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Effects of Interfacial Topography on Adhesion and Fracture at the Nanoscale

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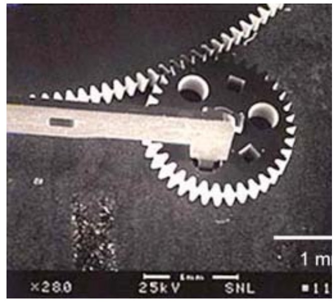
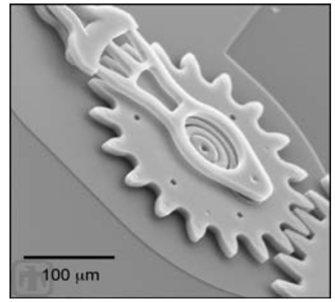
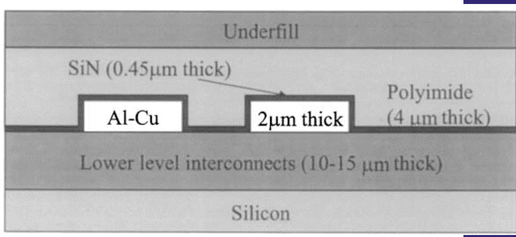
Many Sandia programs incorporate thin films and nanostructured materials where performance and reliability must be assured.

LIGA

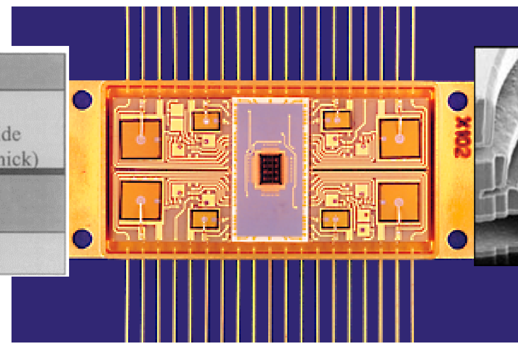


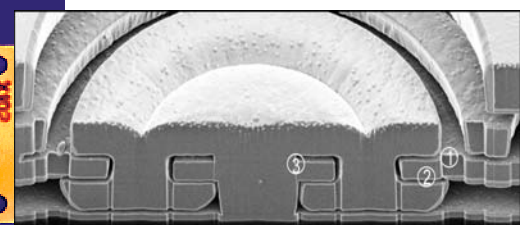


MEMS

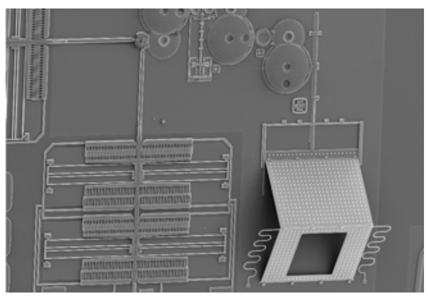


microelectronics

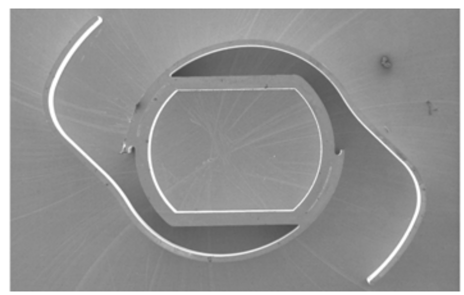




protective coatings



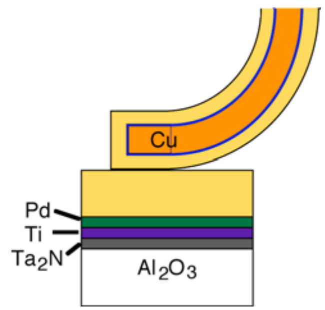
MEMS mirrors

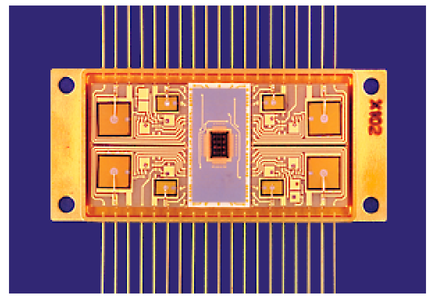


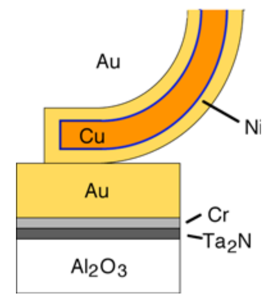
Micro springs

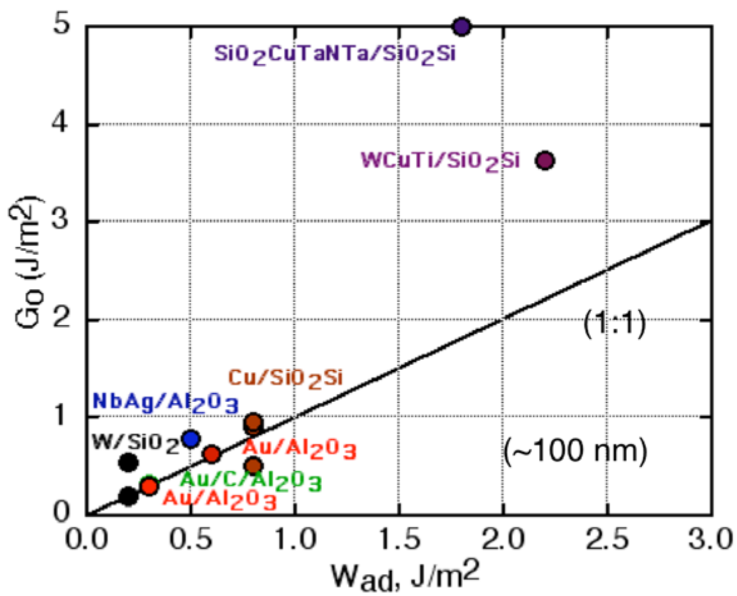
Adhesion and fracture of interfaces is critical to performance and durability of nanostructured materials and devices.

