INTERFACE FRACTURE TOUGHNESS

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OUTLINE

• Introduction
• Stresses in thin films
• Interface fracture mechanics
• Experimental techniques for measurement of interface fracture toughness
INTRODUCTION

- There are several systems and technologies that use materials in film form to achieve both their structural and functional requirements
  - Microelectronic Integrated Circuits
  - Magnetic Information Storage Systems
  - Microelectromechanical Systems (MEMS)
  - Coatings for Thermal, Oxidation, Corrosion and Wear Resistance

- The characterization of the mechanical properties of the individual constituents (thin films) as well as that of the interfaces are critical for designing as well as ensuring reliability of these systems

- In this talk the focus will be on interface fracture
STRESSES IN THIN FILMS

- Stresses in films and multilayers have three primary origins:
  - Intrinsic
  - Thermal
  - Mechanical

- Intrinsic stresses arise during the deposition process.
  - Intrinsic stresses are distinct from thermal stresses in that they are the stresses present at the deposition temperature.
  - The mechanisms which generate intrinsic stresses include grain growth, defect annihilation, phase transition and evaporation of a solvent.

- Thermal stresses arise due to changes in temperature when the film and substrate (or the layers in a multilayer) have different coefficients of thermal expansion (CTE).
Away from the edges, in the film you get biaxial strain due to temperature change

This results in a biaxial stress in the film

If the film also contains intrinsic stresses, then the interior of the film is subject to the equi-biaxial in-plane stress state
Failure Modes: An Overview

There are many modes of failure of films and multilayers which result from stresses which are too large.

Failure modes in tension

- Surface Crack
- Channeling
- Substrate Damage
- Spalling
- Debonding

Failure modes in compression

- Interface delaminations
- Circular blister
- "Telephone cord" blister
Consider a body consisting of two dissimilar materials, labelled 1 and 2, bonded by a planar interface and containing a crack.

Each material is homogeneous, isotropic, and linearly elastic.

Subject to a load, the body deforms under the plane-strain conditions.

The plane-strain moduli of the two materials is given by

\[
\begin{align*}
\overline{E}_1 &= \frac{E_1}{1-v_1^2} = \frac{2\mu_1}{1-v_1} \\
\overline{E}_2 &= \frac{E_2}{1-v_2^2} = \frac{2\mu_2}{1-v_2}
\end{align*}
\]

When the load reaches a critical value, the crack extends along the interface.

The central object of the interfacial fracture mechanics is to formulate this critical condition.

For the crack extending on the interface, the energy release rate $G$ is still defined as the reduction in the potential energy associated with the crack advancing a unit area.

All the familiar methods of determining the energy release rate still apply. For example, the energy release rate can be determined by measuring the load-displacement curves for bodies containing cracks of different sizes.
The energy release rate characterizes the amplitude of the load.

The critical condition for the extension of the crack also depends on the mode of the load.

To characterize the mode of the load, we need to analyze the field near the tip of the interfacial crack.

Williams (1959) was the first to solve this problem. He discovered that the singular field around the tip of the interfacial crack is not square-root singular, but takes a new form.

At a distance \( r \) ahead the tip of the crack, the stresses on the interface are given by

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

\[i = \sqrt{-1} \quad \text{and} \quad r^{i\varepsilon} = e^{i\varepsilon\ln r} = \cos(\varepsilon\ln r) + i\sin(\varepsilon\ln r)\]

The stress intensity factor \( K \) is complex-valued and has the dimension

\[K = \text{[stress][length]}^{1/2 - i\varepsilon}\]
The constant $\varepsilon$ is dimensionless and depends on the elastic constants of both materials.

