Fracture in Thin Films

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4.2.1.i Fracture in Thin Films

Thin films are grown on substrates in many technologies. Examples include zirconia coatings as thermal barriers on superalloys in engines, silicon nitride films as environmental barriers on metals and polymers in microprocessors, and gallium nitride films as optoelectronic materials on sapphire substrates in light-emitting diodes. Residual stresses may cause cracks to grow in the film, or in the substrate, or on the film-substrate interface. The phenomena have long been a nuisance in daily life: paints peel and pavements crack. Systematic applications of fracture mechanics to film-substrate composites started in the 1980s. Hutchinson and Suo (1991), and Evans and Hutchinson (1995) have provided extensive reviews. This article outlines empirical observations, theoretical concepts, and research trends.

1. Origins of Stress

As a film grows on a substrate at a fixed temperature, T_G, a mismatch strain field arises in the film due to, e.g., defects annihilation, epitaxy, phase transition, and new material growing into grain boundaries in the film (Evans and Hutchinson 1995, Tolpygo *et al*. 1998). The film accommodates the mismatch by inelastic and elastic deformation. It is usually difficult to predict from first principles the stress generated in the film during growth. In practice, the growth stress is measured experimentally by using methods such as wafer bending, X-ray diffraction, and luminescence piezospectroscopy (Nix 1989, Ma and Clarke 1993). Unless otherwise stated we assume that the substrate is much thicker than the film, and both are flat. We further assume that the stress field developed during film growth is uniform throughout the film, and equal biaxial in the plane of the film. Under these assumptions, the substrate is stress-free.

After the film is grown, the temperature may be changed from T_G to a different level, T. The thick substrate acquires a thermal strain, but remains stress-free. The film also acquires a thermal strain, which differs from that of the substrate by

$$\varepsilon_T = \int_{T_G}^{T} (\alpha_f - \alpha_s) dT , \tag{1}$$

where α_f and α_s are the thermal expansion coefficients of the film and the substrate. When the film and the substrate are well bonded, the net in-plane strain in the film must be the same as the thermal strain of the substrate. Consequently, the mismatch strain, Eqn. (1), need be accommodated by elastic and inelastic deformation in the film. If the film remains elastic during the temperature change, this mismatch strain induces a biaxial stress in the plane of the film, σ_T, given by

$$\sigma_T = \frac{E_f \varepsilon_T}{1 - \nu_f} , \tag{2}$$

where E_f is Young's modulus and ν_f is Poisson's ratio of the film.

Additional stress can be generated by, e.g., a bending moment applied to the film-substrate composite. Indentation and scratching are other means to generate stress; however, the stress field so generated is complicated and is beyond the scope of this article. The total stress in the film is the sum of the growth stress, the thermal stress, and the applied stress.

2. Crack Driving Force and Crack Resistance

Following the Linear Elastic Fracture Mechanics, we adopt a crack growth approach. Cracklike flaws are assumed to pre-exist in the film, in the substrate, and on the interface. When the stress in the composite is large enough, one of the flaws will grow. The crack driving force, *G*, is the elastic energy reduction associated with the crack advancing per unit area. For a given crack geometry, the crack driving force is calculated by solving an elasticity boundary value problem. The crack resistance, Γ, is the energy needed to advance the crack per unit area. A crack cannot grow when the driving force is below the resistance, and grows when the driving force equals the resistance.

The crack resistance is measured experimentally for a crack running in the film, or in the substrate, or on the interface. The three locations have different values of crack resistance, denoted as Γ_f, Γ_s and Γ_i. The crack resistance also depends on the environment and the crack velocity. For a crack running on the interface, the crack resistance in addition depends on the interfacial chemistry, the interfacial morphology, and the mode mixity. Experimental methods to determine the crack resistance in film-substrate composite are discussed by Evans and Hutchinson (1995).

