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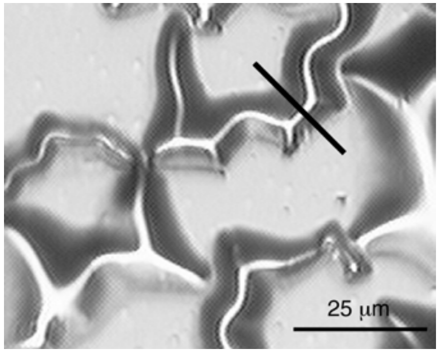
Modeling Thin Film, Buckle-Driven Delamination along a Metal/Polymer Interface in a Stressed Overlayer Test

Dave Reedy and Edmundo Corona
Sandia National Laboratories, Albuquerque, NM, USA
edreedy@sandia.gov

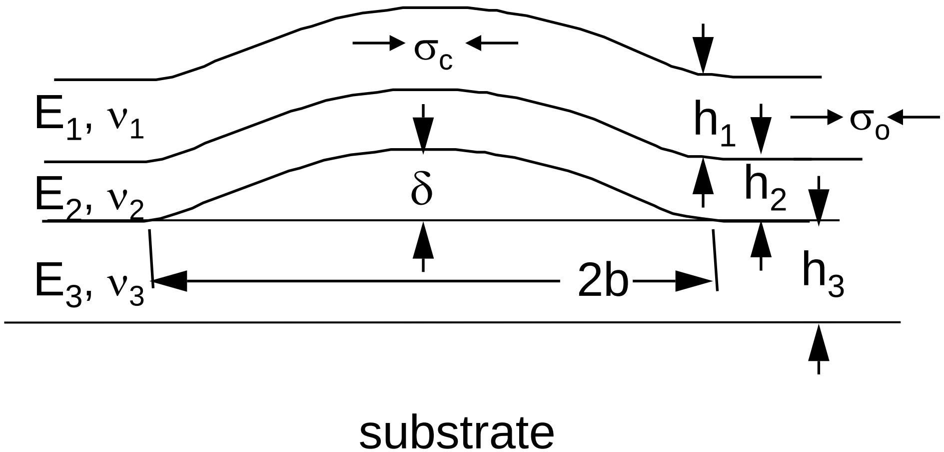
N. R. Moody,
Sandia National Laboratories, Livermore, CA, USA

Modeling Stressed Overlayer Test

- The reliability of components with thin film polymer/metal interfaces is often controlled by the toughness of the interface.
- One method of measuring the toughness of such interfaces is the stressed-overlayer test:
  - –metal substrate coated with thin polymer film to create interface of interest.
  - –deposit overlayer with very high residual compressive stress on top of polymer.
  - – height of induced blisters used to infer toughness using mechanics models.

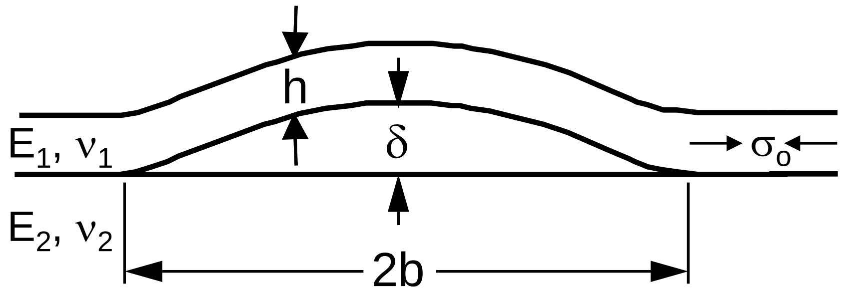


Tungsten/Epoxy/Aluminum deposited on a thick glass substrate



Buckle-driven thin film delamination: one-dimensional, straight-sided blister

- Analytic results for a thin elastic film on a rigid substrate are well established (Chai et.al, 1981; Evans and Hutchinson, 1984; Gille, 1985; Whitcomb, 1986).
- There are some published results for the case of a compliant substrate (Cotterell and Chen, 2000; Yu and Hutchinson, 2002), however, results for a very stiff film on a very compliant substrate have not been fully determined (e.g., W/PMMA).
- There appears to be little work aimed at including the effects of substrate yielding and crack flank friction in FEA simulations.



•Requires a pre-existing delamination.

•Nonlinear, large deflection analysis.

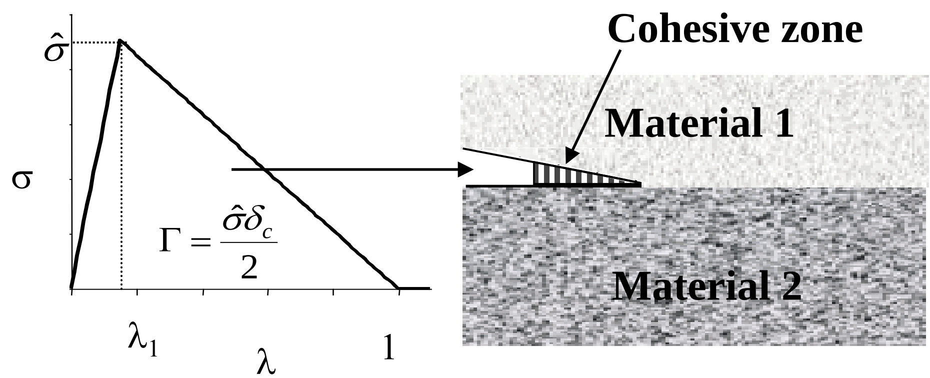
•No crack growth until σ_o exceeds the critical buckling stress.

