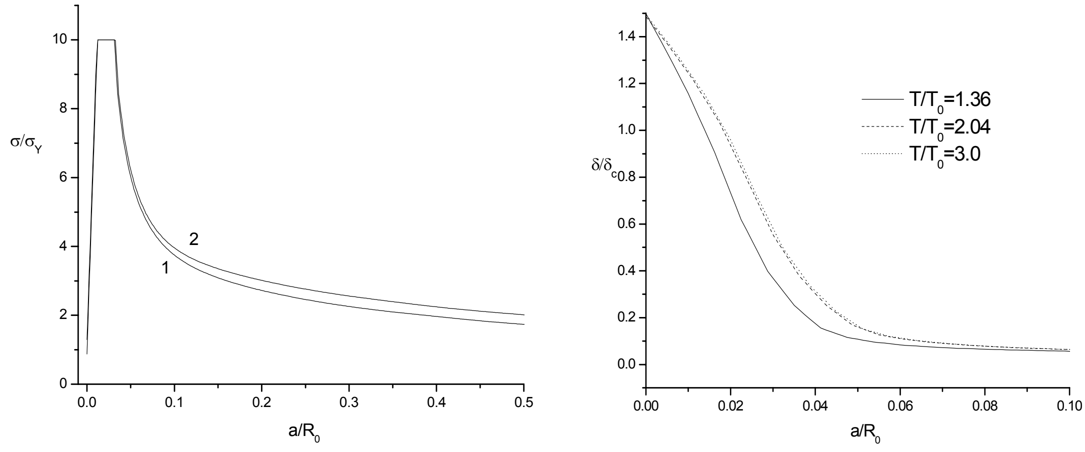
We take the calculation under plane strain conditions and $\delta_1/\delta_c=0.15$, $\delta_2/\delta_c=0.5$, $E(x)/\sigma_y(x)=300$, $v=0.3$, $t/R_0=0.05$, $\hat{\sigma}/\sigma_y=10$, $h/R_0=4$. For comparing with the result of the uniform film, the same T_0 in uniform film was taken. The relations between the true T_0 and the T_0 used in uniform film will be discussed later. We have

$$T^0=\frac{1}{\alpha}\sqrt{\frac{4.5*10^{-3}(1-v)}{1+v}}\sqrt{\frac{k\delta_c}{h}} \tag{4.}$$

The linear change of the mechanical and thermal parameter in the direction of thickness was assumed.For enhanced graded film ,we have $E_m>E_c$, $\alpha_m>\alpha_c$,, $\sigma_m>\sigma_c$ and take $E_m=2E_c$, $\alpha_m=2\alpha_c$, $\sigma_m=2\sigma_c$, and can get the results of stress distribution near crack tip.

We take $E_m=3E_c$, $\alpha_m=3\alpha_c$, $\sigma_m=3\sigma_c$ (signed 2), and compared the stress distribution near crack tip with the results of $E_m=2E_c$, $\alpha_m=2\alpha_c$, $\sigma_m=2\sigma_c$ (signed 1), which was shown in Fig. 2. It can be seen that there is only minor different between these two curves. On the basis Fig. 2, we can draw a conclusion that the graded structure in thin film has only a minor influence on the stress distribution and the three parameters of cohesive model have major influence on the distribution.