Many methods are available to increase durability at the macro and micro scales

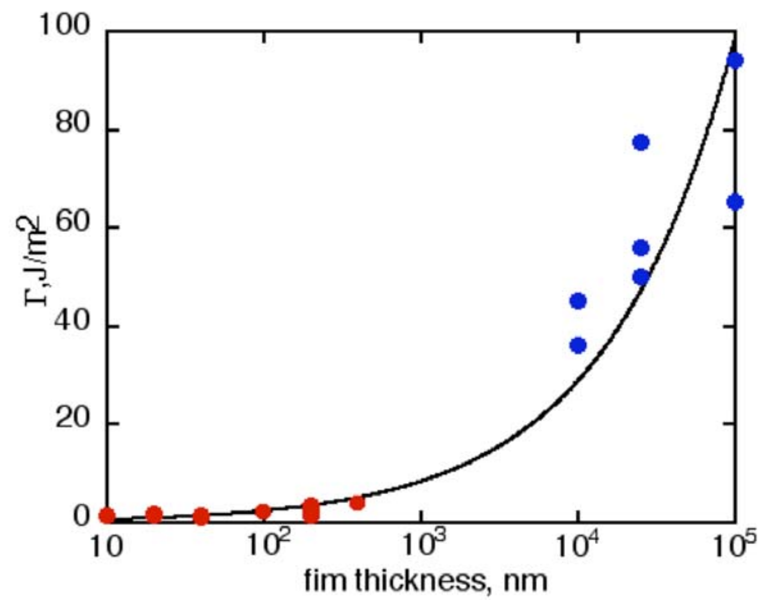








Composition



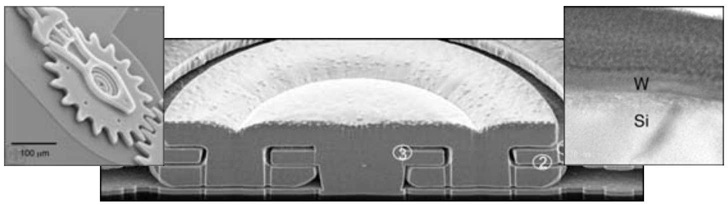
Thickness

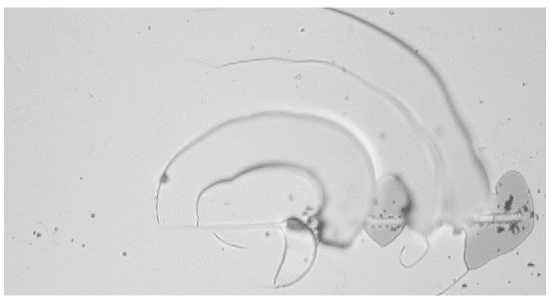
Composition, structure, and scale affect adhesion

Options become limited at the nano scale

Mismatch strains, interactions, and residual stresses can lead to failure.

Tribological coatings





ALD tungsten on silicon.

Well known that surface roughness increases interfacial fracture toughness.

Mechanisms that can increase interfacial toughness include:

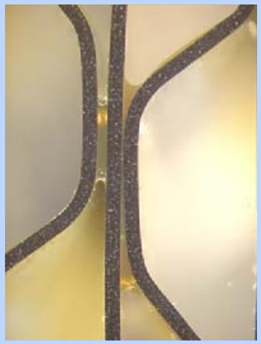
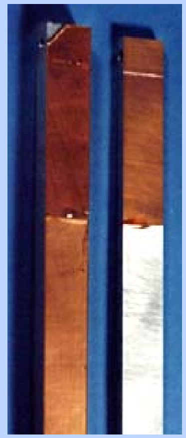
- –increase in surface area
- –mechanical interlock
- –increased crack path tortuousity
- –mixed-mode crack-tip loading

Expect similar mechanisms operate on the nano-scale.

Look to roughness for enhanced adhesion and durability

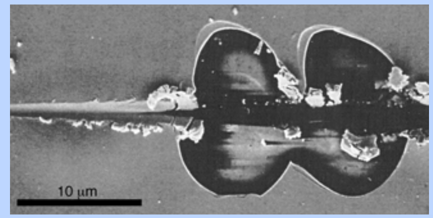
Roughness has been successfully used to enhance adhesion and durability at the macro and micron scales

