SAND2015-2530D

A cohesive zone-based fracture modeling capability for polymer/solid interfaces

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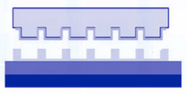
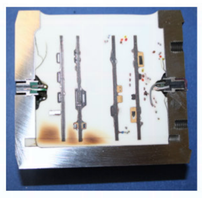
Polymer/solid interfaces are ubiquitous

- The performance and the reliability of many Sandia components depend on the integrity of interfaces between dissimilar materials
- Goal: Develop a finite element-based simulation capability to predict how variations in processing, environment, geometry, and loading affect the integrity of polymer/solid interfaces

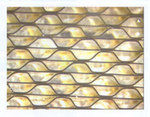


Nanoimprint lithography

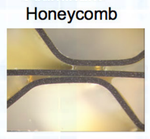


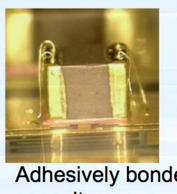
Fuze canister

Adhesively bonded stainless steel rupture disk

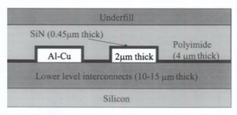


Aluminum Honeycomb

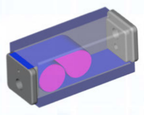




Adhesively bonded capacitors



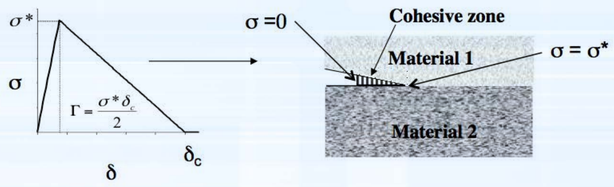
Thin films in microelectronics

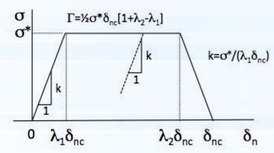


Bonded end caps in a switch

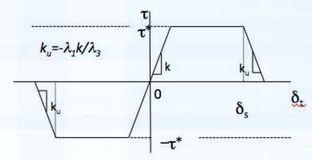
Developed a Novel Ψ – dependent Cohesive Zone Model (CZM)

CZM defines interfacial separation





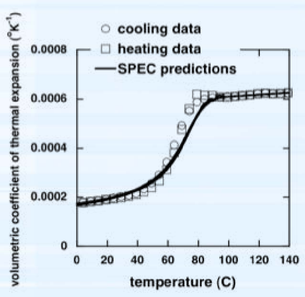
- Mode I dissipation depends only on normal separation



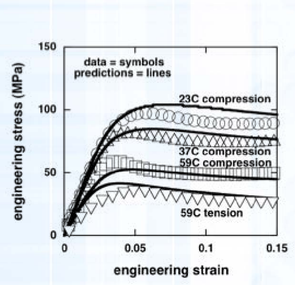
- Mode II dissipation by shear yielding along intact interface in front of CZ
- τ^* from SPEC model

CZM generates a Ψ–dependent toughness (Reedy and Emery, IJSS 2014)

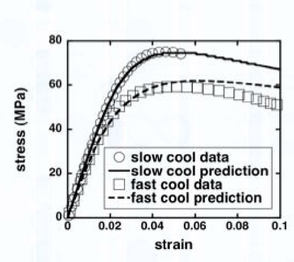
Epoxies: Complex Material Response



Thermal Expansion, Tg



Yielding

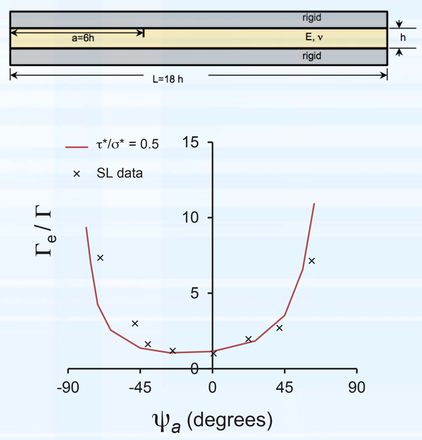


Physical Aging

Thermal expansion and yield strength are not material properties
Depends on time and temperature history
Described by SNL's nonlinear viscoelasticity SPEC model (Polymer 2009)
Used to determine residual stress generated during fabrication and lifecycle

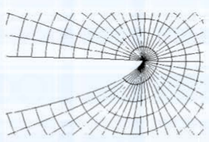
CZM Predictions Match Published Data

- Swadener and Liechti, measured the interfacial toughness of a glass/epoxy interface (JAM, 1998)
  - E = 2 GPa, h=0.25 mm, and Γ=1.5 J/m^2
- Calculated effective toughness Γ_e in good agreement with data
  - displays similar asymmetric response
- Shape of calculated Γ_e/Γ *vs.* ψ_a relationship is not predefined