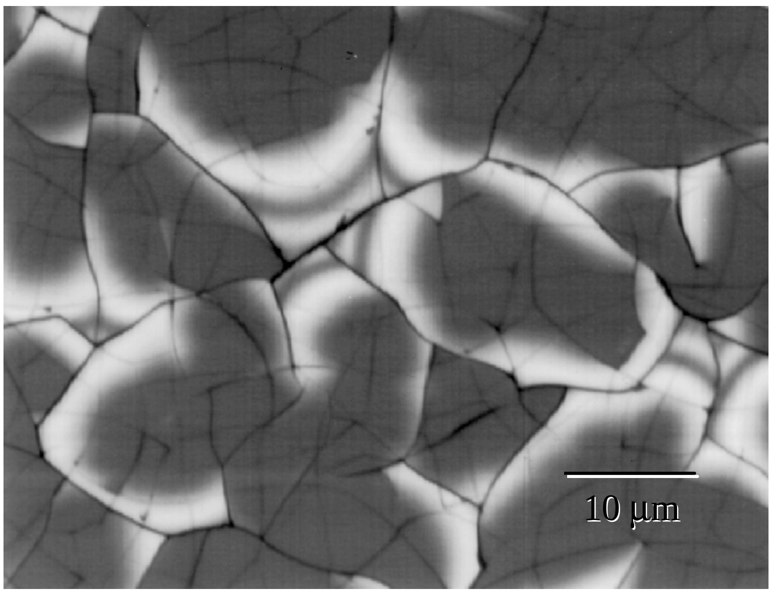

Figure 1. A plan view of a silicon nitride film of about 1 μm thick grown on a silicon substrate. The tensile stress in the film causes channel cracks. The contrast indicates that the film also partially debonds from the substrate. (Courtesy of Q. Ma of Intel Corp)

3. *Cracking in a Film under Tension*

If a film is under tension and is brittle, a possible failure mode is cracking in the film. Starting from a flaw in the film, a crack runs across the film thickness. For the time being, the crack is taken to arrest at the interface, leaving the interface and the substrate intact. The crack, however, elongates laterally in the film, uninhibited until it meets a film edge or another crack. The lateral crack length can be many times the film thickness. Such a crack is known as a channel crack. Because the film may have many pre-existing flaws, under a large stress, many channel cracks can form. A cracked film looks like a field of dry mud (Fig. 1).

The complex morphology of a cracked film is difficult to quantify. A more practical question, Can the film sustain a given stress without cracking? Consequently, attention is focused on the formation of the first channel crack, originated from the worst pre-existing flaw in the film. For the time being both the film and the substrate are taken to be elastic. Let *h* be the film thickness, σ the stress in the film, and *a* the size of the pre-existing crack in the film. Figure 2 distinguishes two cases. In case A, the pre-existing crack size is much smaller than the film thickness, $a \ll h$, so that the crack front runs both toward the interface and laterally in the film. The crack driving force is given by

$$G = 3.94 \frac{\left(1 - \nu_f^2\right)\sigma^2 a}{E_f} . \tag{3}$$

This expression comes from an edge crack of depth *a* in an infinite homogeneous material. The form of the equation applies to cracks of other shapes, with the numerical coefficient being shape-dependent (Tada *et al.* 1985). The pre-existing crack grows when the crack driving force equals the crack resistance, namely,

$$3.94 \frac{\left(1 - \nu_f^2\right)\sigma^2 a}{E_f} = \Gamma_f . \tag{4}$$

Once started, the crack will grow and form a channel. In condition (4), the crack resistance, Young's modulus, and Poisson's ratio are all material constants. Consequently, the critical stress needed to form a channel crack varies with the size of the pre-existing flaw. Flaws are generated during film growth or subsequent use, and measuring the flaw sizes on a routine basis is impractical. Condition (4) is therefore difficult to use.

The above consideration leads us to examine case B illustrated in Fig. 2. When the pre-existing crack size is comparable to the film thickness, $a \approx h$, the crack can only elongate laterally in the film. When the lateral crack length exceeds several times the film thickness, the driving force at the growing front attains a steady-state value, given by (Hutchinson and Suo 1992)

$$G = \beta \frac{\left(1 - \nu_f^2\right)\sigma^2 h}{E_f}. \tag{5}$$

The dimensionless number β depends on the elastic constants of the film and the substrate. When the substrate is stiffer than the film, β is between 1 to 2. When the substrate is much more compliant than the film, β can be very large.