•Based upon dimensional considerations

$$\frac{b}{h} = f\left(\frac{\Gamma}{G_o}, \frac{\sigma_o}{\overline{E}_1}, \alpha, \beta\right) \quad \text{where} \quad G_o = \sigma_o^2 h/(2\overline{E}_1)$$

Cohesive Zone Model

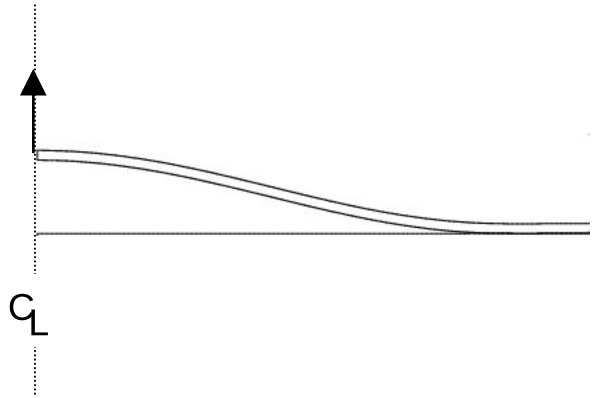
- Material separation based on a specified traction-separation(σ –δ) relationship.
- Well-suited for modeling interfacial crack growth when crack path is well defined.
- Crack growth is a natural outcome of the solution, bond failure is a gradual process with tractions resisting separation.
- Key parameters are the interfacial strength $\hat{\sigma}$ and the work of separation/unit area Γ (i.e., the intrinsic interfacial toughness).
- Mesh-independent results.

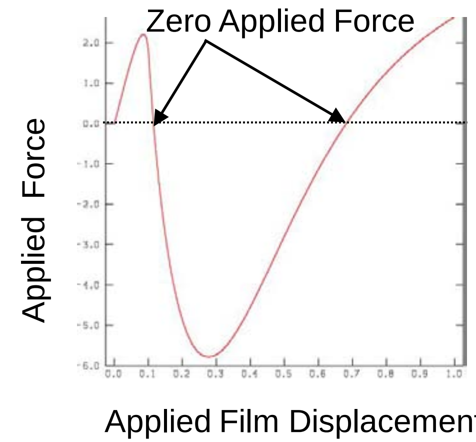


- Usually defined in terms of a potential that depends on a scalar effective separation.
- Similar to model introduced by Tvergaard and Hutchinson (J. Mech. Phys. Solids, **41**, 1119, 1993).

Technique for analyzing a buckle-driven delamination

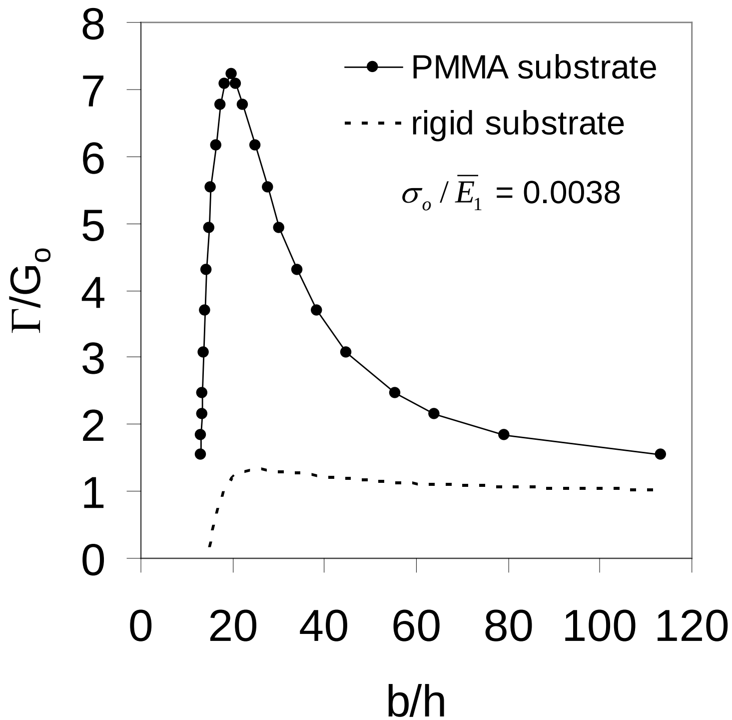
For a prescribed σ_o, apply monotonically increasing film displacement and monitor associated force.

