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CRACK INTERACTION AND PROPAGATION—STABILITY IN A THIN FILM/SUBSTRATE SYSTEM

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Abstract—We first investigate the configurational stability of a semi-infinite crack in the substrate of an isotropic, linearly elastic film/substrate system under residual tension in the thin film. The crack runs parallel to the film/substrate interface. The propagation is found to be generally unstable. We further consider the interaction of the crack, under the same loading, either with a crack in the thin film perpendicular to the interface, or with a finite length interface crack. We calculate the stress intensity factors for both cracks, as well as the non-singular T stress for the substrate crack. The path of the substrate crack under the attraction of film cracking or interface debonding is qualitatively studied based on Cotterell–Rice theory. While the interface debonding does not have a great effect on the probable path of the substrate crack, the presence of a perpendicular crack in the thin film leads to three possible paths for the substrate crack. These are discussed.

1. INTRODUCTION

Understanding the failure mechanism of film/substrate systems and evaluating their mechanical reliability is necessary to optimize their design and safeguard their performance. These have been the subject of extensive studies for the last few years [e.g. Canon *et al.* (1986), Drory *et al.* (1988) and Suo and Hutchinson (1988)].

Failure modes of these systems depend strongly on the mismatch of material properties and the sign of residual stress, among other factors. When films are subject to residual compression, the films may buckle and separate from the substrate, or the substrate itself may develop a crack, perpendicular to the interface. There has been evidence that for a specimen subject to residual tension in the film or general edge loading, cracks would initiate at its edges and tend to deviate into the substrate and, after an initial transitional period of propagation, enter a stage of steady-state propagation along a tracjectory parallel to the interface (Canon *et al.*, 1986). This steady-state propagation of cracks has been studied both experimentally and theoretically [e.g. Thouless *et al.* (1987) and Suo and Hutchinson (1988)]. These investigations were focused on predicting the characteristic depth from the interface at which local symmetry can be achieved and the crack can run in a straight path. The study by Suo and Hutchinson (1988) also provides information on the critical combination of film thickness and external loads under which delamination by substrate cracking can be suppressed.

In these previous studies, the films were assumed to be crack free with perfect interfacial bonding. However, in practice, this is not always the case. For a film under residual tension, it is very likely that some cracks may initiate and extend onto the interface and cause decohesion; they may also interact with other defects in the structure. It has been observed in experiments that in an alumina/silica structure under residual tension which has a Young's modulus ratio of 4–5, the substrate crack runs along a wavy, rather than a straight path. The disturbance of the crack path is attributed to micro-cracks in the thin film (Drory *et al.*, 1988). The fracture pattern under the disturbance of thin film cracks suggests that the substrate crack, in some stage of propagation, may be directionally unstable. Theoretical analysis needs to be carried out to investigate the stability of the crack and its propagation patterns under the perturbation of surrounding defects and therefore to explain the observed wavy path. This is the subject of our present work.

The issue of path selection and stability of cracks in a homogeneous isotropic solid can be addressed in terms of the asymptotic stress field around the crack tip, i.e. as described by the well-known Williams asymptotic expansion of stresses in terms of polar coordinates (r, θ) centered at the crack tip:

$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{xy} & \sigma_{yy} \end{bmatrix} = \frac{K_{\mathrm{I}}}{\sqrt{2\pi r}} \begin{bmatrix} \tilde{\sigma}^{\mathrm{I}}_{xx}(\theta) & \tilde{\sigma}^{\mathrm{I}}_{xy}(\theta) \\ \tilde{\sigma}^{\mathrm{I}}_{xy}(\theta) & \tilde{\sigma}^{\mathrm{I}}_{yy}(\theta) \end{bmatrix} + \frac{K_{\mathrm{II}}}{\sqrt{2\pi r}} \begin{bmatrix} \tilde{\sigma}^{\mathrm{II}}_{xx}(\theta) & \tilde{\sigma}^{\mathrm{II}}_{xy}(\theta) \\ \tilde{\sigma}^{\mathrm{II}}_{xy}(\theta) & \tilde{\sigma}^{\mathrm{II}}_{yy}(\theta) \end{bmatrix} + \begin{bmatrix} T & 0 \\ 0 & 0 \end{bmatrix} + O(r^{1/2}), \quad (1)$$

where the constants K_{I}, K_{II} are intensity factors and T is the non-singular stress acting parallel to the crack plane. The stresses ahead of the crack tip ($\theta = 0$) are given by