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

It can also be expressed in terms of two non-dimensional Dundurs parameters

$$\alpha = \frac{\mu_1 (\kappa_2 + 1) - \mu_2 (\kappa_1 + 1)}{\mu_1 (\kappa_2 + 1) + \mu_2 (\kappa_1 + 1)} = \frac{E_1 - E_2}{E_1 + E_2} \quad \beta = \frac{\mu_1 (\kappa_2 - 1) - \mu_2 (\kappa_1 - 1)}{\mu_1 (\kappa_2 + 1) + \mu_2 (\kappa_1 + 1)} \quad \kappa = 3 - 4\nu$$

$$\varepsilon = \frac{1}{2\pi} \ln \frac{1 - \beta}{1 + \beta}$$

The constant is bounded, $|\varepsilon| < (1/2\pi) \ln 3 \approx 0.175$.
One complex number corresponds to two real numbers. For example, we can write a complex number in terms of its amplitude and phase angle, namely

\[ K = |K| \exp(i\phi) \]

The amplitude of the stress intensity factor is defined by

\[ |K| = \sqrt{KK} \]

This real-valued quantity has the familiar dimension

\[ |K| = \left[ \text{stress} \cdot \text{length} \right]^{1/2} \]

\( |K| \) relates to the energy release rate \( G \) as

\[ G = \frac{1}{2} \left( \frac{1}{E_1} + \frac{1}{E_2} \right) \frac{|K|^2}{\cosh^2(\pi\varepsilon)} \]

The phase angle specifies the mode of the load
Oscillatory stresses

The Williams field predicts that the stresses a distance $r$ ahead of the tip of the crack in the interface are given by

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

$$
K = |K| \exp(i\phi)
$$

$$
\sigma_{22} + i\sigma_{12} = \frac{|K|}{\sqrt{2\pi r}} \exp[i\phi + i\varepsilon \log r]
$$

$$
\sigma_{22} = \frac{|K|}{\sqrt{2\pi r}} \cos[\phi + \varepsilon \log r]
$$

$$
\sigma_{12} = \frac{|K|}{\sqrt{2\pi r}} \sin[\phi + \varepsilon \log r]
$$

Thus, the Williams field predicts that the stresses are oscillatory as $r$ approaches the tip of the crack.

The ratio of the shear stress to the tensile stress is

$$
\frac{\sigma_{12}}{\sigma_{22}} = \tan[\phi + \varepsilon \log r]
$$

When $\varepsilon = 0$, as for a crack in a homogenous material, the ratio $\sigma_{12}/\sigma_{22}$ is independent of the distance $r$ in the K-annulus, and the mode angle $\phi$ characterizes the relative proportion of shear to tension. When $\varepsilon \neq 0$, the ratio $\sigma_{12}/\sigma_{22}$ varies with the distance $r$. 
On the virtues of taking $\epsilon = 0$

The stress field becomes square-root singular, namely

$$\sigma_{22} + i\sigma_{12} = \frac{K}{\sqrt{2\pi r}}$$

Separate the complex-valued $K$ into the real and imaginary parts

$$K = K_I + iK_{II}$$

We obtain that

$$\sigma_{22} = \frac{K_I}{\sqrt{2\pi r}}$$
$$\sigma_{12} = \frac{K_{II}}{\sqrt{2\pi r}}$$

The two parameters $K_I$ and $K_{II}$ measure the amplitudes of two fields. Consequently, we can treat a crack on an interface the same way as we treat a crack in a homogeneous material under mixed-mode loading.

However, even when we set $\epsilon = 0$, there is a significant difference between an crack on an interface and a crack in a homogeneous material. When a mixed-mode crack in a homogeneous material reaches a critical condition, the crack kinks out of its plane. By contrast, when a mixed-mode crack on an interface reaches a critical condition, the crack often extends along the interface.
For the case $\varepsilon \neq 0$

The stress intensity factor $K$ is complex-valued and has the dimension

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

and the dimension of the absolute value of the stress intensity factor

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

Following Rice (1988), we define the mode angle $\psi$ by

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

where $l$ is an arbitrary length. The complex-valued $K$ represents the external boundary conditions, the choice of an arbitrary length does not affect $K$ and $|K|$.

To keep $K$ and $|K|$ unchanged by the different choices of the length, we require that

$$l^{-i\varepsilon} \exp(i\psi_A) = l^{-i\varepsilon} \exp(i\psi_B)$$

$$\psi_B - \psi_A = \varepsilon \log \left( \frac{l_B}{l_A} \right)$$

This formula shows how the mode angle $\psi$ changes with the length $l$.