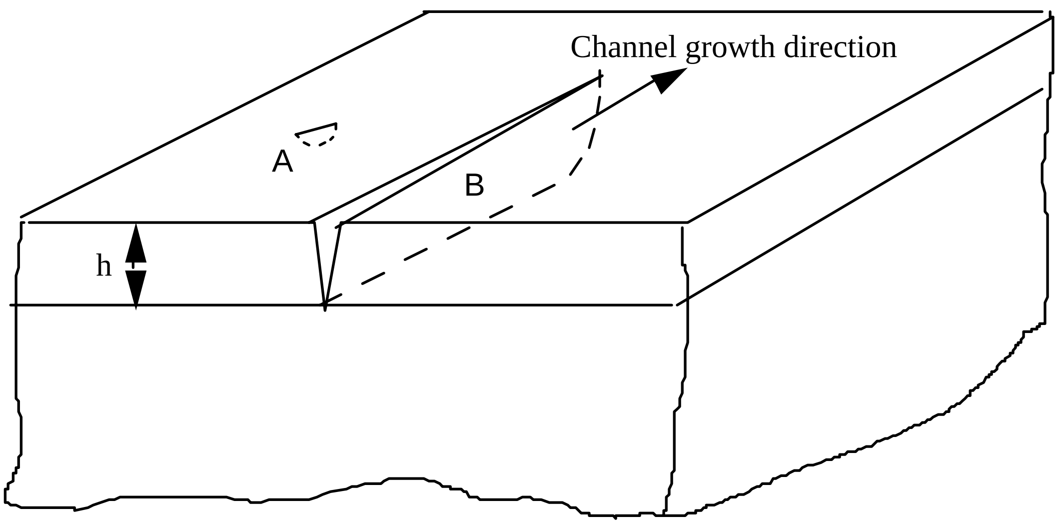

Figure 2 Case A: the initial flaw size is much smaller than the film thickness. Case B: the initial flaw size is comparable to the film thickness.

For a given film-substrate composite, Eqn. (5) gives the largest driving force for flaws of any size to form a channel. Consequently, regardless of the details of the initial flaws, no channel can form if this driving force is below the crack resistance, namely,

$$\beta \frac{\left(1 - \nu_f^2\right)\sigma^2 h}{E_f} < \Gamma_f. \tag{6}$$

This condition depends on the film thickness, rather than on the pre-existing flaw size. When the condition is satisfied, no channel can form. When the condition is violated, channels may or may not form. Because the lateral dimension of a film is typically much larger than the film thickness, the probability is high to have flaws, especially at film edges, that are comparable to the film thickness. It is therefore prudent to use condition (6) as a conservative design rule. It frees the designer from inquiring into the details of the flaws. The rule, however, does become overly conservative when the pre-existing flaws are much smaller than the film thickness (Leung *et al*. 1995). Furthermore, for a film on a very compliant substrate, as mentioned above, β is very large, condition (6) may be difficult to satisfy. In this case a knowledge of initial flaw size becomes indispensable, and the designer need to find a way to use a flaw-based condition like Eqn. (4).

4. Debonding of a Film under Tension

A film under a tensile stress may debond from the root of a channel crack (Fig. 1), or from the edge of the film (Fig. 3). When the debond length exceeds several times the film thickness, the debonding process attains a steady-state, and the driving force becomes independent of the debond length. Under the plane strain conditions, the debond driving force is given by

$$G = \frac{\left(1 - \nu_f^2\right)\sigma^2 h}{2E_f}. \tag{7}$$

The film debonds steadily when the driving force equals the resistance, $G = \Gamma_i$.