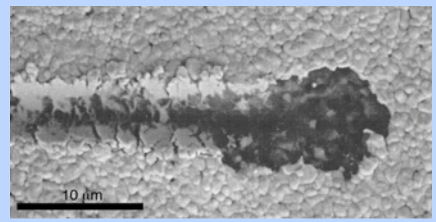
epoxy on aluminum

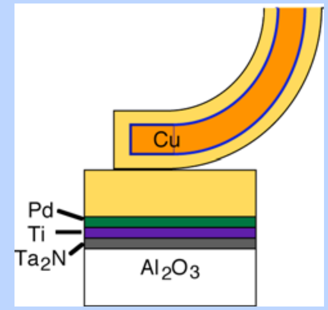




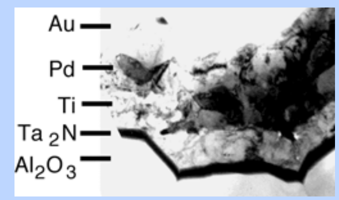
surface roughness (μm)	G_c (J/m^2)
0.2	22
1.0	31
5.0	126
7.0	168

tantalum nitride on alumina









surface roughness (nm)	P_{cr} (mN)	A (μm^2)
2	100	200
1000	350	50

Roughness significantly increases fracture energy at the micro scale

Purpose

Develop a fundamental understanding of how patterned nanoscale heterogeneities affect interfacial strength and toughness

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Experimental

Determine the effect of nanopatterned interfaces on interfacial fracture toughness.

- Sputter deposit highly stressed tungsten films
- Polished and patterned silicon substrates
- Determine fracture energies from spontaneous buckles

Modeling

Explicity model the effect of heterogeneities on interfacial cracking

- Use detailed finite element analysis
- Define separation using a cohesive zone model
- Determine effects of mode mixity

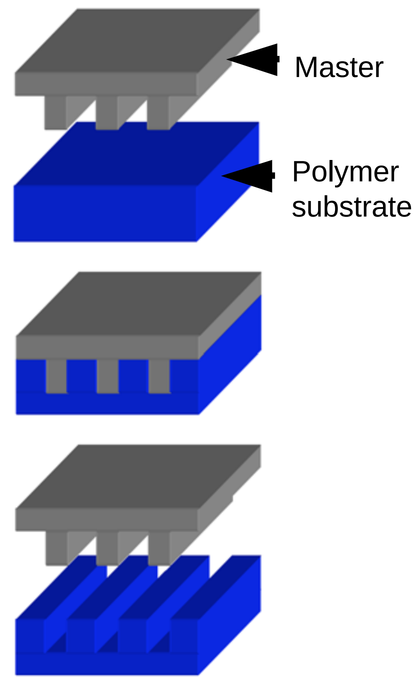
> Develop an approach to simulate strength and toughness of engineered interfaces in micro and nanoscale devices

Nanoimprint lithography is used to create patterned interfaces

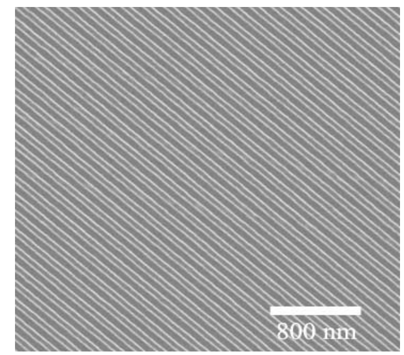
A master is fabricated using laser interference lithography

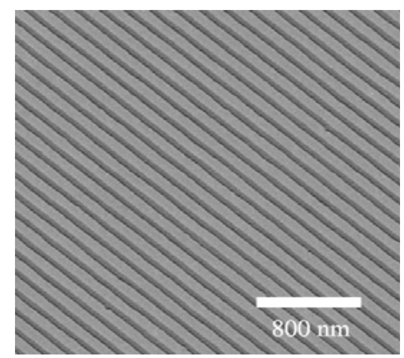
The master is used to repeatedly emboss the pattern into polymer substrates using a Nanonex 2000 NIL tool.

Mechanical Patterning: Nanoimprint Lithography



Ni master





imprinted polymer

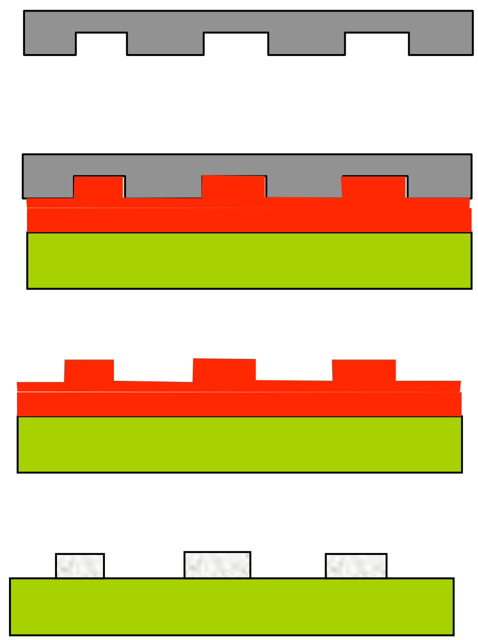
Rapid, top-down nano-patterning of large areas with well-defined surface topographies of controlled shape and dimension

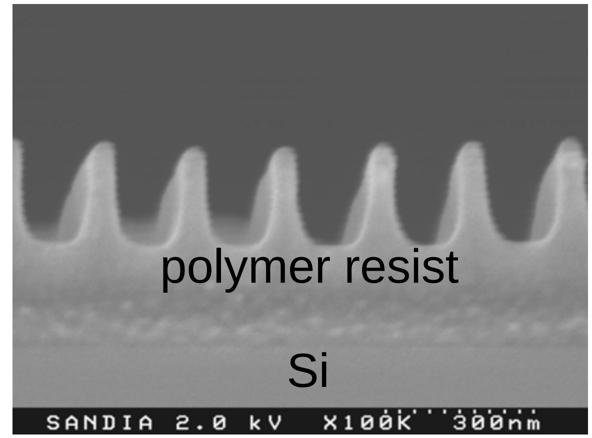
We used the technique to fabricate a 200 nm pitch 100 nm deep channel pattern on four inch diameter silicon wafers