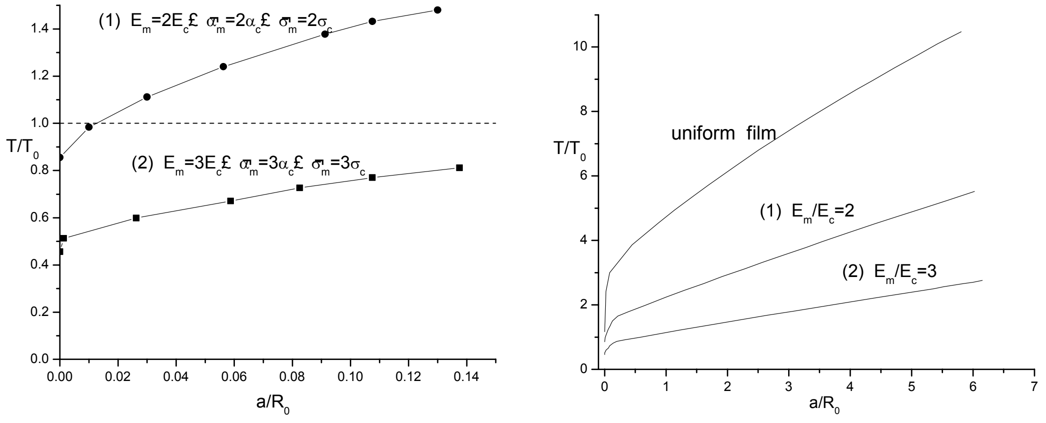
On the basis of the stress distribution, we can also acquire the displacement distribution. We take $E_m=2E_c$, $\alpha_m=2\alpha_c$ and $\sigma_m=2\sigma_c$ and plot the distribution in Fig. 3b. The similar conclusion can also be drawn that graded structure in thin film has only a minor influence on the displacement distribution.



(a) (b)

Fig. 2 Stress and displacement distribution near crack tip

The different structures of graded films have influence on the resistance curve of crack propagation. First, we compared the results of the two structures, $E_m=3E_c$, $\alpha_m=3\alpha_c$, $\sigma_m=3\sigma_c$ (signed 2) and $E_m=2E_c$, $\alpha_m=2\alpha_c$, $\sigma_m=2\sigma_c$ (signed 1). The result was show in Fig. 4. In Fig.4a, the initial resistance force was discussed. It can be seen that the two structures have different initial resistance force. For structure (1), the true resistance force is about $0.855T_0$, which is the value in uniform film. For structure (2), the true value is $0.456T_0$. So It can be concluded that the crack between enhanced graded film and ceramic substrate is easier to propagate compared with that of the uniform film, and the more E_m/E_c, the easier to propagate. The reason is that the enhanced structure makes the film more difficult to come into plastic and easier to propagate. The similar result was acquired in crack propagation, which was shown in Fig. 3b. It can be seen that the graded film can greatly decrease the fracture toughness of interfacial crack propagation compared with the uniform film, and the more E_m/E_c, the more decrease. For example, for structure (1), the critical resistance force is about 40% of that of the uniform film. For structure (2), the critical resistance force is about 20% of that of the uniform film.



(a) (b)

Fig. 3 The influence of graded structure on crack initiation and propagation

In the process of making graded film on substrate, the rate of two materials can be controlled and different curve of parameter's change can be attained. The influence on the resistance curve will be discussed. We still take $E_m=2E_c$, $\alpha_m=2\alpha_c$, $\sigma_m=2\sigma_c$, and take different changing curves which were shown in Fig.4.

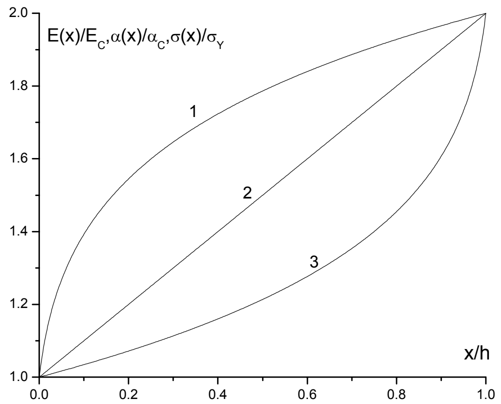


Fig. 4 Different changing curve

Curve 1 followed the expression below ($E(x)/E_c$, $\alpha(x)/\alpha_c$ and $\sigma(x)/\sigma_c$ are all equal to $f(x)$),

$$f(x)=0.67951[640\frac{x}{h}+10.159)]^{\frac{1}{6}} \tag{5.}$$

Curve 3 is symmetrical with curve 1 in point (0, 5, 1.5) and followed the expression below.