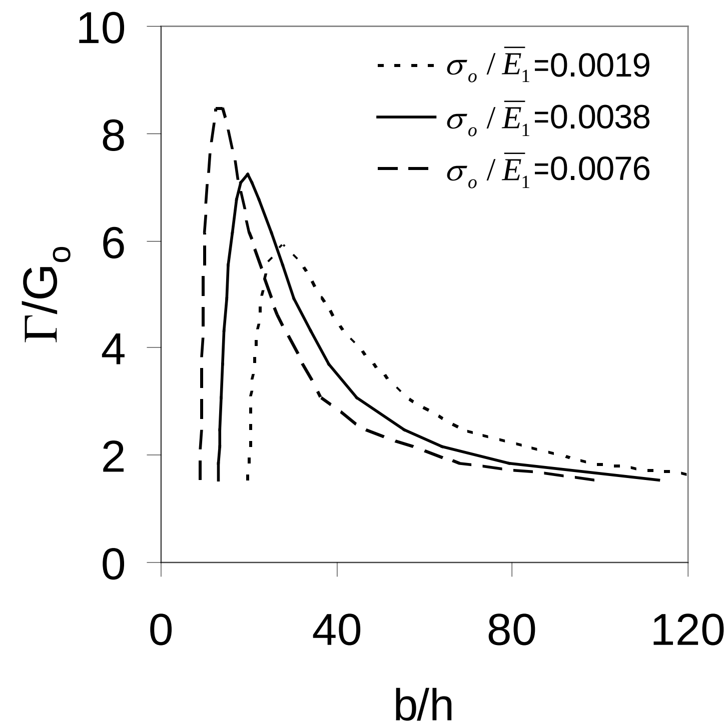




- For a prescribed σ_o, perform CZ finite element simulation to determine delamination width (b) and height (δ) for interface with toughness Γ.
  - displace center of buckle upwards (i.e., an external agent prescribes the buckle height δ).
  - monitor the associated applied force
  - when the applied force does equal zero, a free-standing, buckled exists.
- Perform calculations for broad range of Γ to determined relationship between delamination height (width) and interfacial toughness for fixed σ_o.
- FE model contains a small pre-existing flaw shorter than the critical buckling length.

Results for a 0.1 μm W film on a thick PMMA substrate with σ_o=1.7 GPa demonstrated effect of substrate compliance.





- Note scaling $\dfrac{b}{h} = f\left(\dfrac{\Gamma}{G_o}, \dfrac{\sigma_o}{\overline{E}_1}, \alpha, \beta\right)$

  where $G_o = \sigma_o^2 h / (2\overline{E}_1)$ is the long crack energy release rate. G_o = 0.325 J/m^2
- These results are for W/PmmA with α = 0.985, β = 0.227
- CZ length in these calculations was ~ 3-5*h*

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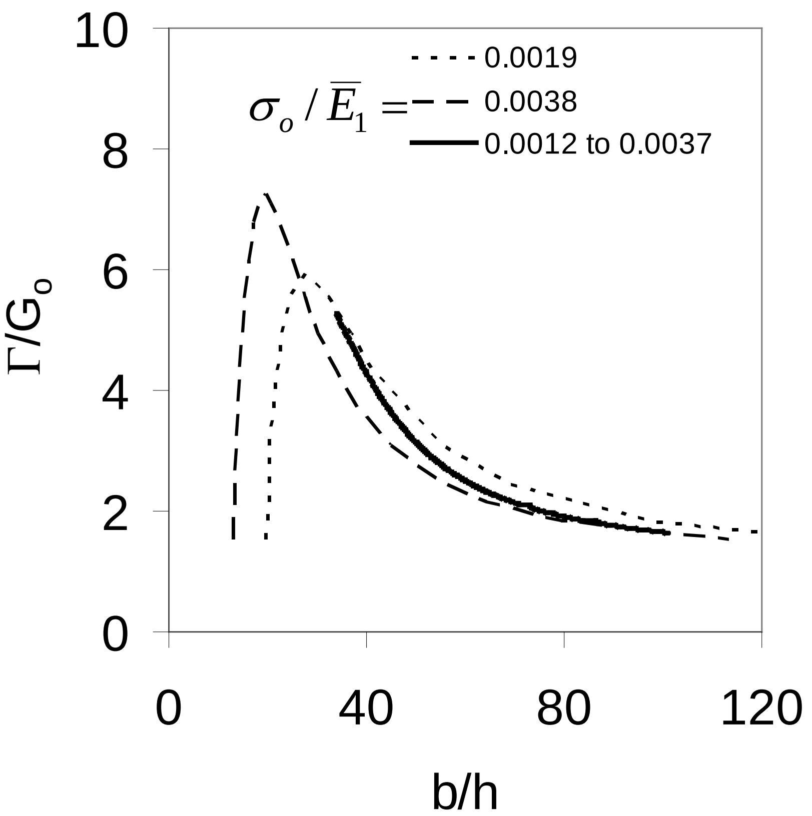
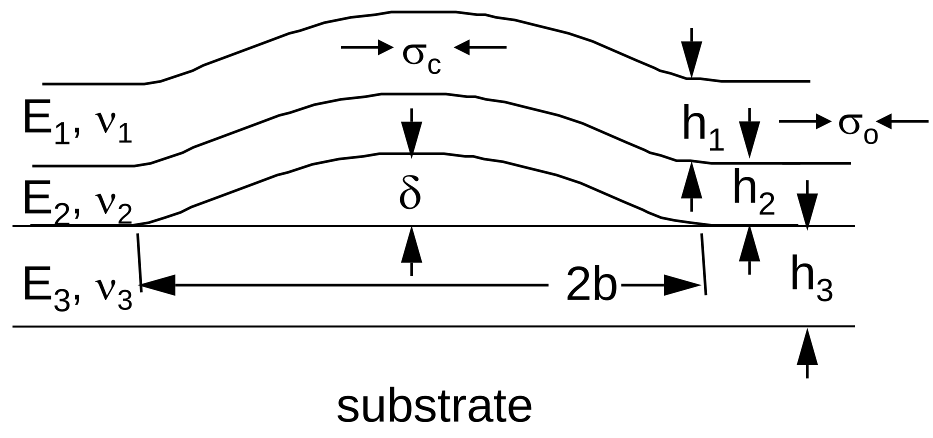
Another calculation approach

- Initially apply load to lift up preexisting delaminated region (create an initial "imperfection").
- Then monotonically increase the film compressive stress while decreasing applied load (fully release applied load prior to any delamination growth).
  - note $\sigma_o / \overline{E}_1$ increases with increasing σ_o.
- Results consistent with previous approach.
- Calculation for W/PMMA with *h* = 0.1 μm, with Γ = 0.5 J/m^2 and for an initial delamination = 3 μm.



