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Nanomechanics of Films on Compliant Substrates

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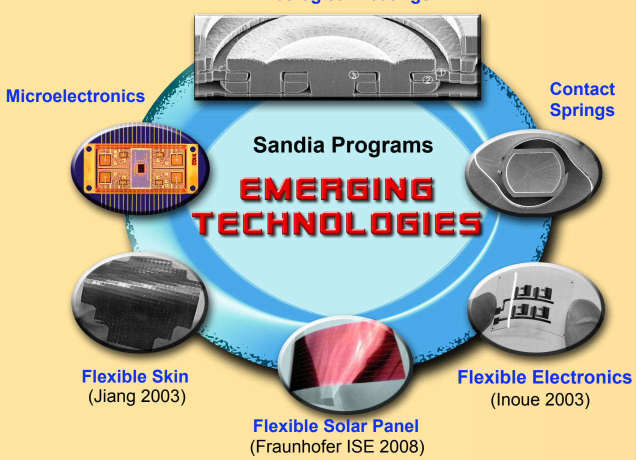
Motivation:

Thin films and compliant substrates are found in many Sandia applications. They are also the basis for emerging technologies of electrotextiles, flexible displays, and tactile sensor arrays. In all these applications, the ability to resist interfacial failure is critical to component performance.



Problem:

There is a large body of elastic rigid substrate solutions describing interfacial failure. However, compliance and the introduction of plasticity significantly complicates the problem.

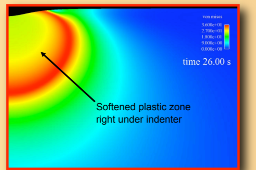
- It is difficult to perform suitable mechanical tests.
- It is difficult to deconvolute film, substrate, and interface contributions

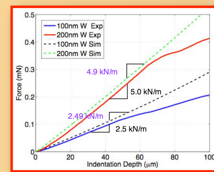
Program:

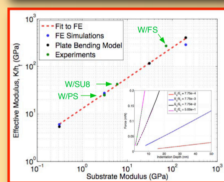
We have integrated nanomechanical tests and advanced modeling and simulations to develop a fundamental understanding of these complex systems.

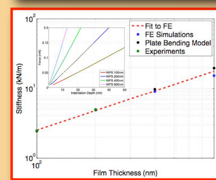
- Employed nanomechanics based tests to characterize deformation and fracture
- Applied analytical and finite element models to describe nanoindentation response
- Developed cohesive zone based modeling techniques to investigate the effects of substrate compliance and yielding on film failure

Elastic and viscoplastic models show good agreement with experimental nanoindentation data

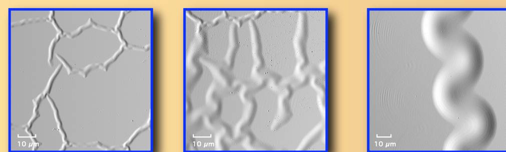








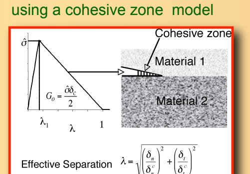
Buckles formed spontaneously in tungsten films on PMMA and silicon substrates with large and small blisters on PMMA



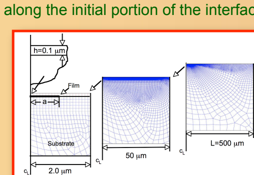
Simulations:

Cohesive Zone finite element simulations were used to investigate the effects of substrate compliance on buckle-driven delamination

Material separation was defined using a cohesive zone model



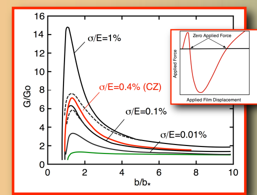
Cohesive zone elements were inserted along the initial portion of the interface



Failure modeled as a gradual process with tractions resisting separation with

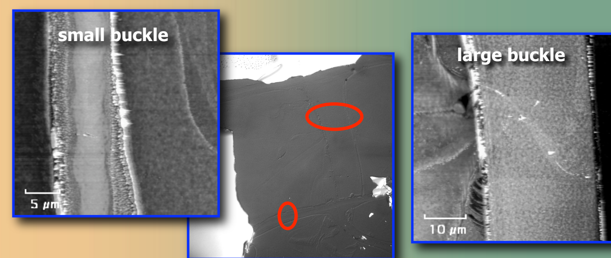
- traction-separation defined by interfacial strength and work of separation/unit area.
- a single layer of cohesive zone elements along the interface to model buckle-driven delamination
- a large substrate to approximate an infinite substrate (5000h for W/PMMA).

Cohesive Zone finite element simulations showed that substrate compliance increased fracture energies.

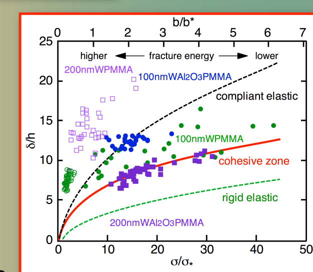


Buckles	Rigid Elastic $\Gamma(\psi)$ (J/m2)	Compliant Elastic $\Gamma(\psi)$ (J/m2)	Cohesive Zone $\Gamma(\psi)$ (J/m2)
200W/SiO2/Si	0.9	1.1	
100W/Al2O3/PMMA	0.4	0.9	0.4
100W/PMMA			
Large	0.4	0.9	0.4
Small	0.4	2.7	2
200W/Al2O3/PMMA	0.9	2.5	1.4
200W/PMMA	1	4.7	3.1

AFM imaging clearly showed that the increase in fracture energies paralleled an increase in localized substrate deformation and change in buckle morphology



The cohesive zone simulations accurately describe the change in buckle morphology with film stress, providing a lower bound to seemingly disparate sets of data



Conclusions:

- Substrate compliance markedly increases susceptibility to buckle driven delamination
- Elastic and viscoplastic models accurately describe indentation behavior leading to film fracture
- Cohesive zone finite element simulations show that increasing substrate compliance increases fracture energies.
- Other W/PMMA simulations that included substrate yielding revealed crack blunting and an increased apparent toughness.

National Nuclear Security Administration

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