Interfacial fracture

Readings

J.R. Rice. Elastic fracture mechanics concepts for interfacial cracks. *J. Appl. Mech.* 1988, **55**, 98-103. (http://esag.harvard.edu/rice/139_Ri_ElFracMechInterf_JAM88.pdf)

J.W. Hutchinson and Z. Suo, "Mixed-mode cracking in layered materials", *Advances in Applied Mechanics*, **29**, 63-191 (1992). (http://www.deas.harvard.edu/suo/papers/139.pdf)

References in the following notes can be found in

Z. Suo, Reliability of interconnect structures. pp. 265-324 in Volume 8: Interfacial and Nanoscale Failure (W. Gerberich, W. Yang, Editors), Comprehensive Structural Integrity (I. Milne, R.O. Ritchie, B. Karihaloo, Editors-in-Chief), 2003. (http://www.deas.harvard.edu/suo/papers/139.pdf)

The Williams singularity

Consider a crack on the interface between two elastic materials. The difference in the elastic constants of the two materials affects the stress field. Williams (1959) discovered that the singular stress field at the interface crack tip is not square root singular. The stresses on the interface a distance r ahead of the crack tip take the form

$$\sigma_{22} + i\sigma_{12} = \frac{Kr^{i\varepsilon}}{\sqrt{2\pi r}}.$$

The notation of complex numbers is used: $i = \sqrt{-1}$ and $r^{i\varepsilon} = e^{i\varepsilon \ln r} = \cos(\varepsilon \ln r) + i\sin(\varepsilon \ln r)$. The bimaterial constant ε is defined by

$$\varepsilon = \frac{1}{2\pi} \ln\left[\frac{(3-4\nu_1)/\mu_1 + 1/\mu_2}{(3-4\nu_2)/\mu_2 + 1/\mu_1} \right],$$

where ν is Poisson's ratio, μ the shear modulus, and the subscripts 1 and 2 refer to the two materials. The constant is bounded, $|\varepsilon| < (1/2\pi)\ln 3 \approx 0.175$.

The stress intensity factor K is complex-valued, and therefore contains two real parameters, analogous to the mixed mode crack in a homogeneous material. According to Irwin's Doctrine, the two parameters are the messengers between the external load and the crack tip process.

The stress intensity factor has the dimension

$$K = [\text{stress}][\text{length}]^{1/2 - i\varepsilon}.$$

The energy release rate

The amplitude of the stress intensity factor has the familiar dimension, $|K| = [\text{stress}][\text{length}]^{1/2}$. Indeed, $|K|$ relates to the energy release rate as

$$G = \frac{1}{2}\left(\frac{1}{\overline{E}_1} + \frac{1}{\overline{E}_2}\right)\frac{|K|^2}{\cosh^2(\pi\varepsilon)} .$$

Mode angle

Following Rice (1988), we define the mode angle ψ by

$$K = |K|l^{-i\varepsilon}\exp(i\psi),$$

where l is an arbitrary length.

Stress oscillation

To see the consequence of this definition, write

$$\sigma_{22} + i\sigma_{12} = \frac{|K|}{\sqrt{2\pi r}}e^{i[\psi+\varepsilon\ln(r/l)]} .$$

The ratio of the shear stress to the tensile stress is

$$\sigma_{12}/\sigma_{22} = \tan[\psi + \varepsilon\ln(r/L)].$$

When $\varepsilon = 0$, as for a crack in a homogenous material, the ratio σ_{12}/σ_{22} is independent of the distance r in the K-annulus, and the mode angle ψ characterizes the relative portion of shear to tension. When $\varepsilon \neq 0$, the ratio σ_{12}/σ_{22} varies with the distance r, and equals $\tan\psi$ at $r = l$. The variation is not rapid, because ε is small and because a logarithm is a slowly varying function. Thus, $\tan\psi$ approximates the ratio σ_{12}/σ_{22} so long as r is not far from l. For a brittle interface, a natural choice is $l = 1$ nm, representative of the bond breaking zone size. With this choice, the mode angle ψ represents the relative portion of shear to tension at the size scale of bond-breaking zone.