$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{xy} & \sigma_{yy} \end{bmatrix} = \frac{K_{\mathrm{I}}}{\sqrt{2\pi r}} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \frac{K_{\mathrm{II}}}{\sqrt{2\pi r}} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + \begin{bmatrix} T & 0 \\ 0 & 0 \end{bmatrix} + O(r^{1/2}). \quad (2)$$

Based on an experimentally established fact that a crack advancing continuously in an isotropic homogeneous brittle solid seeks a path at which $K_{\mathrm{II}} = 0$, Cotterell and Rice (1980) presented a theory which says: If $K_{\mathrm{II}} \neq 0$ for a straight crack, then the crack will kink at an approximate angle of $\theta^* = -2K_{\mathrm{II}}/K_{\mathrm{I}}$ (in radians) either up if $\theta^* > 0$ or down if $\theta^* < 0$; also if the crack advances with $K_{\mathrm{II}} = 0$, it is directionally stable if $T < 0$ and unstable if $T > 0$. The determination and the use of T stress to predict the stability and path of crack propagation has been well established in recent years by, notably, Fleck *et al.* (1991), Sham (1991) and Nakamura and Parks (1991).

We begin with the study of steady-state cracking in the substrate under residual tension in the thin film. The crack is assumed to be long enough, so that it can be treated asymptotically as semi-infinite in length. Though this problem has been studied by several investigators, we examine it with a focus on the T stress of the crack. We found the T stress to be positive and therefore according to Cotterell–Rice theory, the assumed *steady-state* cracking is directionally *unstable*. We thus believe that the instability of a long substrate crack can be the cause of the buckling of specimens in experiments (Thouless *et al.*, 1987).

Once the instability of a very long substrate crack is understood, we consider separately two commonly seen forms of micro defects near the crack tip and investigate the interaction between the defect and the substrate crack.

The first kind of defect we consider is a film crack: An edge crack perpendicular to the free surface. The stress intensity factors for both cracks and the T stress of the substrate crack are computed. With these quantities, we are able to qualitatively explain, based on Cotterell–Rice theory, the phenomenon observed by Drory *et al.* (1988). We also find three possible substrate cracking patterns, and look at how these crack paths depend on the material properties of the film and substrate.

We also investigate the case in which there is a pre-existing debonded zone along the interface of the film and the substrate. It is found, not surprisingly, that the interface debonding does not have a noticeable effect upon the K_{II} of the substrate crack. Hence its influence on the crack path will not be as great as that of film cracking, but bearing in mind the fact that the long substrate crack is directionally unstable, it is possible that interface debonding can cause the steady-state crack path to deviate. Numerical calculation is required to determine the true path of cracking, but this is beyond the scope of our present work.

2. PROBLEM FORMULATION

The elastic fields in isotropic bimaterial systems are conveniently characterized by the two Dundurs' parameters (Dundurs, 1969) which are

$$\alpha = \frac{\Gamma(\kappa_2+1)-(\kappa_1+1)}{\Gamma(\kappa_2+1)+(\kappa_1+1)}, \qquad \beta = \frac{\Gamma(\kappa_2-1)-(\kappa_1-1)}{\Gamma(\kappa_2+1)+(\kappa_1+1)}. \quad (3)$$

Subscripts 1 and 2 refer to the film and substrate materials, respectively. Further, μ and ν

are the shear modulus and Poisson's ratio, $\kappa = 3-4\nu$ for plane strain and $(3-\nu)/(1+\nu)$ for plane stress while $\Gamma = \mu_1/\mu_2$. The physically admissible values of α and β are restricted by

$$-1 \leqslant \alpha \leqslant 1, \qquad -1 \leqslant \alpha-4\beta \leqslant 1. \tag{4}$$

