SAND2012-0576P

35th Annual Meeting of the Adhesion Society

Adhesion/Atomistic Friction Surface Interaction Model with Application to Interfacial Fracture and Nano-Manufacturing

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This work was performed at Sandia National Laboratories. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

Supported in part by the Laboratory Directed Research and Development program at Sandia National Laboratories.

February 27th, 2012

Adhesion/Atomistic-Friction (Ad/AF) model for weak surface interactions

- Motivated by shear force microscopy measurements.
- Scanning probe tests that measure lateral force (friction) force as a function of the applied normal force.
- Published work suggests that in some cases there is a load-independent interfacial shear strength can be used to describe molecular-level friction.

$$F = \tau^* \cdot A(L)$$

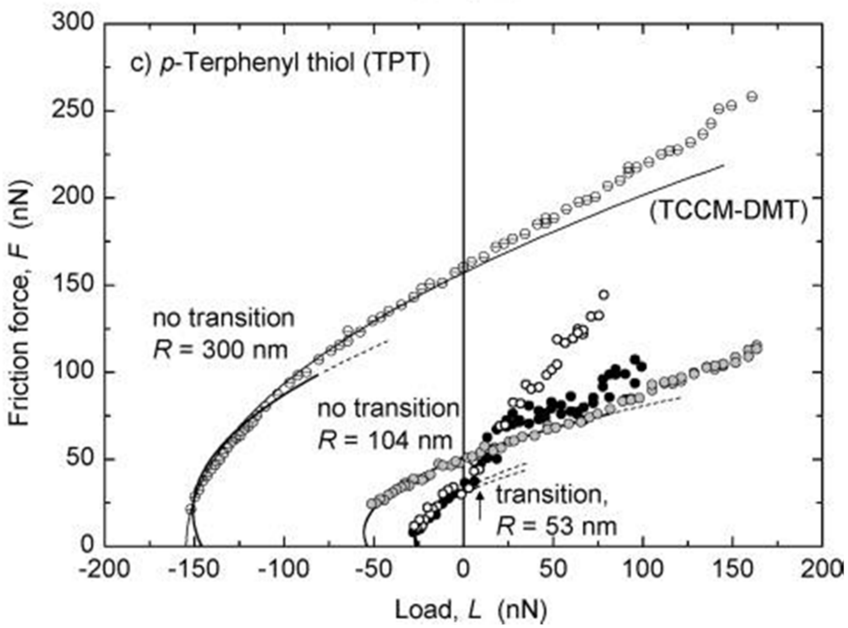
- F: friction force
- τ^*: interfacial shear strength
- $A(L)$: contact area (depends on normal load *L*)

- see for example Carpick, et.al, JOM, V56 2004.

Ad/AF model for weak surface interactions

Yang, Y. and M. Ruths (2009). "Friction of Polyaromatic Thiol Monolayers in Adhesive and Nonadhesive Contacts." Langmuir 25: 12151-12159.

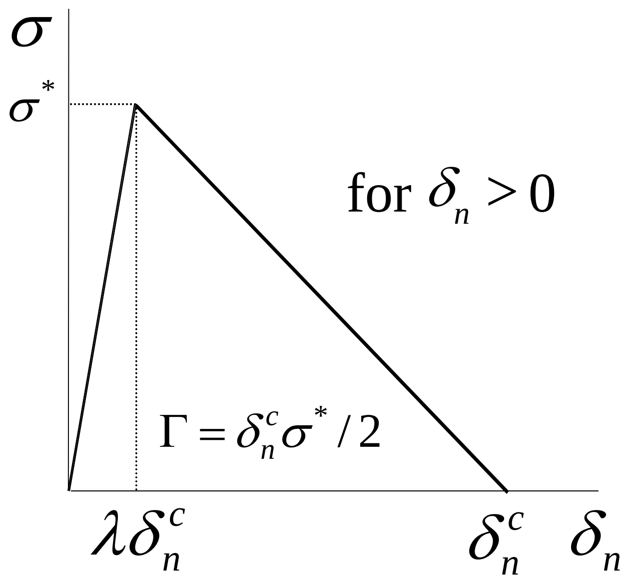
- Friction force microscopy results (from Table 2 and Fig. 3 of reference).
- Gold-coated tip and substrate are coated with the 1.5 nm thick p-terphenyl thiol (TPT) SAM.
- Found they could fit data well to $F = \tau^{*} \cdot A(L)$.
- *A(L)* from TCCM analysis that includes adhesion (Reedy, JMR 2006, 2007).