Small scale contact

In a homogeneous material, crack faces come into contact under compression. By contrast, interface crack faces may come into contact even the remote load has a tensile component. When the contact zone is large, one has to take into account of the forces on the crack faces in solving the boundary value problem. In many situations, however, the contact zone is small compared to the overall dimension. Consequently, the K-annulus exists, with the inner radius enclosing the contact zone, as well as the bond-breaking process zone. Rice (1988) has examined the condition for small-scale contact.

Williams's elastic solution shows that the displacement jump at a distance r behind the crack tip is

$$\delta_2 + i\delta_1 = \left(\frac{1}{\overline{E}_1} + \frac{1}{\overline{E}_2}\right)\frac{Kr^{i\varepsilon}}{2(1+2i\varepsilon)\cosh(\pi\varepsilon)}\sqrt{\frac{2r}{\pi}} .$$

The jump in the displacement component normal to the crack faces is

$$\delta_2 = \delta \cos\left[\psi + \varepsilon \ln(r/l) - \tan^{-1}(2\varepsilon)\right],$$

where $\delta = \left(\delta_1^2 + \delta_2^2\right)^{1/2}$ is the magnitude of the displacement jump. If the crack is required to be open within $l < r < 100l$, the mode angle must be restricted within

$$-\pi/2 + 2\varepsilon < \psi < \pi/2 + 2.6\varepsilon, \text{for } \varepsilon > 0$$
$$-\pi/2 - 2.6\varepsilon < \psi < \pi/2 + 2\varepsilon, \text{for } \varepsilon < 0$$

The number 100 is arbitrary, but the above conditions are insensitive to this number. When $\varepsilon = 0$, the above condition simply says that the contact does not occur when the crack is under tension, which is known for homogeneous materials.

Example 1: A small crack on the interface

For a given crack configuration, the stress intensity factor K is determined by solving the elasticity boundary value problem. Finite element method and other numerical methods have been developed to determine the stress intensity factor (Matos et al., 1990). Hutchinson and Suo (1991) have compiled solutions for layered materials.

As an example, consider a crack, length $2a$, on the interface between two semi-infinite materials, subject to remote tensile stress σ and shear stress τ. Write $\sigma + i\tau = Te^{i\omega}$, so that T is the magnitude, and ω the direction, of the remote load. This elasticity boundary value problem has been solved analytically, giving the stress intensity factor (Rice, 1988)

$$K = (1 + 2i\varepsilon)\sqrt{\pi a}(2a)^{-i\varepsilon}Te^{i\omega}.$$

The mode angle is

$$\psi = \omega + \tan^{-1}(2\varepsilon) + \varepsilon \ln(l/2a).$$

When $\varepsilon = 0$, the mode angle ψ equals the angle ω of the remote load. The two angles are different when $\varepsilon \neq 0$. Consider representative values, $\varepsilon = -0.05$, l = 1 nm, and $2a$ = 1 mm. Under remote tension, $\omega = 0$, one finds that $\psi = 34°$, indicating a significant shear component near the crack tip, at the size scale of bond breaking zone.

Example 2: Thin film debonding

As a second example, consider the debond of a thin film from a substrate. A film, thickness h, is under a tensile inplane stress σ and initially bonded to the substrate. The film may debond from the root of a channel crack, or from the edge of the film. When the debond length exceeds several times the film thickness, the debonding process attains a steady-state, in which the energy release rate is independent of the debond length. Under the plane strain conditions, an elementary consideration gives the energy release rate

$$G = \frac{\sigma^2 h}{2\overline{E}_f}.$$

The debond crack is under the mixed mode conditions. The mode angle must be determined by solving the elasticity boundary value problem. When the film and the substrate have similar elastic constants, the stress intensity factors are given by the previous lecture, setting $P = \sigma h$ and $M = 0$. The mode angle is $\psi \approx 52°$.