The two Dundurs' parameters are related to two other commonly used parameters: Σ, the stiffness ratio, and ε, the oscillatory index, by

$$\Sigma = \frac{c_2}{c_1} = \frac{1+\alpha}{1-\alpha}, \qquad \varepsilon = \frac{1}{2\pi}\ln\frac{1-\beta}{1+\beta}, \tag{5}$$

where $c = (\kappa+1)/\mu$. These two parameters measure the elastic dissimilarity of two materials in the sense that both vanish if the materials are identical. α is a measure of the dissimilarity of stiffness of the two materials, i.e. material 1 is stiffer than material 2 if $\alpha > 0$ and relatively more compliant if $\alpha < 0$. The parameter β is related to the oscillatory behavior at an interfacial crack tip. Since the stress intensity factors for the substrate crack depend only weakly on β (Suo and Hutchinson, 1988), we assume that $\beta = 0$ in all calculations.

The Eshelby cut-and-paste scheme is adopted here to reduce the internal residual stress inside the thin film to boundary loading (Fig. 1) which is further reduced to a compression force P and bending moment M on the edges (Fig. 2). To study the perturbation of the crack path by the thin film fracture, a uniform compression is applied on the surface of the film crack [Fig. 3(a)]. A crack or interfacial debonding is represented by the continuous distribution of edge dislocations. The procedures used to obtain both the Green functions due to a single edge dislocation and the integral equations governing dislocation density are broadly similar to those adopted by previous studies [e.g. Thouless *et al.* (1987) and

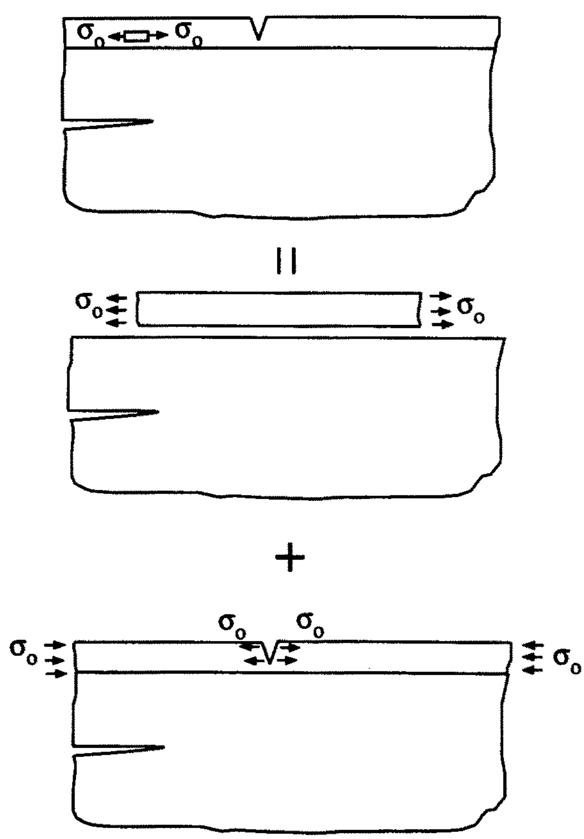

Fig. 1. Scheme of superposition for the film crack case.

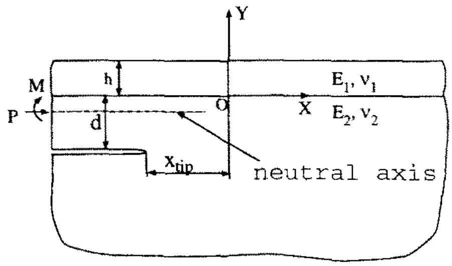

Fig. 2. Elasticity problem of steady-state cracking.

Suo and Hutchinson (1988)] and thus will not be presented here. The T stress is evaluated from the stress field on the crack surface near the crack tip from which the K_{II} field has been excluded.