The debond crack is under mixed mode loading. For example, when the film and the substrate have identical elastic constants, the tensile residual stress in the film, σ, gives rise to both mode I and mode II stress intensity factors at the debond crack tip:

$$K_I = \sigma\sqrt{\frac{h}{2}}\cos\omega, \quad K_{II} = \sigma\sqrt{\frac{h}{2}}\sin\omega, \tag{8}$$

with $\omega \approx 52°$. Effect of modulus mismatch between the film and the substrate has been discussed in Hutchinson and Suo (1991). The debond resistance Γ_i depends on the mode mixity.

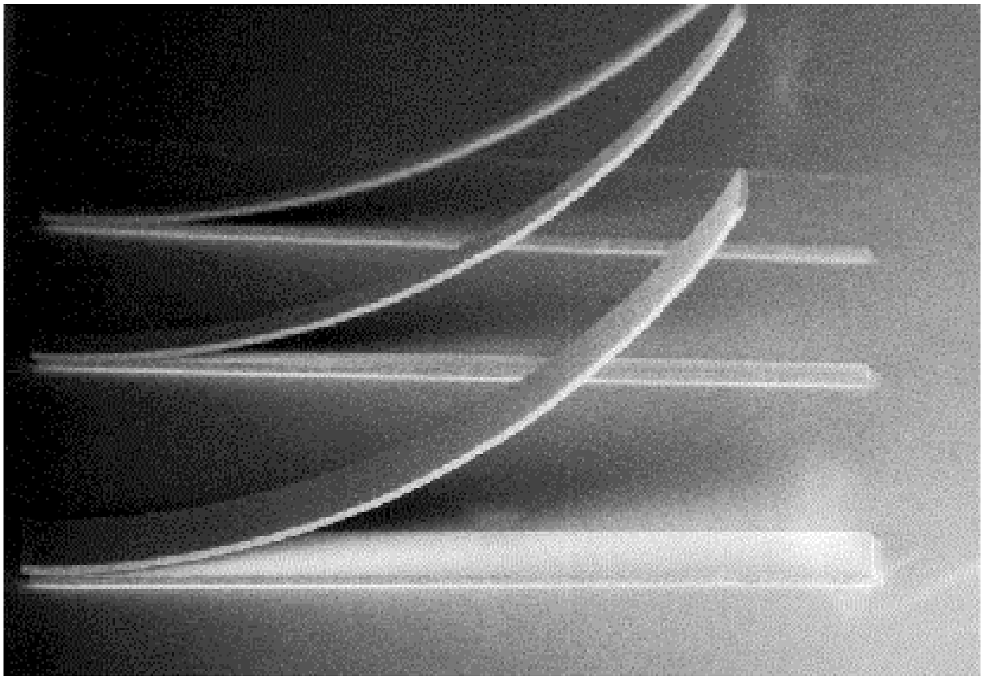

Figure 3 Debond from an edge of the film, driven by residual tensile stress in the film. When the debond front approaches the other edge of the film, the debond driving force decreases, so that the debond arrests before it reaches the film edge. (Courtesy of Q. Ma of Intel Corp)

5. Debonding of a Film under Compression

When a film is under compression, it may still debond from the substrate, but will do so in quite different manners from a film under tension. To appreciate basic behaviors, first assume the plane strain conditions. Figure 4 illustrates a debond crack initiated from an edge of a film under compression. The debonded film remains in contact with the substrate. This can be understood as follows. If the two crack faces were not in contact, they would be traction-free, and the stress intensity factors would be given by Eqn. (8). The residual stress in the film is now compressive, so that $K_I < 0$, suggesting that the crack should be in contact. The two crack faces may slide relative to each other against friction. Such a crack will stop after a certain length. Assume that the sliding friction has a constant value, τ_0. The crack length l may be estimated by the shear lag model. Force balance of the sliding segment of the film requires that $l\tau_0 = \sigma h$.