W-overlayer on an epoxy film on an aluminized glass substrate

- To provide focus, analyzed a previously reported, stressed overlayer test configuration (SAND2002-8567).
  - Substrate: 0.2 μm Al sputtered on a glass microscope slide.
  - Film: 0.024, 0.164 or 0.615 μm thick Epon 828/T403 epoxy layer spin-coated on the substrate (film is material 2).
  - Stressed overlayer: 0.22 μm W with a σ_o=2.2 GPa residual biaxial compressive film stress sputtered on top of the epoxy film (overlayer is material 1).
  - Failure at the epoxy/Al interface.

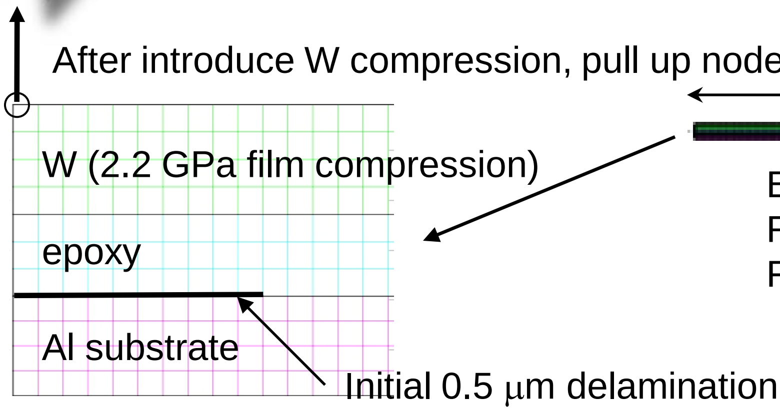


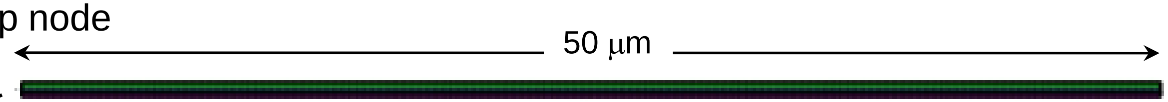
Tungsten (W): E_1=410 GPa ν_1=0.28
Epoxy: E_2=3.5 GPa ν_2=0.35
Aluminum (Al): E_3=70 GPa ν_3=0.33
Substrate: thick and rigid