3. RESULTS AND DISCUSSION

Problem I. Steady-state substrate cracking under general edge loading

The edge loadings, shown in Fig. 2, are considered to be independent. This problem was dealt with by Thouless *et al.* (1987) for the elastically homogeneous case and by Drory *et al.* (1988) and Suo and Hutchinson (1988) for the heterogeneous case. In both situations, the stress intensity factors can be written, via arguments of dimensional analysis and the path-independence of the J integral, as

$$K \equiv K_I + iK_{II} = a\frac{P}{\sqrt{2Ah}} + b\frac{M}{\sqrt{2Ih^3}}, \tag{6}$$

where

$$i = \sqrt{-1} \quad \text{and} \quad A = \lambda + \Sigma, \quad I = \{\Sigma[(1+\Delta)^3 - \Delta^3] + \Delta^3 - (\Delta - \lambda)^3\}/3 \tag{7}$$

in which

$$\Delta = \frac{\lambda^2 - \Sigma}{2(\lambda + \Sigma)}, \qquad \lambda = d/h$$

and the complex constants a and b satisfy the following consistency equations:

$$|a| = 1 \qquad \bar{a}b + a\bar{b} = 0 \qquad |b| = 1. \tag{8}$$

Thus

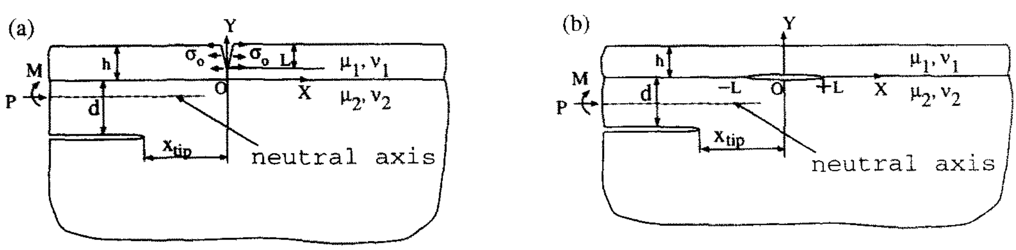

Fig. 3. Elasticity problems of crack interaction.

$$K = \left(\frac{P}{\sqrt{2Ah}} - \mathrm{i}\frac{M}{\sqrt{2Ih^3}}\right)e^{\mathrm{i}\omega}. \tag{9}$$

Hence analysis has to be carried out for only one loading case to find ω, which is a function of geometry and elastic mismatches, so as to fully determine the stress intensity factors for the general loading case. In the previous studies, the case $M = 0$ was always chosen for rigorous numerical computation. As pointed out before, $M \neq 0$ can be troublesome because it induces a term in the dislocation density which increases infinitely far away from the crack tip. This causes difficulty in evaluating integrals accurately. When T stresses and the interaction between cracks are the focus of our study, M cannot be taken to be zero because there is no analogue to eqn (9) relating P and M. We therefore include non-zero M in our calculations, and any combination of edge loadings can be fully analysed.

For a crack at a depth d below the interface, we calculated K_{I}, K_{II} and T for loadings P and M separately, and these quantities under combined loadings can be computed by linear superposition.

Particular attention is paid to the case in which the thin film is subject to residual tension (Fig. 1). Because the film is very thin, the residual stress σ_0 is assumed to be uniform across the film thickness and the resulting edge loadings are

$$P = \sigma_0 h, \qquad M = \sigma_0 h^2 \frac{\lambda(\lambda+1)}{2(\lambda+\Sigma)}. \tag{10}$$

The steady-state substrate crack depth is found by setting $K_{\mathrm{II}} = 0$ and the depth which is characteristic of the elastic mismatch of the structure is plotted in Fig. 4. Our result agrees very well with the graphic information extracted from Suo and Hutchinson (1988).

An apparently surprising result of our calculation is that the T stress for the steady-state substrate crack is *positive* (Fig. 5). Hence according to the Cotterell–Rice theory, the steady-state crack is directionally unstable. So it seems unlikely for the crack to maintain a straight path of propagation for a long distance. This apparently contradicts the experimentally established fact that the straight crack at some characteristic depth below the interface undergoes a steady-state propagation. Yet further consideration excludes the contradiction. It can be explained this way: When cracking begins in the substrate, the composite beam of materials from the upper surface of the crack to the free surface is short and dominated by compression which may give a *negative* T stress, but when the beam