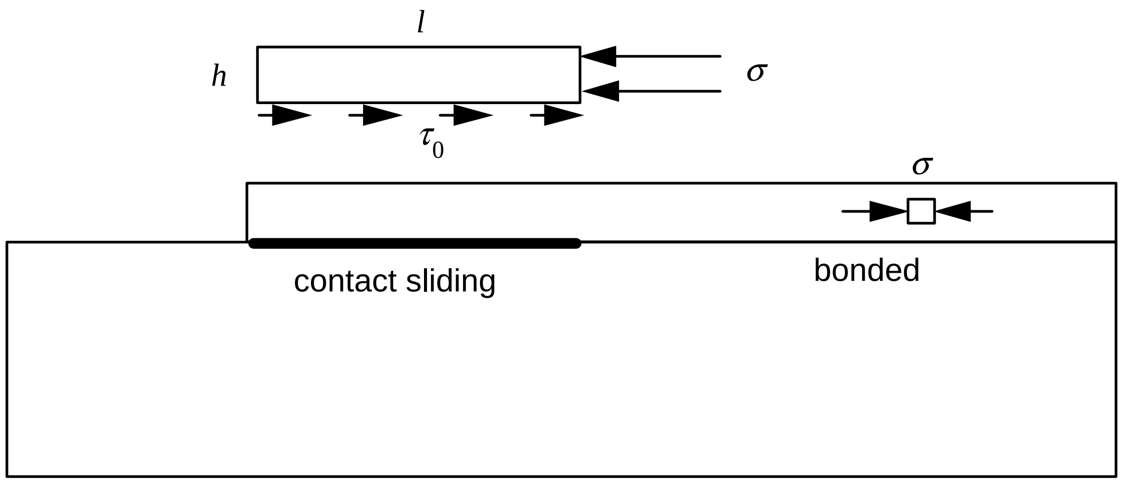

Figure 4 A debond crack initiated from an edge of the film.

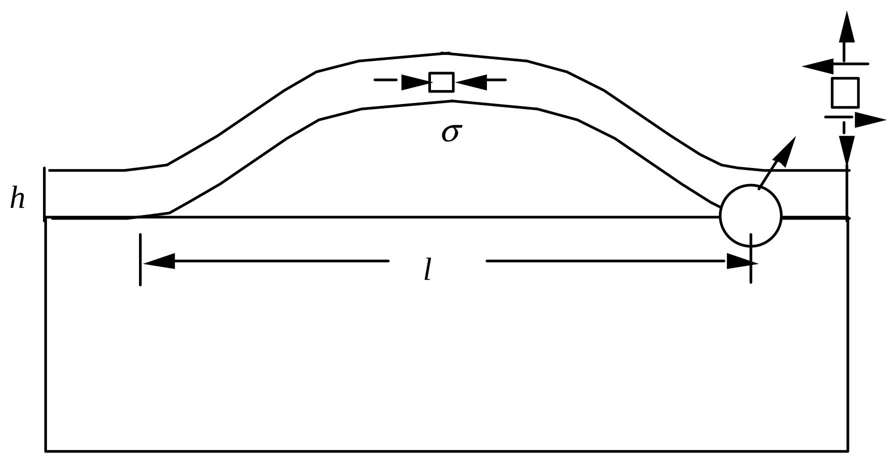

Figure 5 After the unbonded film buckles, stress arises on the interface.

Next consider debond underneath a film, far away from the edges of the film. When the film is perfectly bonded with the substrate, the film is under compression, but the interface is stress-free. Even when an area underneath the film is unbonded, so long as the film remains flat, there is no stress acting on the interface. However, a large enough area of unbonded film may buckle (Fig. 5). After buckling, on the interface at the buckle front both normal and shear stresses develop, which may motivate the unbonded area to grow like a crack.

Three aspects need be considered: pre-buckling development of an unbonded area, buckling of the unbonded film, and post-buckling growth of the unbonded area. Despite their practical significance, pre-buckling processes are little understood beyond a few qualitative observations. A dirty substrate may lead to large unbonded areas after the film is grown. Voids are sometimes seen on the interface. Further research into the pre-buckling processes holds a key to averting failure of films under compression.