Measured half-buckle width *b*

h_2 (μm)	*b (μm)*
0.024	*4.4*
0.164	*6.5*
0.615	*6.0*

Test calculations for W/0.164 μm epoxy/Al specimen



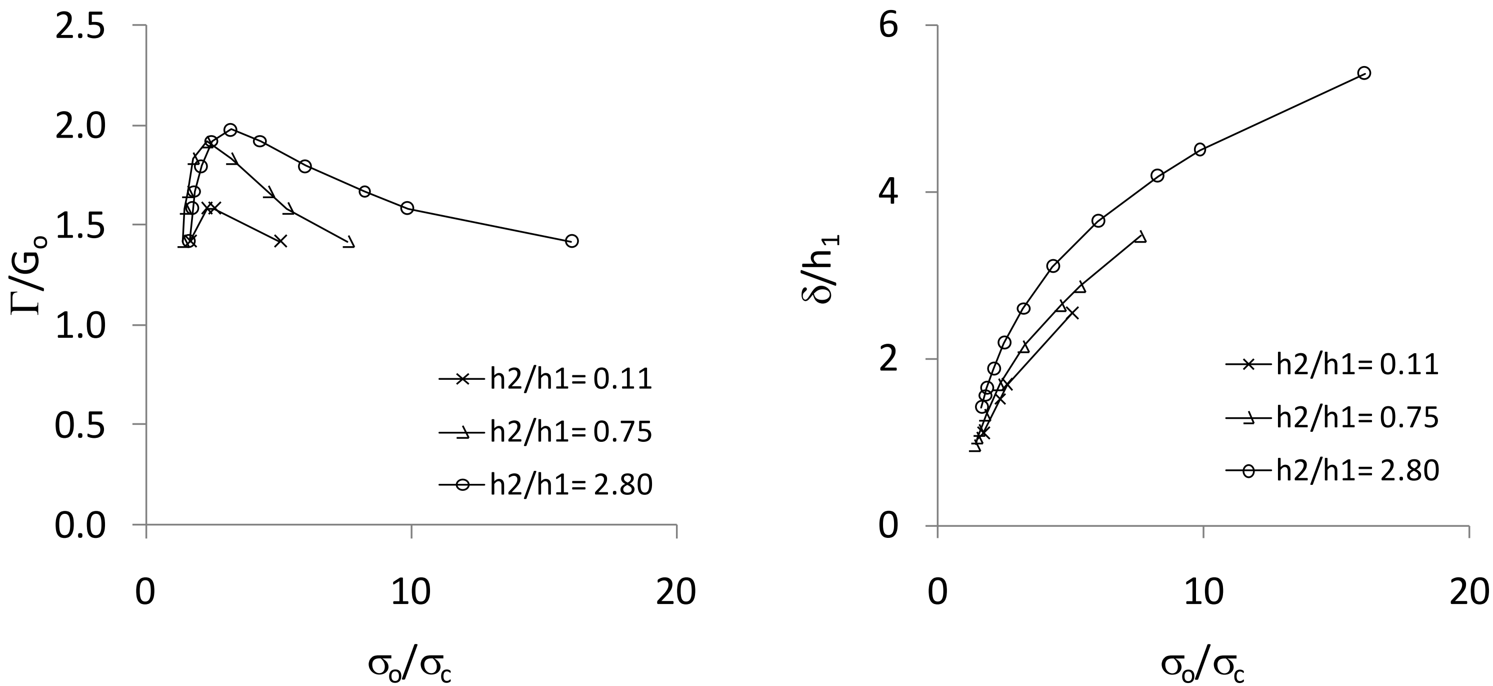


Bottom of substrate fixed.
Rhs and lhs edges constrained against lateral displacement.
Front and back constrained so in plane strain.

- Examined how choice of interface strength $\hat{\sigma}$ affects solution.
  - A higher $\hat{\sigma}$ is associated with a lower δ_c.
  - Length of the cohesive zone scales with δ_c.
  - Results for a W/0.164 μm epoxy/Al lay-up with Γ = 1.7 J/m^2
  - b measured from tip of cohesive zone
  - chose $\hat{\sigma}$ so that CZ length/h_1 ~ 1-2

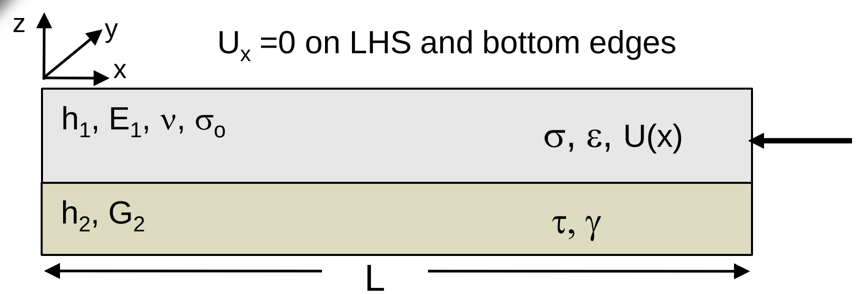
	$\hat{\sigma}$ = 120 MPa	$\hat{\sigma}$ = 170 MPa	$\hat{\sigma}$ = 240 MPa
δ/h_1	3.5	3.5	3.4
b/h_1	36.4	34.5	33.9
CZ length/h_1	4	2	1

Results: effect of epoxy thickness



- Calculated Γ/G_o and δ/h_1 depend on W overlayer-to-epoxy film thickness ratio h_2/h_1.
- Maximum $\Gamma/G_o > 1.33$ exceeds the rigid substrate ratio; as is the case for a thick compliant substrate.
- FEA shows that there is horizontal deflection of the overlayer at the buckle front towards the center of the buckle (will call this overlayer edge-displacement).

Shear-lag analysis estimate of overlayer edge-displacement during buckling



$$N_c = \left(\frac{\pi}{b}\right)^2 D_e$$

$$\frac{d\sigma}{dx} = \frac{\tau}{h_1}$$ (eq.1, equilibrium)

$$\varepsilon = \frac{d}{dx}U(x) = (\sigma_o + \sigma)/\overline{E}_1 \quad \text{where } \overline{E}_1 = E_1/(1-\nu^2)$$ (eq.2, W overlayer)

$$\gamma = \frac{U(x)}{h_2} = \tau / G_2$$ (eq. 3, epoxy)

$$\frac{d^2U(x)}{dx^2} - k^2U(x) = 0 \quad \text{where } \mathrm{k}^2 = G_2/(h_1 h_2 \overline{E}_1)$$ (eq. 4, governing ODE; combine eqs. 1-3)

$$U(0) = 0 \text{ and } \frac{\mathrm{dU(L)}}{\mathrm{dx}} = \frac{\sigma_o}{\overline{E}_1} - \frac{N_c}{h_1\overline{E}_1}$$ (eq. 5, BCs for governing ODE)

$$U^* = U(L) = (\sigma_o - N_c/h_1)/(k\overline{E}_1)$$ (eq. 6, solution for edge-displacement, *U**, in limit of long strip; i.e., *kL*>>1)

- The shear-lag analysis assumes
  - W-overlayer carries only axial loads
  - epoxy layer carries only shear loads
- Note:
  - $\varepsilon_y = 0$ (plane strain) and $\sigma_z = 0$ (beam-like)
  - σ_o is the residual overlayer stress (positive in compression)
  - N_c= critical classical buckling load
  - Analyzing unbuckled portion of strip (i.e., buckle would be beyond rhs of model)

Extended rigid substrate analytic solution

- Extension for a stiff overlayer (e.g., W) on a very compliant film (e.g., epoxy) that fails at the film/substrate interface where the substrate is also relatively stiff (e.g., Al).
- Modify rigid substrate analytic solution (see Mixed Mode Cracking in Layered Materials, Hutchinson and Suo, Advances in Applied Mechanics,1992) by:

  1) Using the effective, plane strain *EI* per unit width for the combined overlayer/film bimaterial beam (see Formulas for Stress and Strain, by Roark and Young for equations to calculate $D_e=(EI)_e$ per unit width).