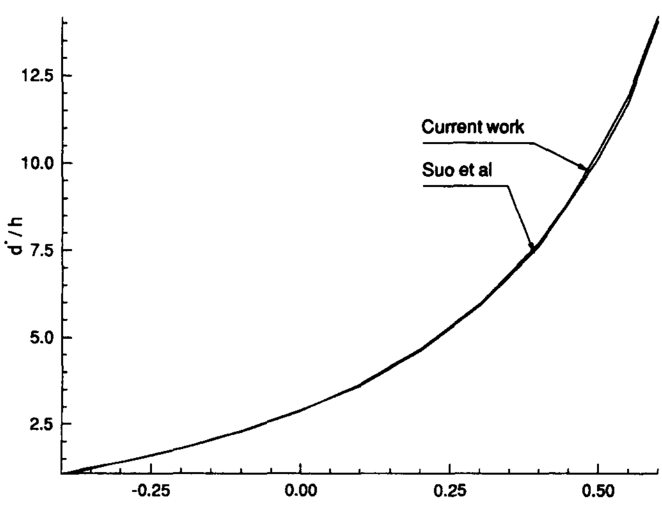

Fig. 4. Depth of steady-state substrate crack determined by $K_{\mathrm{II}} = 0$ criterion versus Dundurs parameter α.

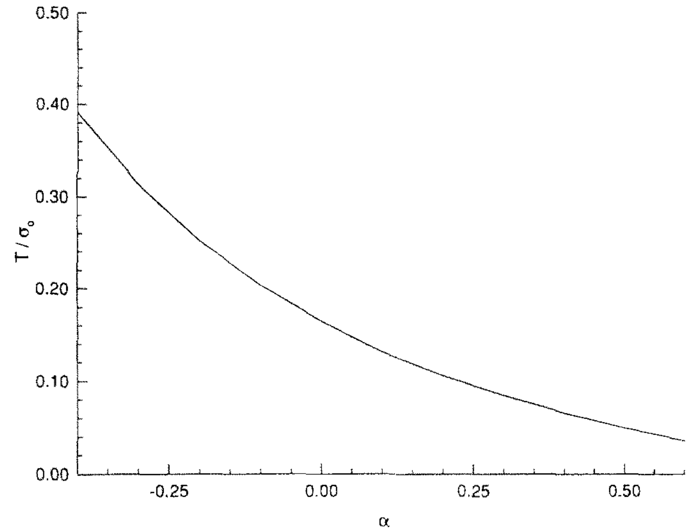

Fig. 5. T stress of the steady-state crack versus Dundurs parameter α.

becomes long enough, the bending effect caused by the moment M will dominate and cause a *positive* T stress.

The combination of the sign of the T stress and the stress intensity factors can be used to explain the cracking patterns of substrate at the three different stages of propagation as illustrated by Thouless *et al.* (1987).

As is well known, a substrate crack usually initiates at the edge of a specimen on the interface and after running along the interface for some distance, it will kink into the substrate (provided the substrate's toughness is lower than that of the interface). At the very early transitional stage of propagation, K_{II} is positive (Drory *et al.*, 1988) so the crack will kink deeply into the substrate. When the crack approaches the steady-state depth, K_{II} is near zero. However, the crack path may still not straighten. If the T stress is positive, the crack path is unstable and thus likely to fluctuate about a straight trajectory under the influence of any defects present in the system. Only if the T stress is negative will the crack path gradually approach the steady-state trajectory where $K_{II} = 0$, and travel on that depth. This is the stage of the *steady-state* propagation of the crack. We thus believe that there is a critical length L_c of the substrate crack such that, if the crack length is finite but smaller than L_c, the crack is stable ($T < 0$) while if the length is greater than L_c, then an unstable crack ($T > 0$) is expected. Since we have taken the crack to be semi-infinite, a positive T stress is a logical result. Further study is required to investigate and characterize this critical crack length L_c.

At the late stage of crack propagation, any small defect near the crack tip might drive the crack away from its original straight path, due to the positive T stress. Thus the positive T stress of a long substrate crack makes possible the buckling behavior observed in experiments by Thouless *et al.* (1987) and the wavy path found in experiments by Drory *et al.* (1988).

Problem II. Interaction with defects

In a film/substrate structure, if the film is flawless and the bonding is perfect, then under the residual tension in the film, a substrate crack tends to propagate along a straight path some characteristic depth beneath the interface. However, because of the directional instability of the crack propagation as discussed above, for an imperfect system, any existing defects near the crack tip could perturb its propagation and change its path. Experiments revealed the wavy path of a substrate crack in an alumina/silica structure. This path was attributed to micro-cracks inside the thin film, yet no explanation within the framework of current theory was provided (Drory *et al.*, 1988). Our work is aimed at rationalizing this phenomenon by Cotterell–Rice theory.