The phase angle $\phi$ was defined before by using the equation $K = |K| \exp(i\phi)$. The phase angle $\phi$ corresponds to the mode angle $\Psi$ associated with a special choice of the length $l = 1$. The unit of the length is left unclear. It is better to clearly specify a length $l$, and use $\Psi$. 


For the case $\varepsilon \neq 0$

To see the significance of the mode angle, recall that the stresses a distance $r$ ahead of the tip of the crack are given by

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

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

$$\sigma_{22} + i\sigma_{12} = \frac{|K|}{\sqrt{2\pi r}} \exp[i\psi + i\varepsilon \log\left(\frac{r}{l}\right)]$$

Separating the real and the imaginary parts, we obtain that

$$\sigma_{22} = \frac{|K|}{\sqrt{2\pi r}} \cos[\psi + \varepsilon \log\left(\frac{r}{l}\right)], \quad \sigma_{12} = \frac{|K|}{\sqrt{2\pi r}} \sin[\psi + \varepsilon \log\left(\frac{r}{l}\right)]$$

The ratio of the shear stress to the tensile stress is

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

When $\varepsilon \neq 0$, the ratio $\sigma_{12}/\sigma_{22}$ varies with the distance $r$. The variation is not rapid, because $\varepsilon$ is small and because logarithm is a slowly varying function. Note that $\sigma_{12}/\sigma_{22} = \tan\psi$ when $r = l$. Thus, $\tan\psi$ approximates the ratio $\sigma_{12}/\sigma_{22}$, so long as $r$ is not far from $l$.

For a brittle interface, for example, a natural choice is $l = 1 \text{ nm}$, representative of the bond breaking zone size. With this choice, the mode angle $\Psi$ represents the relative proportion of shear to tension at the size scale of 1 nm.
Interpenetrating faces of a crack

The Williams field predicts that, at a distance \( r \) behind the tip of the crack, the two faces of the crack move relative to each other by the displacement

\[
\delta_2 + i\delta_1 = \left( \frac{1}{E_1} + \frac{1}{E_2} \right) \frac{K r^i \epsilon}{2(1+2i\epsilon)\cosh(\pi\epsilon)} \sqrt{\frac{2r}{\pi}}
\]

Rewrite this equation by using \( K = |K| \exp(i\phi) \), we obtain that

\[
\delta_2 + i\delta_1 = \left( \frac{1}{E_1} + \frac{1}{E_2} \right) \frac{|K|}{2\sqrt{1+4\epsilon^2}\cosh(\pi\epsilon)} \sqrt{\frac{2r}{\pi}} \exp[i\phi + i\epsilon \log r - i\tan^{-1}(2\epsilon)].
\]

The component of the displacement normal to the interface is

\[
\delta_2 = \left( \frac{1}{E_1} + \frac{1}{E_2} \right) \frac{|K|}{2\sqrt{1+4\epsilon^2}\cosh(\pi\epsilon)} \sqrt{\frac{2r}{\pi}} \cos[\phi + \epsilon \log r - \tan^{-1}(2\epsilon)].
\]

When \( \epsilon = 0 \), this expression is similar to that for a crack in a homogenous material. When \( \epsilon \neq 0 \), this expression indicates that, for some values of \( r \), the two faces of the crack interpenetrate.

• Contact of the crack surfaces should be considered (not traction free any more!)
For the case $\varepsilon \neq 0$ and small scale contact

Interpenetration clearly is a wrong prediction.

To use the Williams field for an interfacial crack, all we really need to do is to ensure that the wrong part of the field occurs in a small zone around the tip of the crack, a zone excluded by the *K-annulus*

When the contact zone is large, one has to take into account of the forces on the faces of the crack 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. The component of the displacement normal to the interface is

$$
\delta_2 = \left( \frac{1}{E_1} + \frac{1}{E_2} \right) \frac{|K|}{2\sqrt{1+4\varepsilon^2 \cosh(\pi\varepsilon)}} \sqrt{\frac{2r}{r}} \cos \left[ \psi + \varepsilon \log \left( \frac{r}{l} \right) - \tan^2(2\varepsilon) \right]
$$
If the crack is required to be open within \( 1 < r < 100 \), the mode angle must be restricted within

\[
-\frac{\pi}{2} + 2\varepsilon < \psi < \frac{\pi}{2} + 2.6\varepsilon, \text{ for } \varepsilon > 0 \\
-\frac{\pi}{2} - 2.6\varepsilon < \psi < \frac{\pi}{2} + 2\varepsilon, \text{ for } \varepsilon < 0
\]

The number 100 is arbitrary, but the above conditions are insensitive to this number.