  2) Appending a term associated with overlayer edge-displacement to the "change in the resultant from the unbuckled state", ΔN, that is used in the formula defining the amplitude of the buckling deflection.

$$\left(\frac{\delta}{h_1}\right)^2 = \frac{4(\Delta N + N^*)}{3N_c} \text{ where } \Delta N = N_o - N_c \text{ with } N_o = \sigma_o h_1,\ N_c = \frac{\pi^2 D_e}{b^2}, \text{ and } N^* = \overline{E}_1 h_1 U^*/b \qquad \text{(eq. 7)}$$

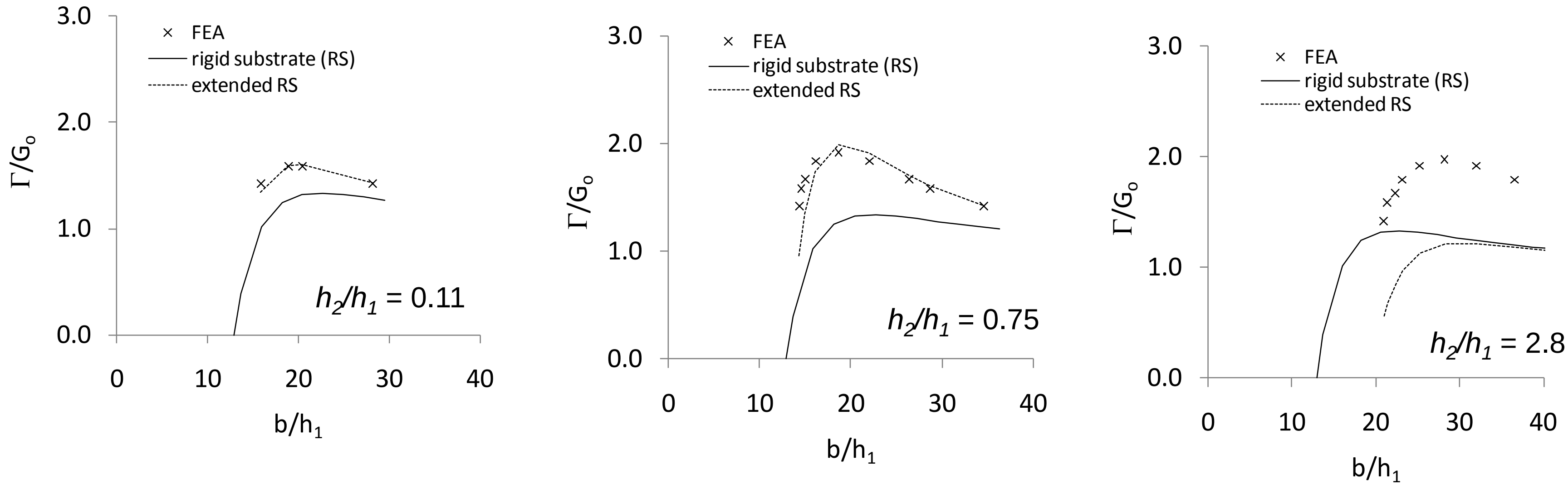
(recall that *U** is the overlayer edge-displacement and *b* is the buckle half-width)

Extended rigid substrate (ERS) analytic solution

Order of calculations for ERS solution; assume know half-buckle width *b*, layer thicknesses and elastic properties.

1. Calculate D_e (see Roark and Young)
2. Calculate N_c eq. 7
3. Calculate U^* eq. 6
4. Calculate δ eq. 7
5. Calculate $$G = \frac{(N_c\delta)^2}{8D_e} + \frac{(\Delta N)^2}{2\bar{E}h_1}$$
6. Calculate G/G_o where $G_o = N_o^2/(2\bar{E}h_1)$

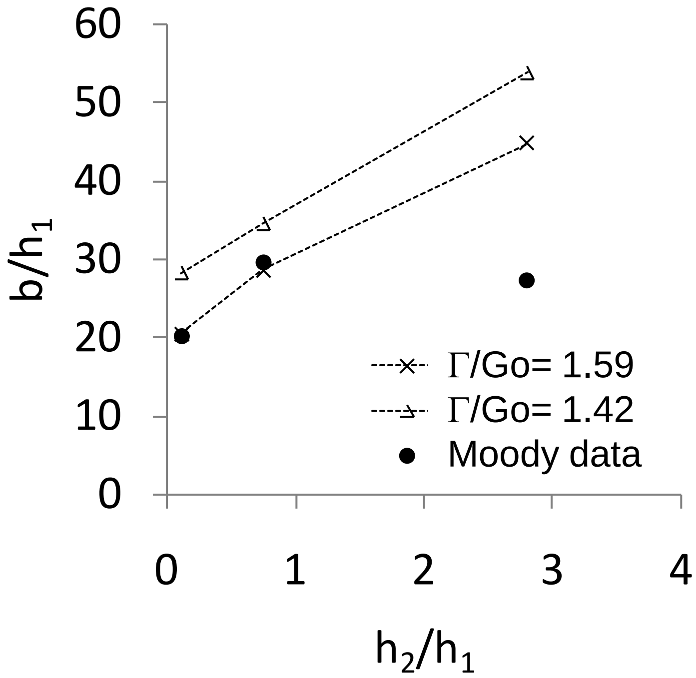
Compare enhanced rigid substrate analytic solution and FEA results



- Enhance Rigid Substrate (ERS) analytic result, which incorporates a shear-lag estimate for horizontal edge-displacement during buckling, is in good agreement with FEA results for the particular specimen analyzed here when h_2/h_1 = 0.11 and 0.75.
- As might be anticipated, the ERS solution was in poor agreement with the FEA results when $h_2/h_1 = 2.8$ (when use of shear-lag analysis is questionable).
- Overlayer edge-displacement provided largest correction to rigid substrate analysis (D_e had small effect).