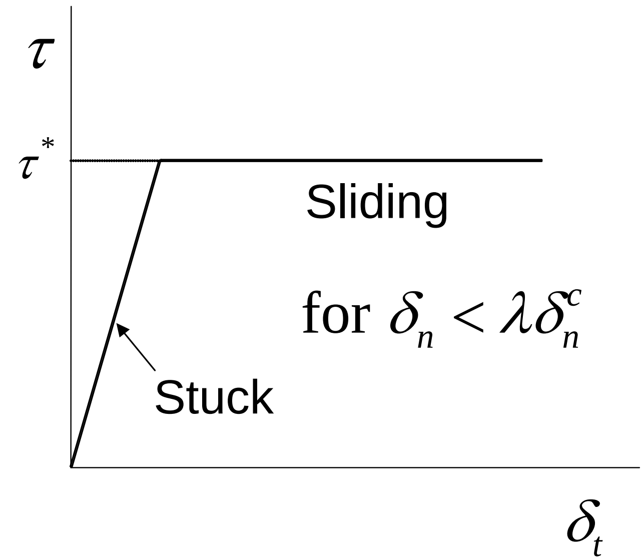


AFM tip radius (nm)	Interfacial strength τ* (MPa)	Work of adhesion (mJ/m²)
53	430	82
53	470	80
104	360	84
300	340	80
300 (alternative TCCM-DMT fit)	460	82

Similar level of agreement for four other SAM coatings.

Ad/AF model for weak interfaces





- δ_n is the normal interfacial separation.
- σ is the normal traction.
- Adhesion force acts across open gap.
- Constrained against normal interpenetration.

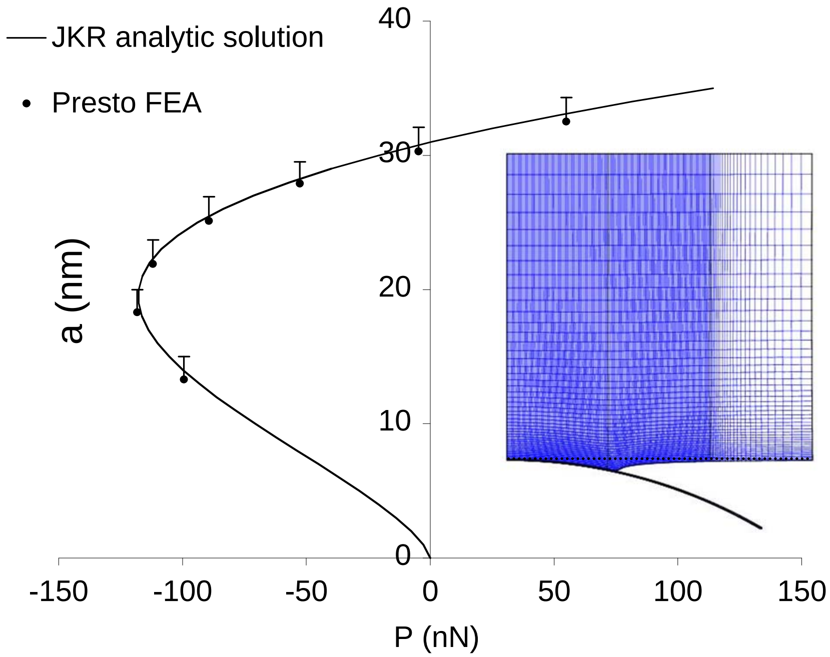
- Tangential traction acts on the interface when in contact.
- When $|\tau| < \tau^*$ the materials stuck together (tied).
- When $|\tau| = \tau^*$ slip with τ^* opposing tangential slip (pressure independent).