By contrast, film buckling is well understood. If the film has a sufficiently large unbonded area, the film over the area buckles. The critical unbonded length for buckling, l_c, is given by

$$\frac{l_c}{h} = \frac{\pi}{\sqrt{3\left(1-\nu_f^2\right)}}\left[\frac{E_f}{-\sigma}\right]^{1/2}. \tag{9}$$

This expression comes from Euler's solution of a buckling column, adjusted for the plane strain conditions. The form of the equation applies to an unbonded area of any shape, with the numerical coefficient being shape-dependent. Taking $-\sigma / E = 10^{-2}$, which is a quite large elastic strain, condition (9) gives $l_c \approx 20h$. Such a large unbonded area is not usually produced in film growth. To avert failure, it pays to investigate the pre-buckling processes that produce large unbonded areas.

Several post-buckling behaviors have been studied (Hutchinson and Suo 1991, Gioia and Ortiz 1997). A large unbonded area can buckle into complicated shapes, an example of which is shown in Fig. 6. Unlike a debond crack initiated from a film edge, a debond crack initiated from a buckled film does have an opening component at the crack front. However, when the crack enlarges, the opening component reduces, and the crack approaches the pure sliding mode. The situation becomes indistinguishable from a debond crack initiated from the film edge. Consequently, a debond buckle under the plane strain conditions will arrest by friction. Similarly, a circular (or any equiaxed) debond buckle cannot grow indefinitely. A debond buckle, however, can grow like a tunnel underneath the film, uninhibited laterally until it approaches another tunnel or an edge of the film (Fig. 7). Initiated from isolated unbonded areas, the tunnels can cause the entire film to disintegrate.

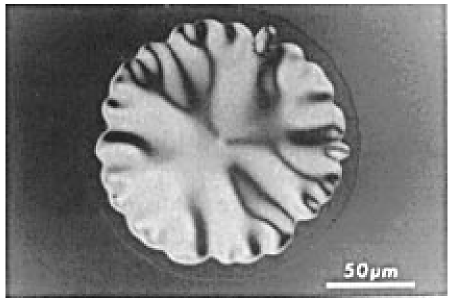

Figure 6 A buckled area in a SiC film on a Si substrate. The outer ring surrounding the buckled film is the zone in which radial slippage occurs. (Argon et al. 1989).

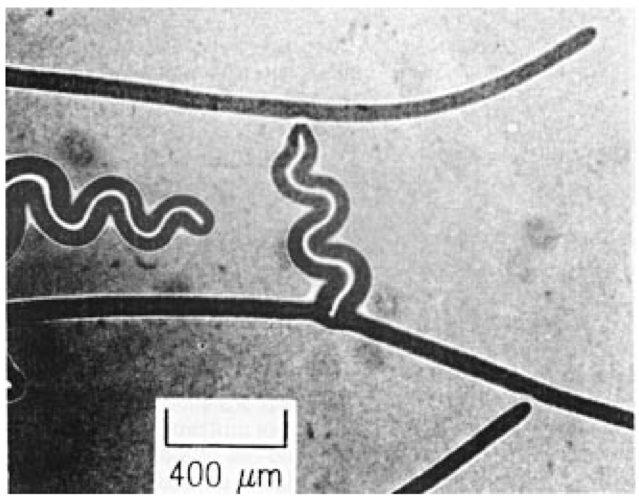

Figure 7 In this plan view of an amorphous silicon film on a glass substrate, debond tunnels grow underneath the film, either straight-sided or meandering (Thouless, 1993).

6. Cracking in Substrate

When the film is under tension and the substrate is brittle, a crack from a film edge or a channel root can enter into the substrate. Under the residual stress, and when the film is much thinner than the substrate, the crack driving force is small when the crack front is deep into the substrate (Ye *et al*. 1992). The crack may, however, grow in the substrate parallel to the interface (Fig. 8). The spacing between the crack and the interface is selected because a crack in a brittle, isotropic, homogeneous material seeks a path to attain the mode I condition at the crack tip (Thouless *et al*. 1987).