Cracking in the thin film is created by the residual tensile stress in the film. A microcrack is assumed to extend from the film's free surface in a direction perpendicular to the interface. Because the film is usually very thin, an edge crack in the film perpendicular to the interface is likely to reach the interface. For such a crack, the stress singularity is a function of elastic mismatch parameters and is, in general, not the square root (Kuang and Mura, 1964). But to focus our attention on the effects of interaction, the film crack length was taken to be less than the film thickness so that the crack is totally embedded in the homogeneous film, hence the stress singularity is always $-1/2$, regardless of the material mismatch. The interaction of the substrate crack with the film crack can be dealt with as an elasticity problem as shown in Fig. 3(a).

We consider the case in which the film crack does not advance. This assumption is justifiable if the toughness of the thin film is very large and its crack length sufficiently small. Our attention focuses on the stress intensity factors K_I, K_{II} and the T stress at the tip of the substrate crack; these are plotted versus the relative position of the substrate crack tip to the film crack in Figs 6–7.

Our calculations show that when the cracks are several film thicknesses apart or farther, the film cracking will induce a substantial negative K_{II} on the substrate crack which, if the film were flawless, would be under pure mode I loading. Thus, according to Cotterell–Rice theory, the substrate crack will deviate upward and the deviation angle from the straight path is approximately measured by $-2K_{II}/K_I$. Because of the positive sign of the T stress, the deviation is unstable. As the substrate crack approaches the film crack, at a distance several times the film thickness, the relative interaction will reach a maximum value and afterwards decrease rapidly to become negative; this implies that when the substrate crack is at a distance 1–2 film thicknesses away from the film crack or closer, it tends to be repelled.

The results of our calculations suggest that three cracking patterns are possible:

I. For a film of sufficiently low relative stiffness containing a large enough crack, the value of $-2K_{II}/K_I$ for the substrate crack can be as great as several degrees, and the T stress is substantial. Furthermore, the steady-state crack path is relatively close to the interface. It is thus reasonable to expect that the crack will deviate at a large angle toward the interface and finally run into it. Afterwards, under the very strong interaction between the two cracks, and provided that the toughness of the film is low enough, the crack will penetrate the film and coalesce with the vertical crack existing in the film. The result is the spalling of the structure as shown in Fig. 8(a).

II. In this case, the substrate crack deviates into the interface as above. But if the toughness of the film is very high, the crack is kept in the interface. After it has traveled away from the film crack, it will, as at the beginning of this process, once again kink into the substrate and eventually evolve into the steady-state path provided that there are no other film defects lying ahead. This pattern is shown in Fig. 8(b).

III. For a film which is stiffer than the substrate, the maximum value of the approximate deviation angle is not very large. Also, the T stress, though still positive, is smaller. Thus, the crack will deviate from the original straight path, but will not meet the interface. As the crack runs into a region close to the film crack, a positive K_{II} is induced, thus slowing the deviation and repelling the crack from the interface. When the substrate crack tip has passed the film defect by a large distance, the influence of the defect diminishes, so the crack ultimately settles down at the initial steady-state path. This mode of crack advance is illustrated in Fig. 8(c).

To determine the exact path of the crack, one has to carry out a step-by-step computation and make use of the K_{II} theory to find the position of the crack tip. Though, in principle, this poses no difficulty, the step-by-step calculation tracing the substrate crack from the far left of the film crack to its far right is very time consuming and hence is not performed.