Finite element analysis

- Used Sandia's Sierra SM explicit, transient dynamics finite element code.
- Such codes (e.g. SNL/Sierra SM, DYNA, ABAQUS Explicit) are well suited for analyzing large deformations with complex contact conditions, discontinuous crack growth, etc.
- Discretizes the equations of motion for a body and solves the resulting system of equations using a central difference time integrator that advances the solution from an initial state.
- Ad/AF model implemented via the contact algorithm.
    - – current, deformed geometry; can have large translations, etc.
- External loads applied sufficiently slowly that external loading is quasistatic.

Verified adhesion portion of Ad/AF model

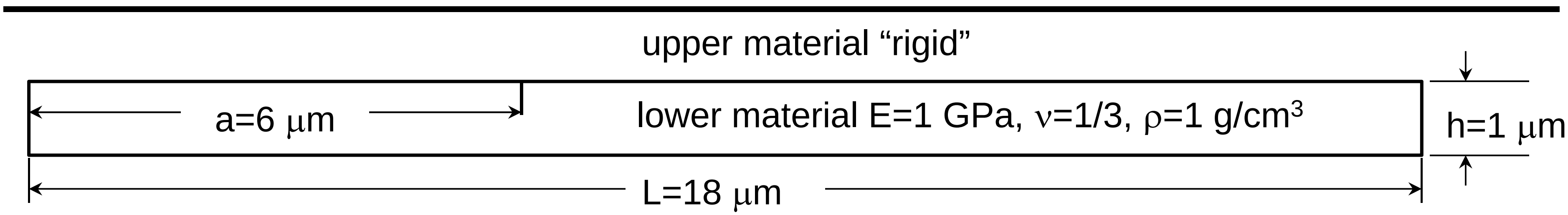
- Simulated problem where JKR adhesion analysis should apply.
  - Rigid sphere contacting a thick compliant substrate.
  - *E*=1 GPa, ν=0.4, *R*=100 nm, *W*=0.25 J/m^2
- Plot contact radius, *a*, versus applied compressive load, *P*.
- Symbol is calculated contact radius, bar indicates length of region where adhesive forces act across open gap. Did not assume JKR-like.
- Ad/AF FEA implicitly assumes interface is locally flat on scale of range on interaction forces.



Illustrative problem:

long edge-cracked bimaterial strip with upper material rigid

Edge-cracked bimaterial strip with upper material rigid



- Plane strain calculation.
- Desire upper material to behave as if rigid.
  - its thickness = $h/200$ and Young's modulus E = 10 GPa.
  - Ad/AF implementation requires interface bounded by opposing elements.
  - can't simply set modulus arbitrarily high without adversely impacting time step.
- Apply uniform edge normal and tangential displacement to upper "rigid" material.
  - applied edge velocity is sufficiently slow (0.1 μm/μs) so that inertial effects due to loading are negligible.
  - lower edge of strip fixed.
- Strip sufficiently long so that large region in central portion of ligament is uniformly stressed with stress levels equal to those in an infinitely long strip.
- Unless indicated otherwise, Ad/AF model parameters are Γ = 0.05 J/m^2,σ^*=50 MPa, τ^*/σ^* = 0.5, and λ=0.05.