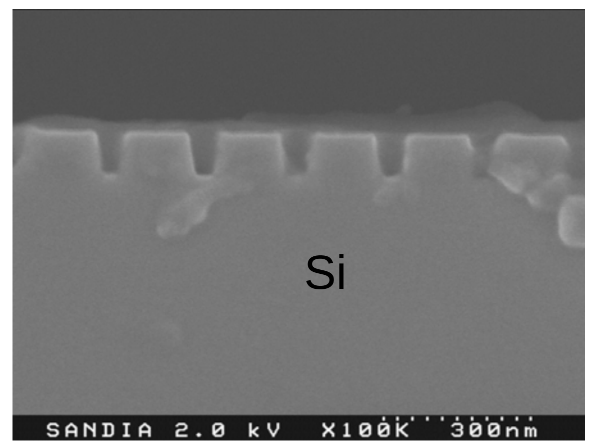
Si master created using laser interference lithography

Thermal NIL used to transfer pattern to a polymer resist coating

A plasma etch (RIE) was used to transfer the pattern to the silicon wafer





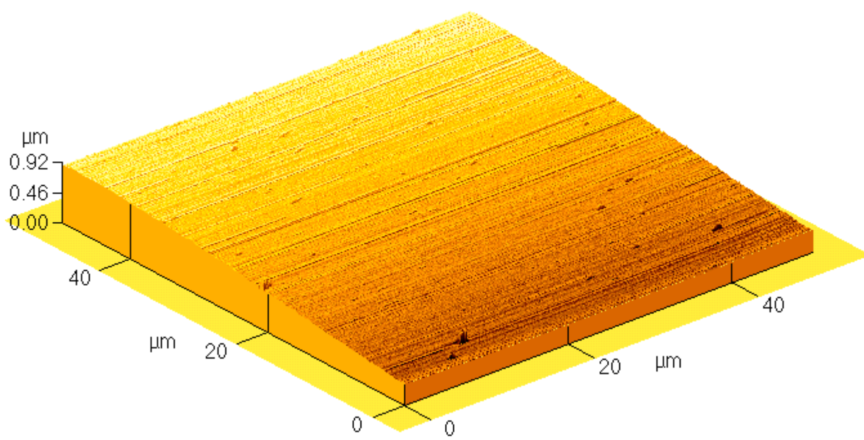


The technique created a uniformly patterned wafer for use in fabricating a variety of interfacial fracture samples