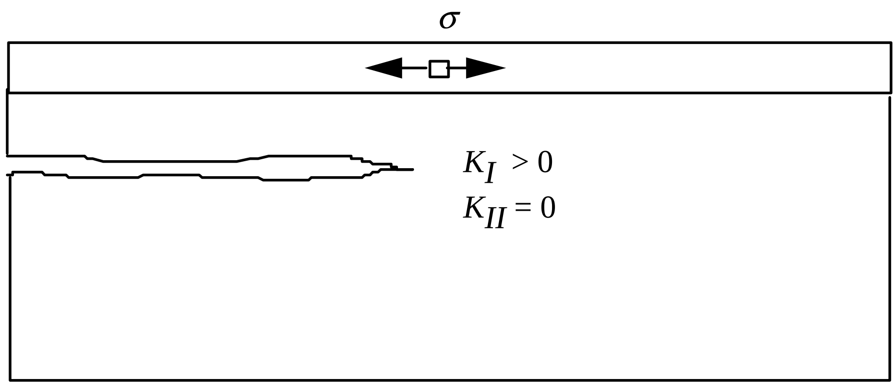

Figure 8 Substrate cracking under a film in tension.

When the film is under residual compression, if the substrate is not too thick, significant tensile residual stress exists in the substrate. For example, after a GaN film is grown on a thin sapphire substrate, upon cooling the film goes into compression and the substrate goes into tension. Cracks grow in the sapphire substrate (Fig. 9, D.R. Clarke, private communication).

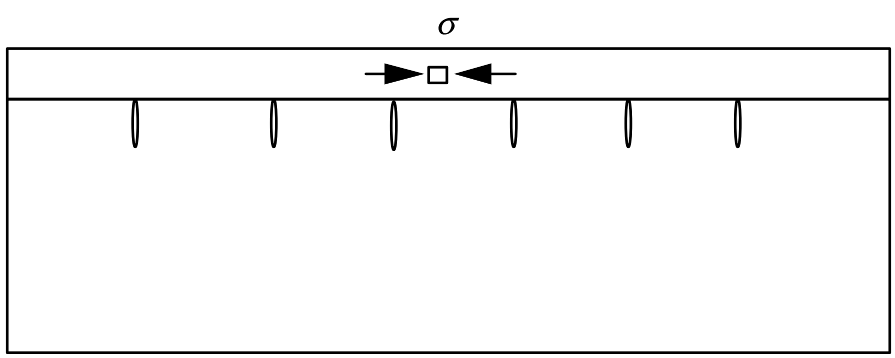

Figure 9 Substrate cracking under a film in compression.

7. Roles of Inelastic Deformation

In the above, we have applied the Linear Elastic Fracture Mechanics (LEFM) to film-substrate composites. A main requirement of the LEFM is that the inelastic zone around the crack tip must be much smaller than the film thickness. The inelastic deformation within the small zone is accounted for by the crack resistance. In computing the crack driving force, both the film and the substrate are taken to be elastic. When the inelastic zone is large compared to the film thickness, however, we must consider the inelastic deformation more explicitly. The following examples illustrate several roles played by plasticity.

First consider a brittle film on a thick, ductile substrate. The film is under tension and is prone to channel cracking (Fig. 2b). Because the film is elastic, the crack driving force at the channel front is well defined. To calculate the driving force, the plastic deformation in the substrate must be accounted for in the boundary value problem. If the substrate were elastic, it would constrain the opening displacement of the channel, so that the driving force at the channel front would be small. This constraint is reduced when the substrate deforms plastically (Bueth and Klingbeil 1996, Hu and Evans 1989). Consequently, the plastic deformation in the substrate promotes channel cracking in the film.