FEA used to reduce experimental data

- For an ~ constant mode-mixity ψ (or if independent of ψ), FEA results for a constant Γ should predict the variation in b/h_1 with h_2/h_1.
- Finite element results suggest that Γ/G_o=1.6 is a good fit to data for h_2/h_1 = 0.11 and 0.75.
  - Corresponds to Γ=*1.9* J/m^2, a relatively high value, suggesting epoxy yielding is contributing to the apparent toughness.
- Data point for h_2/h_1 = 2.8 lies well below the Γ/G_o=1.6 prediction.
  - Finite element results suggest contact behind the cohesive zone --- crack flank friction is not accounted for in the analysis and could generate an enhanced mode-mixity effect.



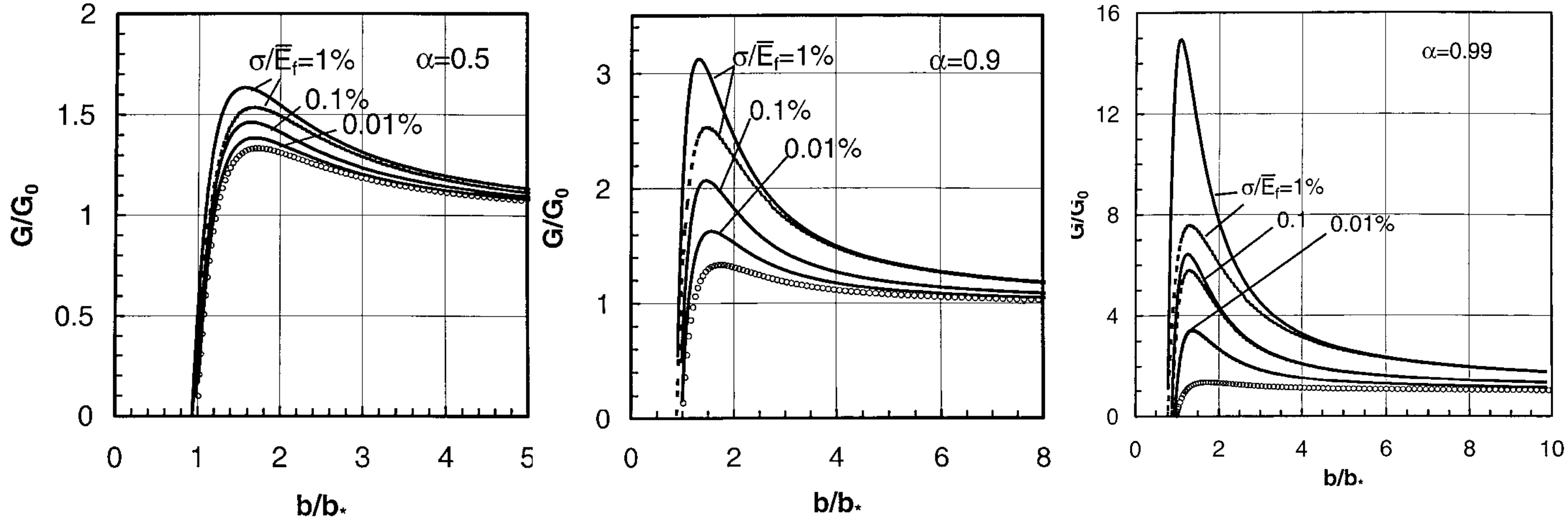
Summary

- Performed cohesive zone finite element analysis of a W/epoxy/Al stressed overlayer specimen that has been used previously at SNL.
  - Showed that variations in the epoxy layer thickness can have a significant effect.
  - Showed that the overlayer "edge-displacement" (enabled by relatively low epoxy compliance) is the primary cause of differences from the rigid substrate idealization.
  - Showed how applicability of rigid substrate analytic solution can be enhanced to include overlayer edge-displacement through a simple, shear-lag based correction (preliminary result, have not determined range of applicability, etc.).
  - Comparison with experimental data indicates that plasticity and crack flank friction affects measured toughness --- topics that must be addressed in future work so can model mode-mixity effects.