Atomic Force Microscopy showed a marked difference in surface roughness

Si (100) Wafer

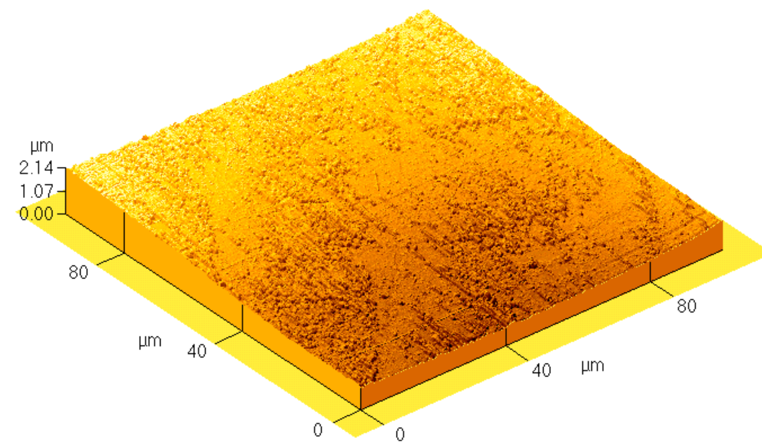
Polished



As-polished

RMS= 3 nm

Patterned

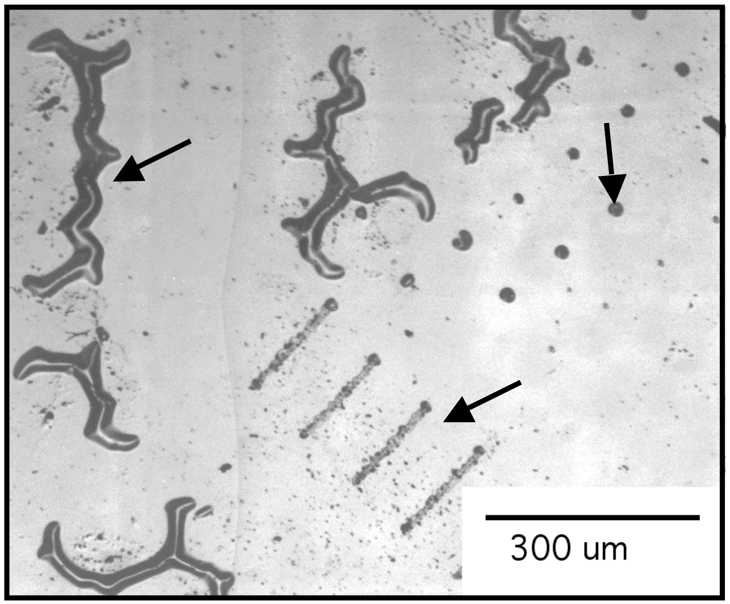


T.A. Etching

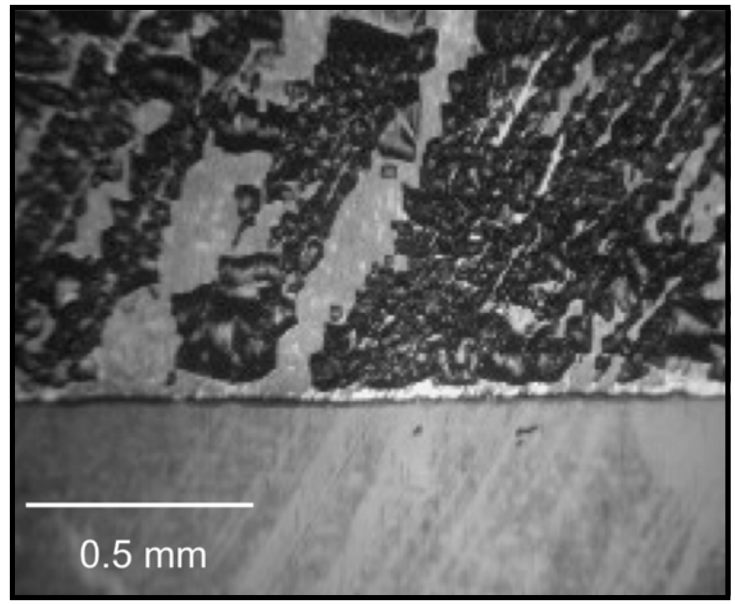
RMS= 97 nm

Tungsten films were sputter deposited onto the polished and patterned silicon wafers under conditions creating high compressive stresses.

polished

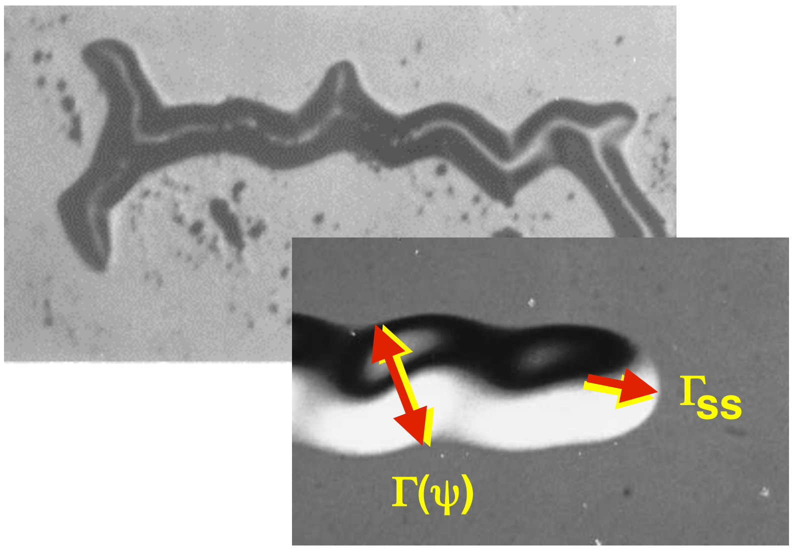


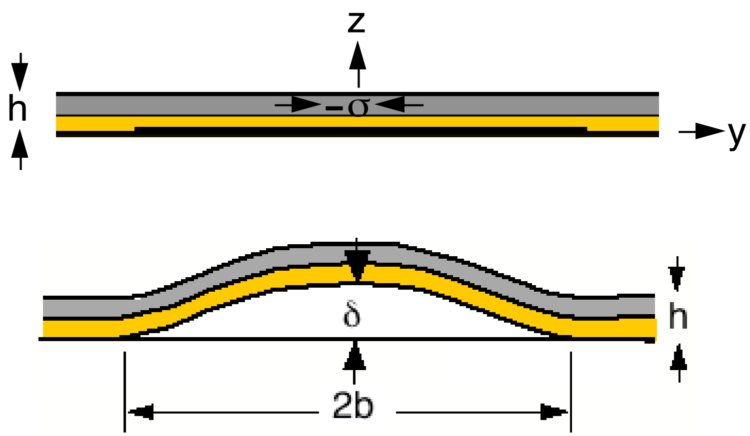
patterned



The high compressive stresses triggered spontaneous blister formation that followed the two dimensional channel patterns.

Mechanics-based modeling gives us the stresses and fracture energies for film failure of compressively stressed films





In terms of a single set of parameters, the stress for delamination is,

$$\sigma_b = \frac{\pi^2}{12}\frac{E}{(1-\nu^2)}\left(\frac{h}{b}\right)^2$$

Residual stress is as follows,

$$\sigma_r = \sigma_b\left[\frac{3}{4}\left(\frac{\delta^2}{h^2}+1\right)\right]$$