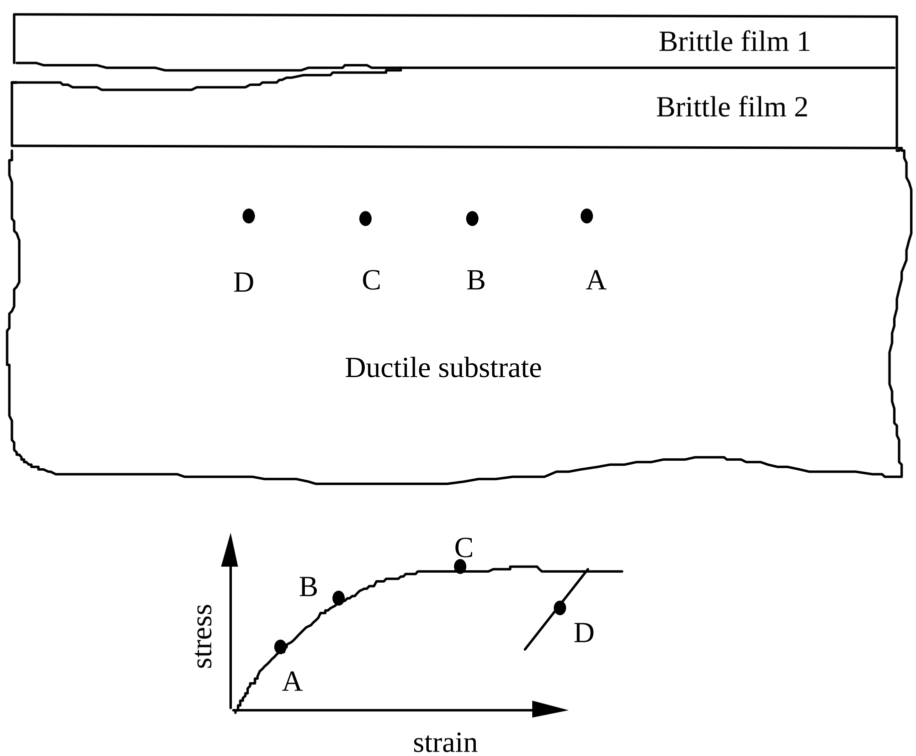

Figure 10 As the crack tip passes by, a material particle in the substrate undergoes a history of deformation: elastic (A), yielding (B), plastic straining (C), and elastic unloading (D).

As a second example, consider a two-layer film on a ductile substrate (Fig. 10). The two materials constituting the film are both elastic, and the crack runs on the interface between them. Because the crack runs on the interface between two elastic materials, one can prescribe the debond resistance Γ_i for this interface, and account for plasticity in the substrate in the boundary value problem in calculating the crack driving force (Suo *et al*. 1993). The plastic hysteresis in the substrate costs energy, and makes the debond crack more difficult to grow.

A third example involves a crack on the interface between a film and a substrate, and yielding can take place either in the film or in the substrate. In all the above discussions, the crack tip is taken to be a structureless mathematical point, and the crack resistance a material constant. When one or both materials deform plastically, the crack tip on the interface blunts, the crack driving force cannot be defined at the crack tip, and there is no unambiguous way to partition plasticity between the crack resistance and the crack driving force. To circumvent this difficulty, we must describe the fracture process with more details than a structureless crack tip equipped with a constant crack resistance. Exactly what details should be included in a model depends on the purpose of the model. At one extreme, we can include all the individual atoms. Such a detailed model, however, may never replace the one-parameter fracture mechanics in practice. Less detailed descriptions are being considered. An economic description is the cohesive zone model, which describes the fracture process by a relation of the separation and the traction between the two crack faces. When the cohesive zone is embedded in materials described by continuum plasticity, the model provides a framework to correlate experimental results; see Hutchinson and Evans (1999) for a review.

8. Summary and Outlook

When constituent materials are elastic, a large body of knowledge exists. The smallness of the film thickness allows one to use a conservative design rule that does not require the knowledge of flaw size. When either the film or the substrate is inelastic, but the crack front is inside an elastic material, inelasticity can be accounted for in the boundary value problem in calculating the driving force. When the crack front is inside an inelastic material, the fracture process must be described with details beyond a constant crack resistance. Theoretical efforts so far have been restricted to time-independent plasticity and monotonic temperature change. The effects of cycle- and time-dependent deformation on thin film fracture remain largely unexplored. The extension of fracture mechanics to small structures more complex than thin films becomes urgent as new interconnect materials are being introduced in the microelectronics industry. For structures of small feature sizes, such as microprocessors and micro-electro-mechanical systems, crack nucleation may take longer time than crack growth. Consequently, the crack growth approach as embodied in the fracture mechanics is doomed. These challenges await serious studies.

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