Extra Slides

Yu/Hutchinson

Energy Release Rate (*G*) vs Blister Width (*b*)



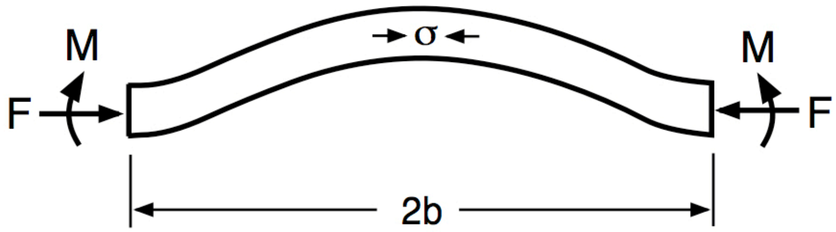
Normalization parameters (1 Film, 2 Substrate):

$$G_0 = \frac{1}{2}\frac{\sigma^2 h}{\overline{E}_1} \qquad b_* = \frac{\pi h}{2\sqrt{3}}\sqrt{\frac{\overline{E}_1}{\sigma}} \qquad \overline{E}_i = \frac{E_i}{1-\nu_i^2}$$

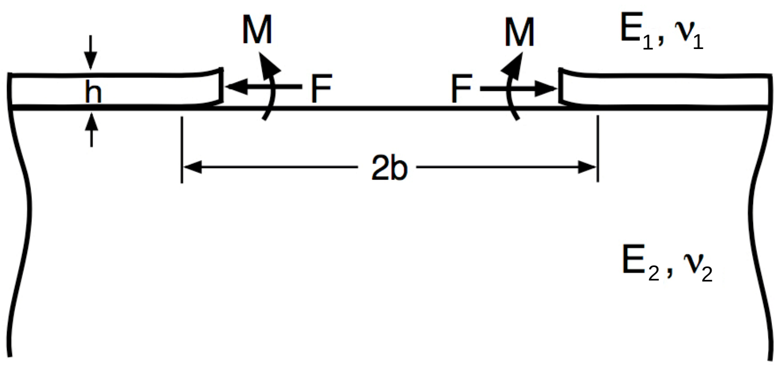
Elastic mismatch characterized by Dundur's parameters:

$$\alpha = \frac{(\overline{E}_1 - \overline{E}_2)}{(\overline{E}_1 + \overline{E}_2)} \qquad \beta = \frac{1}{2}\frac{\mu_1(1-2\nu_2) - \mu_2(1-2\nu_1)}{\mu_1(1-\nu_2) + \mu_2(1-\nu_1)} = 0$$

Yu/Hutchinson (2002)



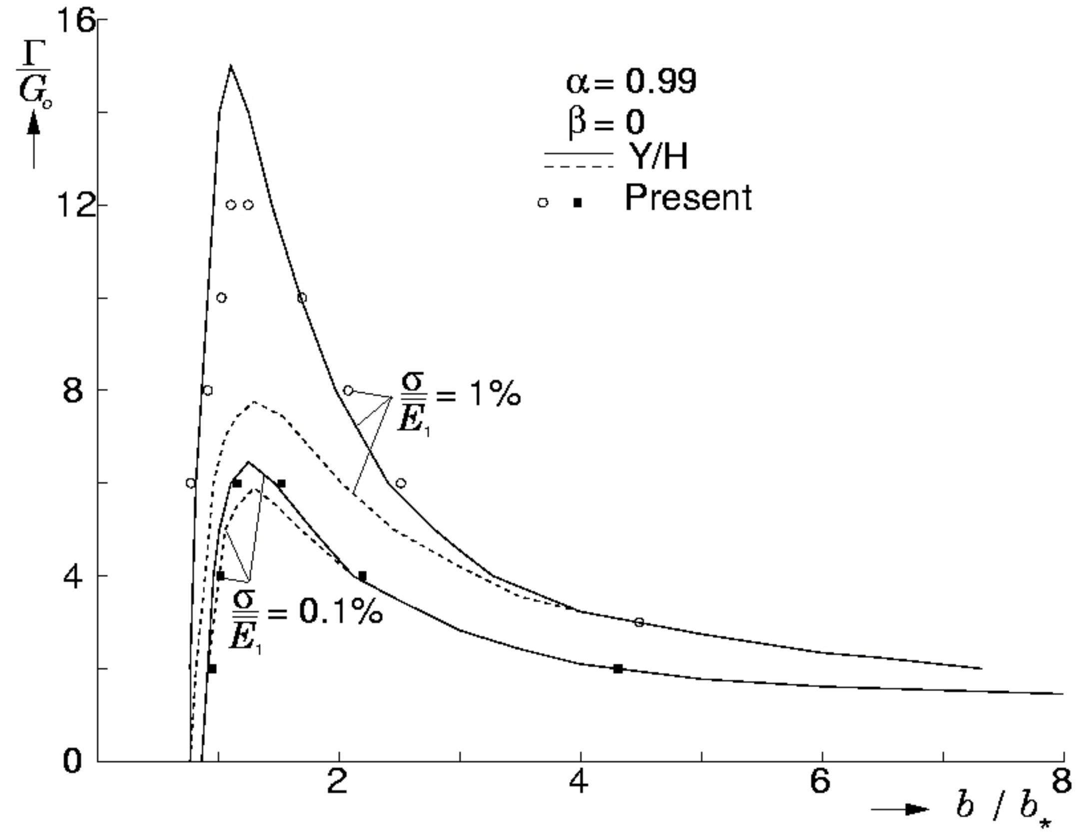
The buckled portion of the film was modeled using von Karman nonlinear plate theory



The film/substrate system is a linear plane strain problem solved using an integral equation formulation

The solutions were matched at the detached edges of the film by requiring continuity of displacements and rotations.

Yu/Hutchinson Results
α=0.99



$$b_* = \frac{\pi h}{2\sqrt{3}}\sqrt{\frac{\overline{E}_1}{\sigma}}$$