The strain energy released along the side wall is given by,

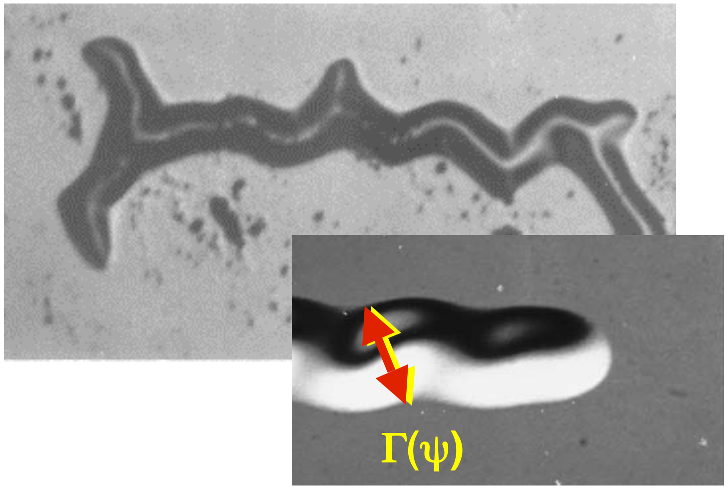
$$\Gamma(\psi) = \left[\frac{(1-\nu^2)h}{2E}\right](\sigma_r - \sigma_b)(\sigma_r + 3\sigma_b)$$

and along the propagating curved front.

$$\Gamma_{ss} = \left[\frac{(1-\nu^2)h\sigma_r^2}{2E}\right]\left(1-\frac{\sigma_b}{\sigma_r}\right)^2$$

Hutchinson and Suo (1992)
Bagchi and Evans (1992)
Kriese, Moody, Gerberich (1998)

Fracture energies show a strong effect of surface topography on interfacial fracture energies.



The strain energy released along the side wall is given by,

$$\Gamma(\psi) = \left[\frac{(1-\nu^2)h}{2E}\right](\sigma_r - \sigma_b)(\sigma_r + 3\sigma_b)$$

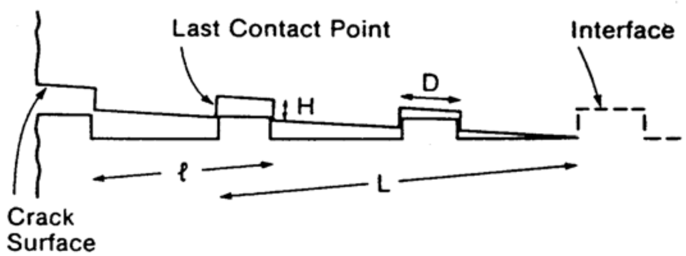
with the mode I contribution defined as,

$$\Gamma_I = \Gamma(\psi) \Big/ \left[1 + \tan^2\{(1-\lambda)\psi\}\right]$$

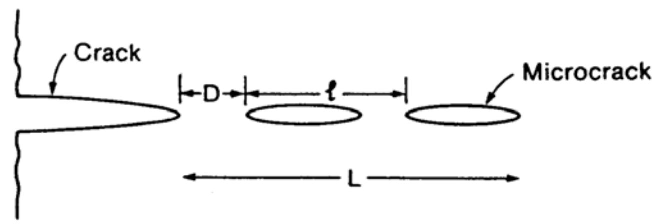
Hutchinson and Suo (1992)

	Thickness	Blister		Stress		Fracture Energy		
sample	h_W	b	δ	σ_b	σ_r	$\Gamma(\psi)$	ψ	Γ_I
	(nm)	(μm)	(μm)	(GPa)	(GPa)	(J/m²)		(J/m²)
smooth	250	14	1.4	0.1	-3.0	2.7	90	0.6
patterned	280	13	1.4	0.2	-3.6	4.3	90	0.9

Evans and Hutchinson analytically described the effect of non-planar crack growth on fracture energy using simple opening and shear mode contact models.



opening mode



shear mode

Superposition of these models leads to a relation between strain energy release rate and the phase angle of loading as follows:

$$\frac{\Delta G}{G} = \frac{\tan^2 \psi \left\{ 1 - k \left[\alpha_o \right) 1 + \tan^2 \psi \right) \left(\frac{\Delta G}{G} + 1 \right) \right] \right\}}{(1 + \tan^2 \psi)}$$

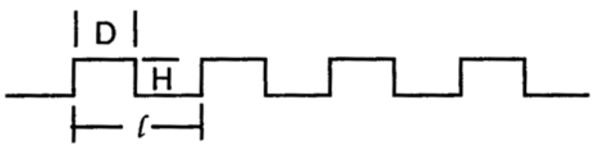
where $$\alpha_o = \pi \left(\frac{EH^2}{\ell G_o} \right) \Big/ 32 \left(1 - \nu^2 \right) \ln \left[1/\sin(\pi D / 2\ell) \right]$$

with α_o and G_o defined at $\psi=0$

(Evans and Hutchinson)