Assume that an annulus exists, whose inside radius is large compared to small-scale events not modeled by the Williams field, and whose outside radius is small compared to the length characteristic of the external boundary conditions.

Inside the annulus, the Williams field prevails, characterized by the complex-valued stress intensity factor \( K \).

For a given crack configuration, the stress intensity factor \( K \) is determined by solving the elastic boundary value problem. Finite element method and other numerical methods have been developed to determine the stress intensity factor.

The critical conditions for debonding can be formulated in terms of the complex-valued stress intensity factors or strain energy release rates.
Under the remote loading, at the right crack tip:

\[ K = K_1 + iK_2 = \left( \sigma_{22}^\infty + i \sigma_{21}^\infty \right) \left( 1 + 2i \epsilon \right) \frac{\sqrt{\pi a}}{(2a)^i\epsilon} \]

Independent of \( \alpha \).

Reduce to Griffith’s solution when \( \beta = 0 \).

Take \( l = 2a \), then:

\[ \tan \psi = \frac{\sigma_{21}^\infty + 2i \epsilon \sigma_{22}^\infty}{\sigma_{22}^\infty + 2i \epsilon \sigma_{21}^\infty} \]

*Hutchinson and Suo, Advances in Applied Mechanics 29, 63-191 (1992).*
K FOR A DOUBLE CANTILEVER BEAM

\[ K = K_1 + iK_2 = \frac{2\sqrt{3}Me^{i\omega(\alpha,\beta)}}{h^i\epsilon \sqrt{(1 - \beta^2)}h^3} \]

Take \( l = h \), then:

\[ \psi = \omega(\alpha, \beta) \quad \omega(\alpha, \beta) \]

Interface fracture resistance (toughness) depends on the true work of adhesion, plastic dissipation in the film and substrate, interface friction as well as the mode mixity at the crack tip.

Following the energy approach by Griffith and Irwin.

**True Work of adhesion:** \[ \Gamma_0 = \gamma_1 + \gamma_2 - \gamma_{12} \]

\( \gamma_1 \) and \( \gamma_2 \) are the specific surface energies of the film and the substrate, respectively, \( \gamma_{12} \) is the energy of the interface.

Other contributions to the interface fracture toughness include plastic dissipation in the film and substrate, interface friction:

**Practical Work of adhesion or Interface fracture toughness:**

\[ \Gamma(\psi) = \Gamma_0 + \Gamma_p(\psi) + \Gamma_f(\psi) \]

**Interface fracture condition:**

\[ G = \Gamma(\psi) \]

\[ G = \frac{1}{2} \left( \frac{1}{E_1} + \frac{1}{E_2} \right) \left| \frac{K}{\cosh^2(\pi \varepsilon)} \right|^2 \]
The most realistic phenomenological descriptions of the functional dependence of the interfacial toughness on the mode mixity are given by Hutchinson and Suo.

\[
\Gamma_{\psi} = \Gamma_0 [1 + \tan^2 \{\psi(1 - \lambda)\}]
\]

\[
\Gamma_{\psi} = \Gamma_0 [1 + (1 - \lambda)\tan^2 \psi]
\]

In these expressions \(\Gamma_0\) is the mode I interfacial toughness for \(\psi = 0\), and \(\lambda\) is an adjustable parameter.
In the case of a brittle, weakly bonded film, indentation tests can be used to delaminate the film from the substrate.