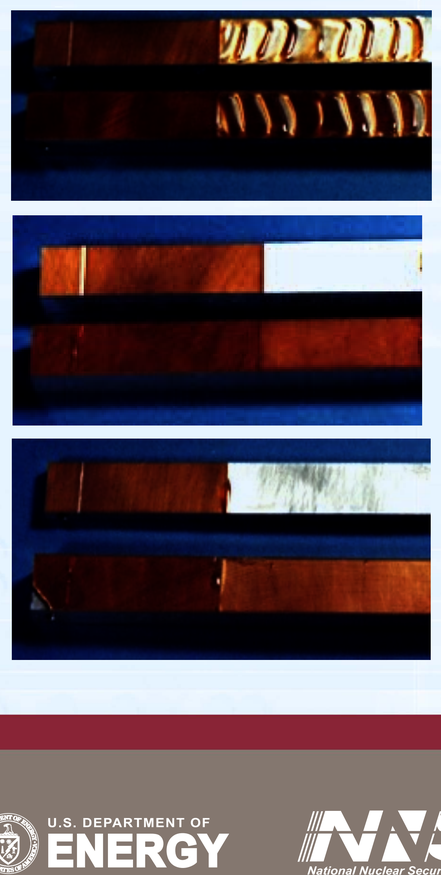


Interfacial Toughness Depends on Mode Mixity Ψ

- Mode mixity $\Psi_{r=l}$ is a measure of shear-to-opening deformation at the crack tip ($\Psi_{r=l}$=0 is pure opening)
- Interfacial cracks are subjected to a mixed mode loading because of material and geometric asymmetries



$$\psi_{r=l_o} \equiv \tan^{-1}(\sigma_{xy}/\sigma_{yy})$$

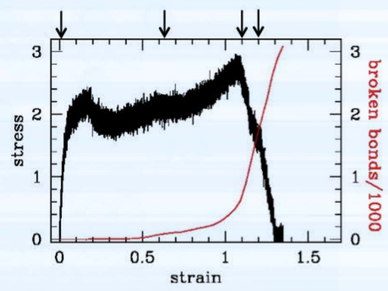


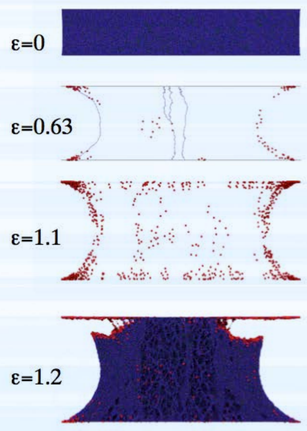
ADHERENDS SAME THICKNESS
G_c = 140 J/m^2
$\psi_{l=10\mu m}$ = 8^o

ADHERENDS SAME THICKNESS
G_c = 2000 J/m^2
$\psi_{l=10\mu m}$ = -83^o

TOP ADHEREND HALF AS THICK
G_c = 60 J/m^2
$\psi_{l=10\mu m}$ = -8^o

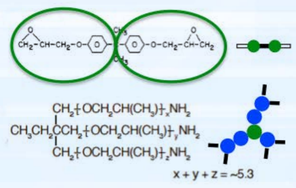
MD Simulations Study Molecular Origins of Fracture





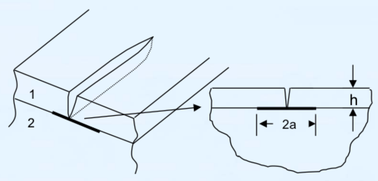
Red spheres are atoms with broken bonds

- New coarse-grain epoxy model enables realistic failure simulations



Impact

- Implemented in SNL's Sierra/Solid Mechanics finite element code
- Enables predictions on how processing/life cycle history affects integrity of polymer/solid bonds in Sandia components
- Have begun to apply our new techniques to SNL problems



Interfacial cracking (delamination) from the root of a channel crack in a thin film.

Publications:

Reedy, E.D., Jr. and Emery, J.M., A Simple Cohesive Zone Model that Generates a Mode-mixity Dependent Toughness, International Journal of Solids and Structures (2014) p3727.

Reedy, E.D., Jr., Cohesive Zone Finite Element Analysis of Crack Initiation from a Butt Joint's Interface Corner. International Journal of Solids and Structures (2014) p4336.

Conference proceedings, presentations, posters

The Adhesion Society, 2014 & 2015 (4), American Physical Society, 2014 & 2015 (3)

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National Nuclear Security Administration

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