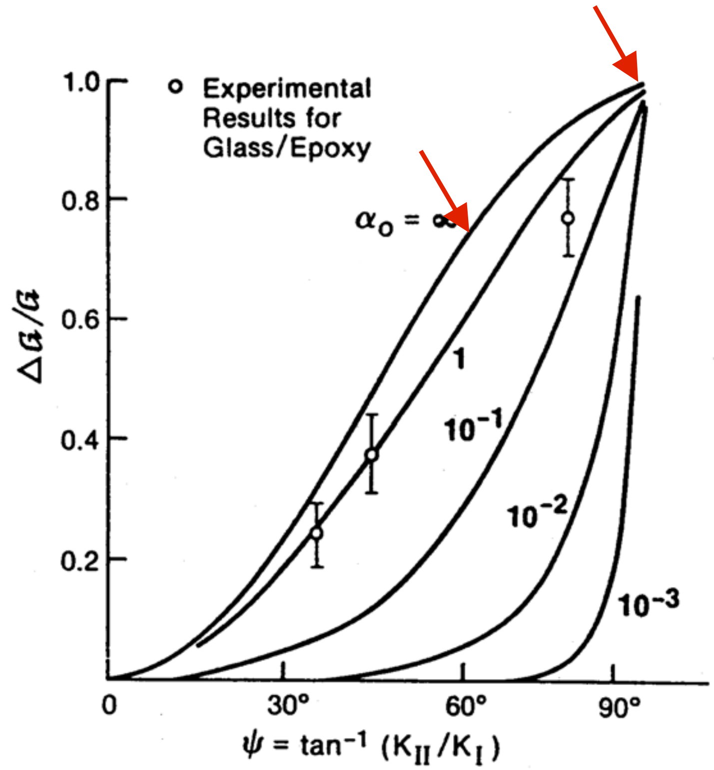
The difference between fracture energies of tungsten films on smooth and patterned silicon substrates follows model estimates.

$$\alpha_o = \pi\left(\frac{EH^2}{\ell G_o}\right)\Big/ 32\left(1-\nu^2\right)\ln\left[1/\sin\left(\pi D/2\ell\right)\right]$$



Nominal dimensions
H = 100 nm
D = 150 nm
L = 200 nm

$\alpha_o \sim 50{,}000 \sim \infty$

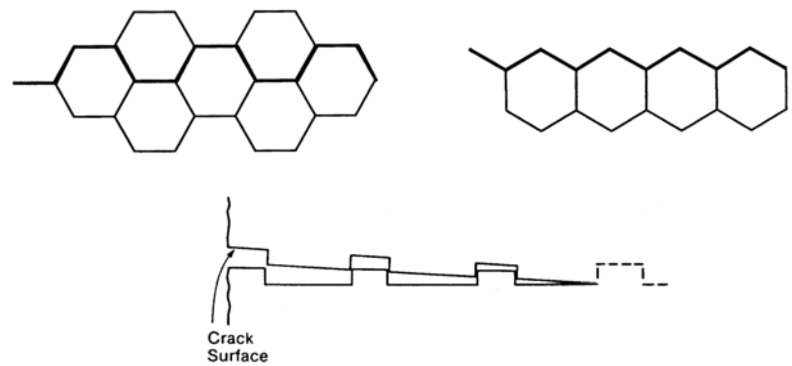


Given ψ between 60° and 90°, $\Delta G/G \sim 0.8\text{-}1.0$ with $G_{patterned} \sim 1.8\text{-}2.0\ G_{polished}$

(Evans and Hutchinson)

Detailed finite element simulations were used to define the effects of surface topography on interfacial fracture

- Need to simulate subcritical crack growth along tortuous paths with deviations from linearity
- Need an accurate representation of the separation process.
- Include material and geometric heterogeneities.
- Ability to model discontinuous or non-sequential crack growth.
- Include the possible cohesive fracture of the heterogeneities themselves.



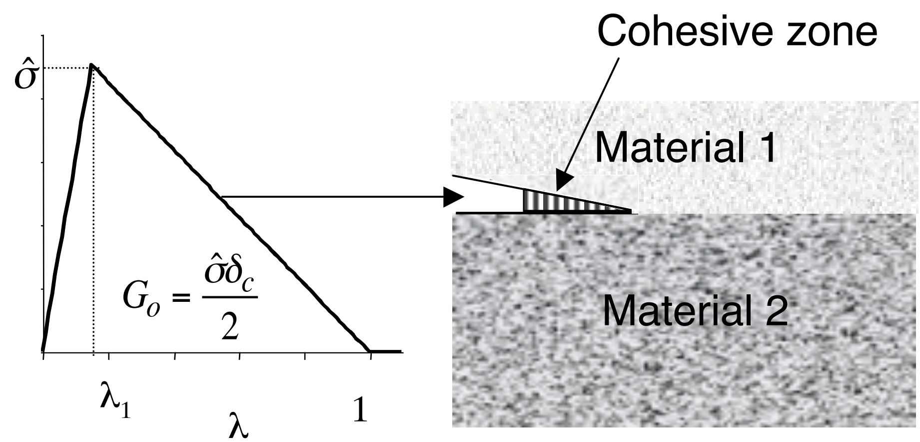
2D and 3D surface features

Crack growth along tortuous crack paths

- Used Sandia's PRESTO explicit, transient dynamics finite element code.
- Well suited for analyzing large deformations with complex contact conditions.

Material separation is defined using a cohesive zone model

- Material separation based on a specified traction-separation ($\sigma-\delta$) relationship.
- Key parameters are the cohesive strength $\hat{\sigma}$ and the work of separation/unit area G_o.
- Mesh-independent results as a length scale is embedded in the $\sigma-\delta$ relationship.
- Defined in terms of a potential that depends on a scalar effective separation.
- Crack growth is a natural outcome of the solution.
- Similar to model introduced by Tvergaard and Hutchinson (J.Mech. Phys. Solids, 1993).