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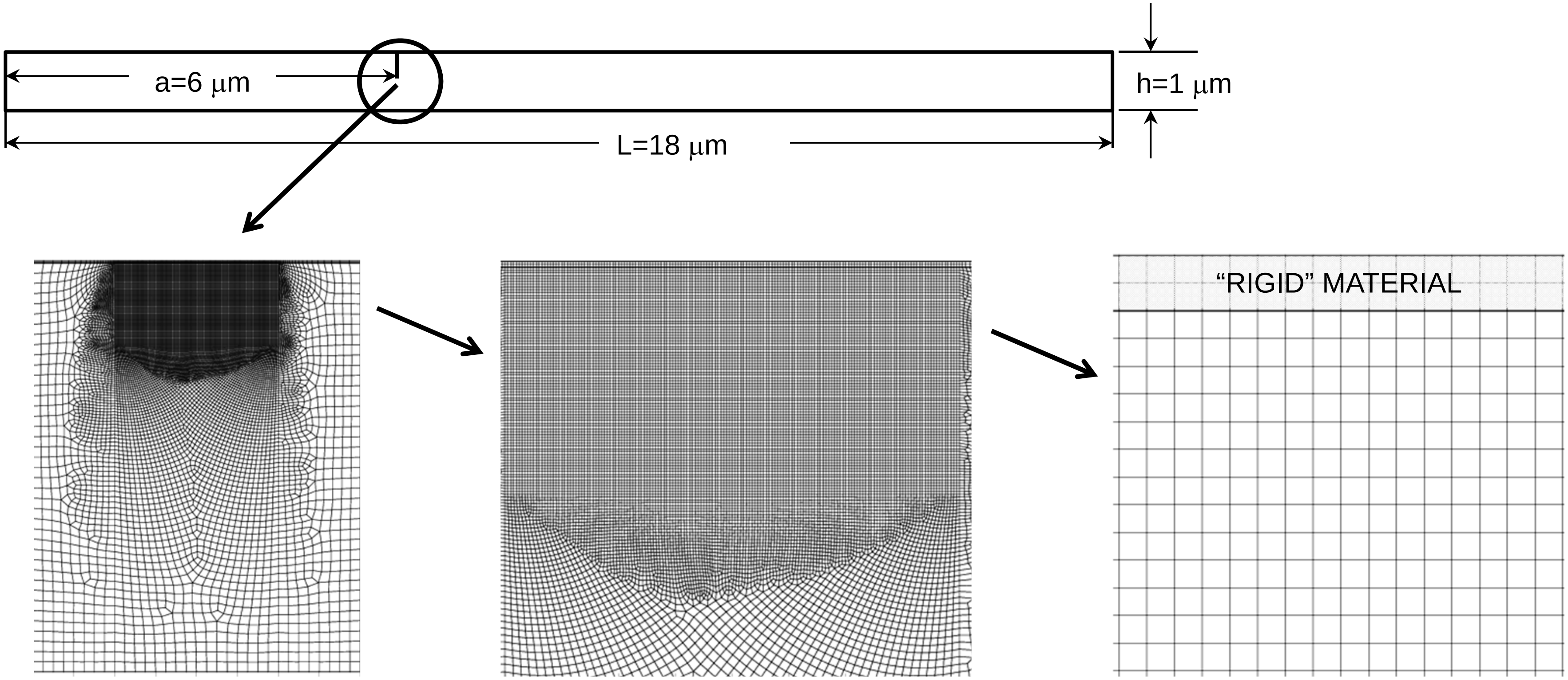
Edge-cracked bimaterial strip with upper material rigid



- Highly refined region surrounds initial crack tip.
  - characteristic element size $\Delta = 0.0025$ μm (h/400).

Nondimensional dependencies

$$\Gamma_e / \Gamma = f\left(\frac{\sigma^c{}_{xy}}{\sigma^c{}_{yy}}, \frac{\tau^*}{\sigma^*}, \frac{\sigma^*}{E}, \frac{h}{(2\Gamma/\sigma^*)}, \nu, \lambda, \frac{2m_d\Gamma}{\sigma^*(E/\rho)^{1/2}} \right)$$

Primary dimensions Γ, σ^*, and ρ

- $L = 2\Gamma/\sigma^* = \delta_n^c$ (μm)
- $F = \Gamma^2/\sigma^*$ (μn)
- $T = (2\Gamma/\sigma^*) / (E/\rho)^{1/2}$ (μs)