Next examine the effect of the modulus mismatch on the mode angle. The complex stress intensity factor is given in the form

$$K = |K| h^{-i\varepsilon} e^{i\omega}.$$

The magnitude $|K|$ relates to the energy release rate. The angle ω depends on elastic mismatch between the film and the substrate, ranging between 40° to 60° if the mismatch is not excessive, as tabulated in Suo and Hutchinson (1990). The mode angle is

$$\psi = \omega + \varepsilon \ln(l/h).$$

For representative values, $\varepsilon = -0.05$, l = 1 nm, and h = 1 μm, the additional angle is $\varepsilon \ln(l/h) = 20°$.

Interfacial fracture energy

When a debond crack extends on a bimaterial interface, mixed mode conditions usually prevail. The fracture energy is a function of the mode angle, $\Gamma(\psi)$. The crack extends when the energy release rate reaches the fracture energy: $G = \Gamma(\psi)$. Due to elastic mismatch in the two materials, one should specify the length l in defining the mode angle ψ. The curve $\Gamma(\psi)$ has been measured for a few interfaces (e.g., Cao and Evans, 1989; Wang and Suo, 1990; Liechti and Chai, 1991). Figure 17 sketches the trend of the $\Gamma(\psi)$ curve. The fracture energy tends to increase as mode angle approaches $\pm \pi/2$. The energy cost for debond varies with the relative proportion of opening and shearing modes, because, e.g., a large amount shear may promote more inelastic deformation in the constituent materials, or promote near-tip sliding against roughness if the interface is not perfectly flat. The curve $\Gamma(\psi)$ need not be symmetric with respect to $\psi = 0$, because the two materials on either side of the interface are dissimilar, breaking the symmetry between $\psi < 0$ and $\psi > 0$. Evans and Hutchinson (1995) have reviewed many test configurations for measuring interfacial fracture energy.

Sandwich specimens

A class of test methods has been particularly versatile for thin film structures. Suppose one needs to measure the interfacial fracture energy of a thin film of material 1, and a substrate of material 2. One can sandwich the thin film between two substrates of material 1. One may use a layer of adhesive, such as epoxy, to glue the bare substrate to the one covered with the film. The substrates are much thicker then the film and the adhesive, so that the whole specimen is easy to load. The interfacial fracture energy can be measured if the crack runs on the desired interface. There are several advantages of methods of this kind. First, the methods are applicable for thin films of any thickness, and can even measure the interfacial energy between

two thin films, when they are both sandwiched. Second, because the film is still bonded to one substrate in the crack wake, the residual stress in the film is unrelieved, and therefore does not contribute to the energy release rate. Third, the experimental data are relatively easy to interpret, as explained below.

Because the substrates are much thicker than the films, the stress field in the substrate, far away from the films, is unaffected by the presence of the films, and is the same as that around a crack in a homogeneous body. The load on the substrate can be represented by the two stress intensity factors K_I and K_{II} for a crack in a homogenous body. Near the crack tip, the stress field is that of an interfacial crack, characterized by the complex stress intensity factor K. The energy release rate is related to both the far field and the near tip field, namely,

$$G = \frac{1}{\overline{E}_1}\left(K_I^2 + K_{II}^2\right) = \frac{1}{2}\left(\frac{1}{\overline{E}_1} + \frac{1}{\overline{E}_2}\right)\frac{|K|^2}{\cosh^2(\pi\varepsilon)}.$$

The energy release rate can be calculated from the homogeneous specimen by neglecting the thin films.

The mode angle, however, has to be determined by solving the boundary value problem that includes the thin films. Let ψ_∞ be the mode angle of the remote load, namely, $\tan\psi_\infty = K_{II}/K_I$. The local mode angle ψ is defined using an arbitrary length l. The local mode angle relates to the remote mode angle as

$$\psi = \psi_\infty + \omega + \varepsilon\ln(l/h),$$

where h is the thickness of one of the films, and ω is an angle that depends on elastic properties of the films and the substrates, as well as the ratios between various films. Suo and Hutchinson (1989) solved the case of a single film between two substrates, and found that ω is less than $10°$ provided the elastic mismatch is not too large. It is rather cumbersome to keep track of the local mode angle, especially when several films are sandwiched, and when some of then deform plastically. A common practice has been to specify the mode angle for the sandwich specimens by the remote value ψ_∞.