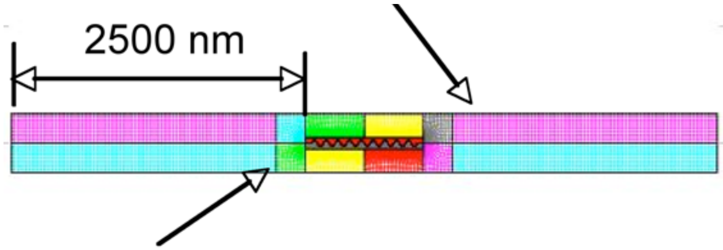


Effective Separation $\lambda = \sqrt{\left(\frac{\delta_n}{\delta_n^c}\right)^2 + \left(\frac{\delta_t}{\delta_t^c}\right)^2}$

A traction-separation relation models bond failure as a gradual process with tractions resisting separation.

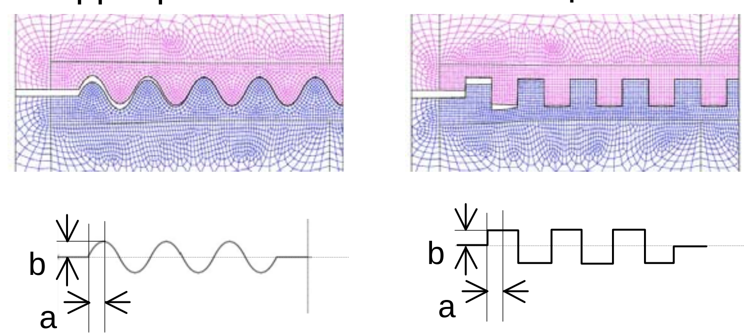
Used fixed-grip loading of a long bimaterial strip to study mode mixity effects on interfacial fracture

Uniformly displace top edge--normal, U_n, and tangential, U_t, motion.



Fixed bottom edge

Ripple patterned   Channel patterned



a = b =25 nm

- Can generate any desired load mode mixity.
- There is an analytic solution for fixed-grip loading with a flat interface:

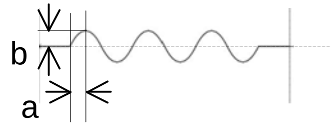
$$G = \frac{U_n^2}{2}\left(h/\bar{E}_1 + h/\bar{E}_2\right)^{-1} + \frac{U_t^2}{2}\left(h/\mu_1 + h/\mu_2\right)^{-1}$$

- Mode mixity can be determined using published results.

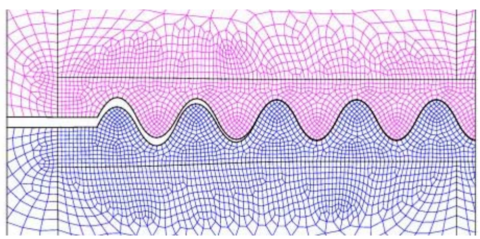
- 250 nm tungsten film on a 250 nm silicon substrate
- Initial 2.5-μm long portion of interface-flat and delaminated.
- Followed by a 1.0 μm patterned region.
- G_o = 0.3 J/m^2, δ_c = 1.0 nm
  $\hat{\sigma}$ = 600 MPa, $\hat{\tau}$ = 300 MPa

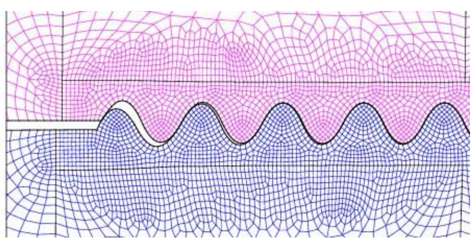
Used fixed-grip loading of a long bimaterial strip to study mode mixity effects on interfacial fracture

Ripple patterned



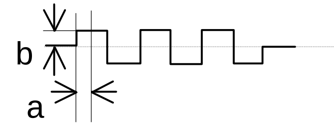
$a = b = 25$ nm
$G_o = 0.3\ J/m^2$

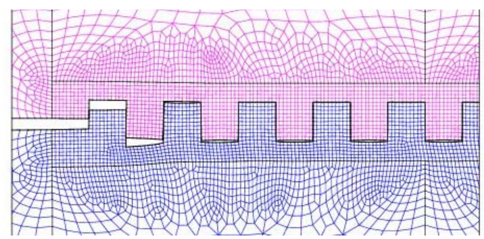


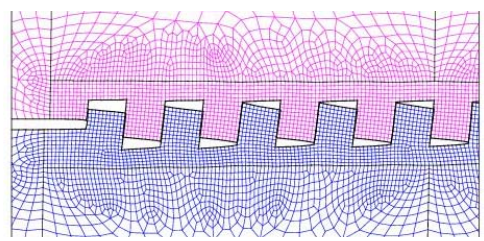


Interface area
1.48 x's higher

Channel patterned







Interface area
2.00 x's higher

G_{ss}/G_o

mode I

Rippled	Channel
1.6	2.3

mode I=mode II

Rippled	Channel
1.7	2.6

G_{ss} is defined as apparent toughness when rapid crack growth begins

Channel patterns appear more effective than ripple patterns

Conclusions

Nanopatterned heterogeneities exert a strong effect on nucleation and growth of thin film blisters.

A 200 nm pitch 100 nm deep channel pattern increased fracture energies by more than 50 percent.

Simulating crack growth using an explicit finite element code with material separation defined by a cohesive zone model shows the same effect on fracture energies.

Develop an approach to simulate strength and toughness of engineered interfaces in micro and nanoscale devices

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