$$f(x)=3-0.67951[640\frac{1-x}{h}+10.159)]^{\frac{1}{6}} \tag{6.}$$

The three crack resistant curves were show in Fig. 5. It can be seen that in curve 1, the crack became unstable when initialing and propagating for a short distance. It is because that the elastic module and other parameters increase rapidly near the crack in thickness direction and the zone of the film near crack is difficult to come into plastic, the crack became unstable when the drive force is a little higher than the initial resistance force. But compared with uniform film, the structure expressed by curve 3 is difficult to propagate because the zone near crack is easier to come into plastic and more work will be dissipated in plastic yielding. But the critical fracture toughness of structure 3 is still much lower than uniform film because the upper part of the graded film was harder and more difficult to come into plastic and the plastic zone was restricted in a thin zone near crack tip.

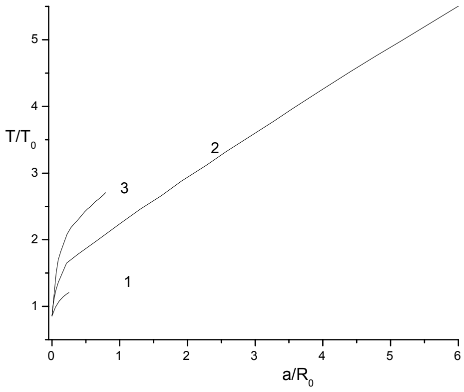


Fig. 5 The influence of different curves on resistance curve of crack propagation

On the basis of the discussion, we can draw a conclusion that for the enhanced thin film on substrate, the most critical fracture toughness and critical propagation length can be attained when the mechanical parameters (elastic module and yield stress) vary linearly. This result can do some favor for the optimizing the film structure and mechanical property.

The mechanical and thermal mismatched thin film on substrate was also investigated and compared with the graded film. The effect of the graded film on decreasing crack propagation between film and substrate was discussed. We also take $E_m=2E_c$, $\alpha_m=2\alpha_c$, $\sigma_m=2\sigma$. The resistance curve was plotted in Fig.6.

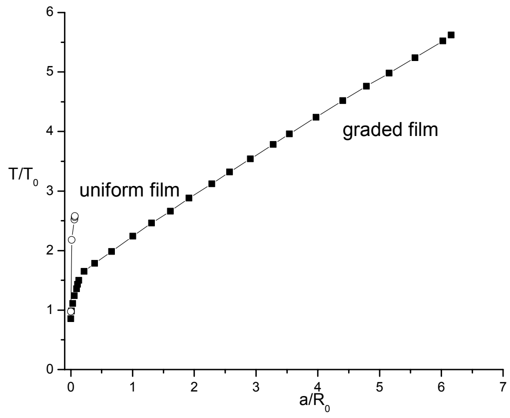


Fig. 6 The effect of graded film on decreasing interfacial crack propagation

It can be seen that because the parameter $\hat{\sigma}$ in mismatch uniform film is two times of that in graded film, the initial fracture toughness improved largely, which is about two times of the toughness in graded film. But the crack propagated in mismatch film became unstable when drive force exceeds the initial value very little. Compared with the mismatched film, the crack propagation of graded film has a much higher critical fracture toughness and a strong restrain on crack propagation.

CONCLUSIONS

A modified three parameter cohesive model embedded with elastic core was introduced to investigated

This model was used to analyze the interfacial crack extension between enhanced graded thin film and substrate. Compared with the uniform film/substrate structure mismatched in mechanical and thermal parameter, the graded film/substrate increased the critical fracture toughness and critical length of crack extension largely. The distribution of stress and displacement in fracture process zone are mainly determined by the parameters of process zone model and the deferent variation of the graded film has a minor influence on them.. The highest critical fracture toughness and critical length of crack extension can be acquired when the material parameters vary linearly on the graded thin film/substrate structure.

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