We further considered the interaction of a substrate crack with an interfacial debonding. Such a debonding is a common defect found in film/substrate structures [Fig. 3(b)]. It may result from several sources. When the stress in the film is compressive, the decohesion

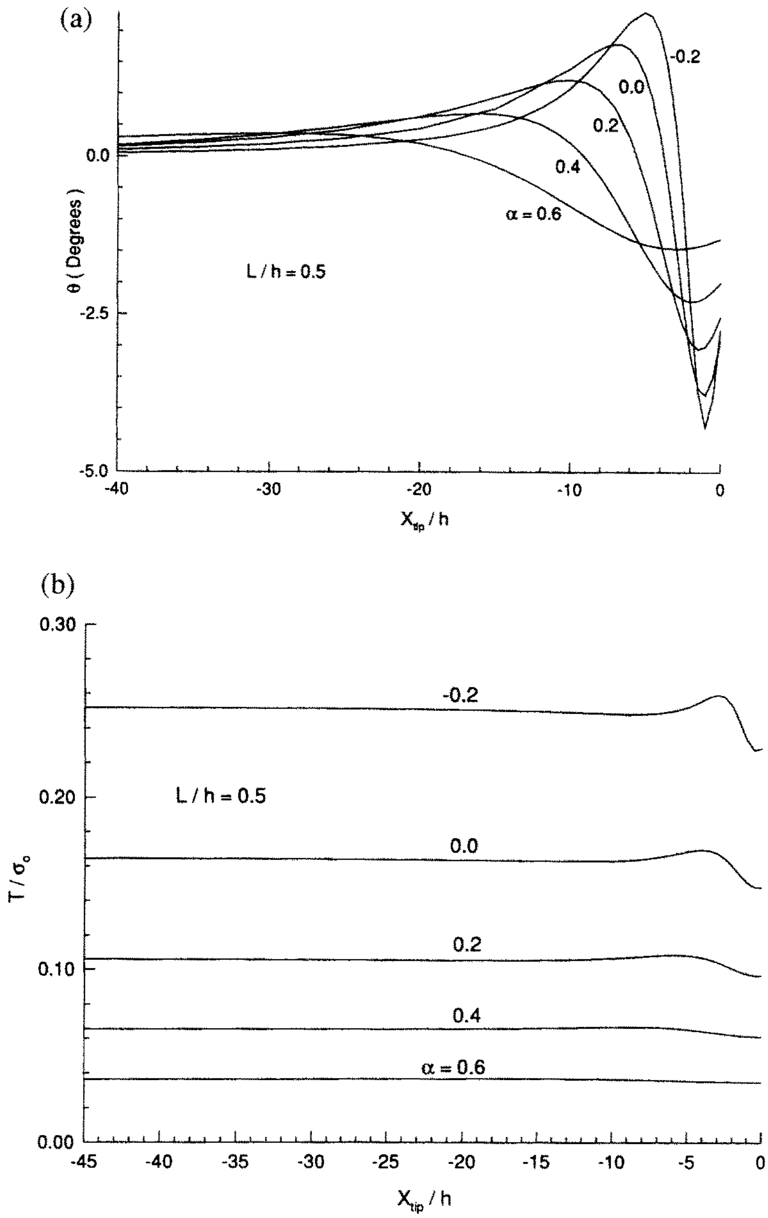

Fig. 6. Rate of deviation from the straight path (a) and the T stress (b) as a function of crack-tip position with relative film crack length $l/h = 0.5$.

or debonding involves buckling above an initial interface separation, followed by a delamination and eventual spalling (Drory *et al.*, 1988). For a film under residual tension, the debonding may be the result of edge crack or improper bonding of the film and substrate. Since the edge crack has been studied in the last problem, we will discuss exclusively pre-existing interfacial debonding. Such a decohesion will not advance because stress acts parallel to the interface and hence stress intensity factors are trivial. Its influence on the propagation of a substrate crack is discussed here. Our calculations show that for a crack starting infinitely far away from the debonded region at a characteristic depth so that K_{II} is zero, as the tip of the crack advances toward the debonding, the change in K_I is negligible and K_{II} is very small, virtually zero, even if the crack tip comes directly under the center of a large debonded area. The K_{II} argument will thus predict the path virtually unchanged, yet instability due to the positive T stress may cause a deviation due to the tiny value of K_{II}. The result of these two competing factors is not apparent and can be determined only