A cone or wedge type indenter is used.
• For a conical indenter, the interface toughness can be determined using

\[
\frac{G E_f}{(1-\nu_f)} = \frac{1}{2} h \sigma_1^2 (1 + \nu_f) + (1 - \alpha)(h \sigma_R^2) - (1 - \alpha)h(\sigma_1 - \sigma_B)^2
\]

where \( E_f \) and \( \nu_f \) are the thin film’s Young’s modulus and Poisson ratio, respectively. 
\( h \) is the film thickness. 
\( \sigma_R \) is the residual stress in the film. 
\( V_i \) is the plastically deformed volume due to indentation.

\[
\sigma_1 = \frac{V_i E_f}{2\pi h a^2 (1-\nu_f)}, \quad \sigma_B = \frac{\mu^2 h^2 E_f}{12 a^2 (1-\nu_f)}, \quad \alpha = 1 - \frac{1}{1 + 0.902(1-\nu_f)}.
\]

Similar expressions are available for wedge indenters.
A relatively new idea of a cross-sectional indentation for thin film delamination has been proposed by Sanchez et al.

An indentation is made into the substrate cross-section, close to the film interface, which causes the film to debond.

The energy release rate can be calculated by measuring the maximum film deflection, \( u_0 \):

\[
G = \frac{Eh^3u_0^2}{12(a-b)^2(1-\lambda)^4(2F + \lambda F')}
\]

where \( a \) and \( b \) are the delamination and contact radii, respectively, \( \lambda = a/b \), and \( F \) is defined as

\[
F(\lambda) = \frac{2 \ln \lambda + \frac{1 + \lambda}{1 - \lambda} \ln^2 \lambda}{[(1 + \lambda) \ln \lambda + 2(1 - \lambda)]^2}
\]

This test is particularly useful, as the film is not directly indented, and the crack initiates in the brittle substrate, which limits the amount of plastic deformation.
The PLST allows measuring the interfacial fracture toughness over a wide range of phase angles.

Here, a thin metal line on a substrate is pushed with the asymmetric diamond wedge from its end.

For ease of fracture, the thin line has a processed precrack in the form of a carbon layer, which makes it a real fracture mechanics specimen.

The precrack portion of the line is deformed elastically in the beginning of the test until the crack propagates.

When the crack reaches its critical buckling length at a certain critical load, $P_{cr}$, the film buckles. At the point of buckling the strain energy release rate can be calculated

$$G = \frac{\sigma^2 h}{2E'_f} = \frac{(P_{cr} - P_{fric})^2}{2b^2 hE'_f}$$

Here $\sigma$ is the stress in the cracked portion of the line, $b$ is the line width, $P_{cr}$ and $P_{fric}$ are the critical buckling load and the friction load, respectively.
Apart from Nanoindentation, other techniques have also been used for Interface debond energy measurements.

For thin films the only method which duplicates the mode mixity found in actual films is based on residual stress induced debonding. However, for most thin films the residual stress induced strain energy release rate $G_{ss}$ is substantially lower than the interface debond energy. $G_{ss}$ can be increased by depositing an additional material layer on the film. One has to ensure that for the additional layer:

- deposition must be carried out at ambient temperature
- the layer must not react with the film
- the layer must have large residual tension upon deposition
• When the superlayer has sufficient thickness, spontaneous decohesion occurs at the interface

• The critical thickness where decohesion occurs can be used to calculate interface fracture toughness
The critical value of $G$ is determined by the critical superlayer thickness.

where $i = 1,2$ refers to the two materials in the bilayer, $h_1$ and $h_2$

$E_i$ are the biaxial elastic moduli, $E_i' = E_i/(1 - v_i)$

the load $P$ is associated with the residual tension stress, $\sigma_i$, in each layer

$k$ is the curvature of the debonded layer

$\varepsilon_i$ are misfit strains: $\varepsilon_i = \sigma_i/E_i'$

$M_i$ are the bending moments along the centerline of each layer due to the load $P$
Sandwich Specimen Tests

For the sandwich type of test a macroscopic fracture mechanics sample is made with a thin film incorporated into the test structure.

Many different sandwich sample geometries are possible.

Expressions are available for calculating critical values of $K$ and $G$.

None of the sandwich specimen tests account for the residual stress in thin films.
THANK YOU
3) Z. Suo, http://imechanica.org/node/7448