Four-point bend specimen

Consider a four-point bend specimen. The method was introduced by Charalambides et al. (1989) and Cao and Evans (1989) to determine interfacial fracture energy, and developed by Dauskardt et al. (1998) for thin film structures relevant for interconnects. The experimental procedure is as follows. Use two silicon wafers to sandwich films of interest. Notch the top wafer to within a few microns of the sandwiched films with a diamond wafering blade. Place the sample in a four-point bend fixture. Record load as a function of displacement, and observe the crack propagation in an optical microscope. At a certain load, a crack initiates from the notch root, approaches the interface, and then bifurcates into two cracks to propagate on the interface. When the interface cracks are long compared to the substrate thickness, the load-displacement curve exhibits a plateau—that is, the crack reaches a steady state, in which the energy release rate is independent of the crack length.

At the steady state, both the energy release rate and the mode angle are obtained analytically. The four-point bend configuration is the superposition of two other configurations,

one being pure mode I, and the other being pure mode II. The energy release rates for the two configurations can be obtained from elementary considerations. Consequently, the energy release rate for the four-point bend specimen is

$$G = \frac{21}{4} \frac{M^2}{\bar{E} H^3},$$

where M is the moment per substrate unit width, H the thickness of each substrate, and $\bar{E}$ the plane strain modulus of the substrates. The mode angle for the four-point bend specimen is

$$\psi_\infty = \tan^{-1}\left(\sqrt{3}/2\right) \approx 41°.$$

Once the plateau load is measured experimentally, one obtains the fracture energy Γ for the mode angle 41°.

Double-cantilever beam

Also commonly used is the double-cantilever beam specimen (Oh et al., 1987; Kook and Dauskardt, 2002). The energy release rate for the double-cantilever beam specimen of a homogenous material is found in handbooks, given by

$$G = 12 \frac{(Pa)^2}{H^3 \bar{E}} \left(1 + 0.677 \frac{H}{a}\right)^2,$$

where a is the crack length, H the thickness of each beam, P the force per beam width, and $\bar{E}$ the plane strain elastic modulus. The specimen is under the mode I condition, $\psi_\infty = 0°$.

The use of the interfacial fracture energy

The measurement of interfacial fracture energy provides a tool for process control (Dr. Q. Ma of Intel Corporation, private communication). Many factors during the interconnect fabrication process can affect adhesion. Because debonding usually occurs after a interconnect structure is fabricated, when stresses arise from, e.g., thermal expansion mismatch. After a debond is identified, one has to modify the processing conditions, fabricate the interconnect structure again, and examine if the new structure has the debond. The iteration is time consuming. Alternatively, without fabricating the whole interconnect structure, one can measure the interfacial fracture energy for the interface at question under various fabrication conditions, and then select the condition that gives an adequate interfacial fracture energy.

The measurement of interfacial fracture energy also provides a tool to select materials to promote adhesion. When copper was introduced into the interconnect structure in late 1990s, new barrier layers are required to prevent copper diffusion into dielectrics, and to provide adhesion of copper to the dielectrics. The sandwiched four-point bend specimens were used to measure the interfacial fracture energy of the thin film structures with Ta and TaN as barrier layers (Lane et al., 2000), and thereby to study the effects of interfacial chemistry, copper layer thickness, and dielectric type on adhesion. More recently, numerous materials of low dielectric constant have been developed to compete to be a replacement for silica in the interconnect structure. To compare these materials, a commonly accepted method is desired to measure the

interfacial fracture energy. Rim et al., (2002) have evaluated adhesion of a carbon-doped oxide in thin film structures.

Interfacial cracks are often susceptible to subcritical growth under static or cyclic load. Environment strongly affects the growth rate. While the implications of subcritical debond growth for long term reliability of the interconnect structure have yet to be fully understood, the fracture specimens discussed above have been used to study subcritical debond growth (Kook and Dauskardt, 2002; Snodgrass et al., 2002).