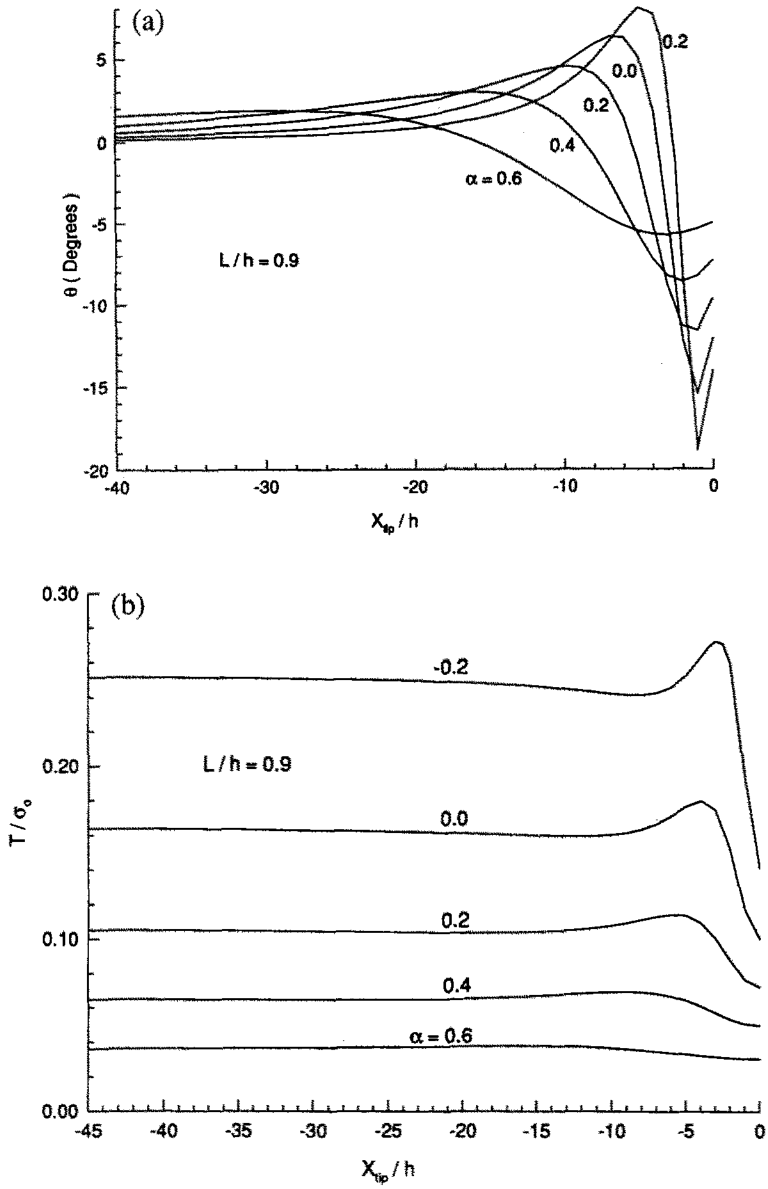

Fig. 7. Rate of deviation from the straight path (a) and the T stress (b) as a function of crack-tip position with relative film crack length $l/h = 0.9$.

through quantitative calculation. What one can expect is that the change of path caused by interfacial debonding will be considerably smaller than that by film cracking.

4. CONCLUDING REMARKS

This study has provided some insight regarding the directional stability of a crack in a brittle substrate driven by residual tension in the thin film. The steady-state crack which is governed by the $K_{II} = 0$ criterion is found to be directionally unstable when the crack is sufficiently long. Secondly, under the attraction of a film crack, the straight path of the substrate crack is deformed and may follow one of three patterns, depending on the relative toughness and elastic mismatches of the film and substrate and also on the film defect size. Finally, interfacial debonding seems not to cause as significant a disturbance on the path of the substrate crack as the film crack.

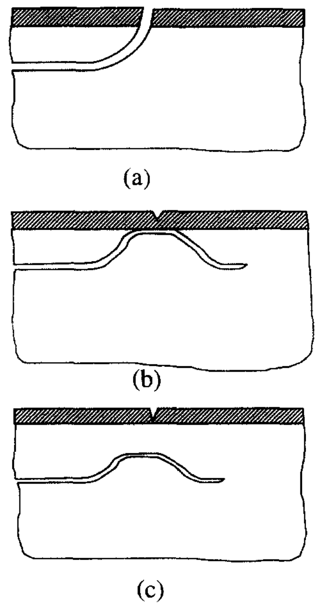

Fig. 8. Schematic illustration of crack patterns for film under residual tension.

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