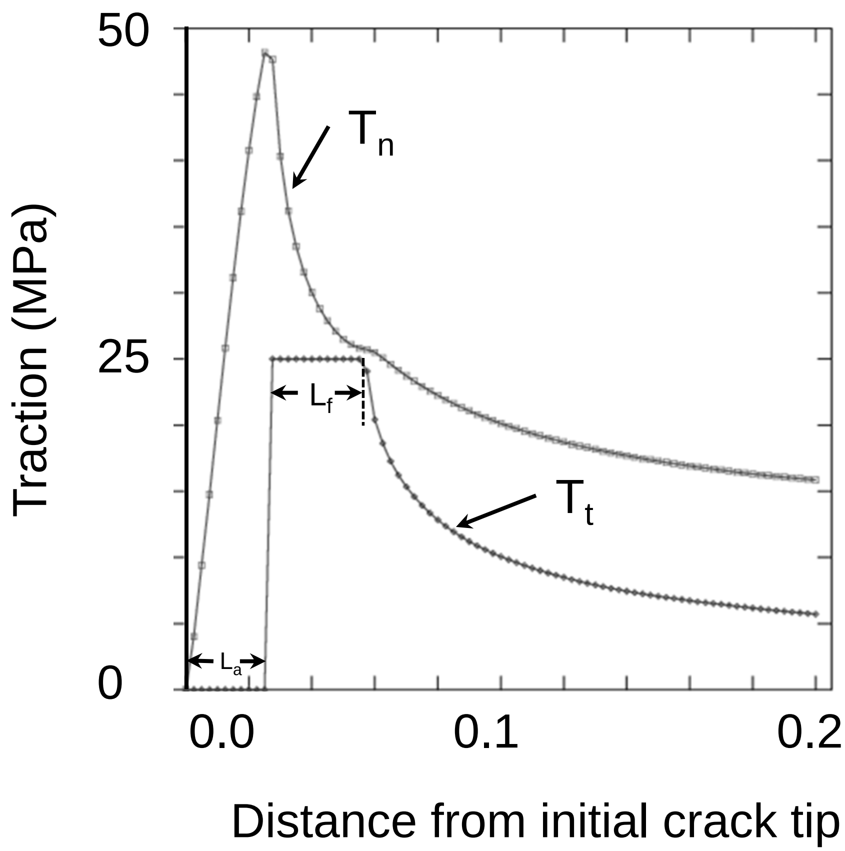
- Γ_e is the energy release rate when the interfacial crack begins to propagate.
  - use well-known analytical *G*-calibration for an edge-cracked bimaterial strip.

$$\Gamma_e = \frac{h}{E_u}\left(\sigma^c_{yy}\right)^2 + \frac{h}{G}\left(\sigma^c_{xy}\right)^2$$

  - σ^c_{xy} and σ^c_{yy} are critical stresses in uniformly stressed ligament and E_u is the uniaxial strain modulus.
- Low level of mass damping m_d (with units of μs^{-1}) included to damp out vibrations (stress waves) generated by release of interfacial shear as adhesive zone forms.
  - in reality, such vibrations will be damped out by energy dissipation mechanism such as polymer viscoelasticity.
  - mass proportional damping is simply a convenient computational approach for applying damping.

Example of calculated interfacial stress distributions

- Calculated interfacial normal traction T_n and tangential traction T_t just prior to crack propagation.
- Results for
  - $\sigma^c_{xy}/\sigma^c_{yy} = 0.25$.
  - $\Gamma = 0.05$ J/m^2
  - σ^*=50 MPa
  - $\tau^*/\sigma^* = 0.5$.
- Length of fully developed adhesive zone $L_a/h = 0.0250$.
- Length of fully developed frictional zone $L_f/h = 0.0275$.
- Note: no T_t within adhesive zone where $\delta_n > \lambda\delta_n^c$.



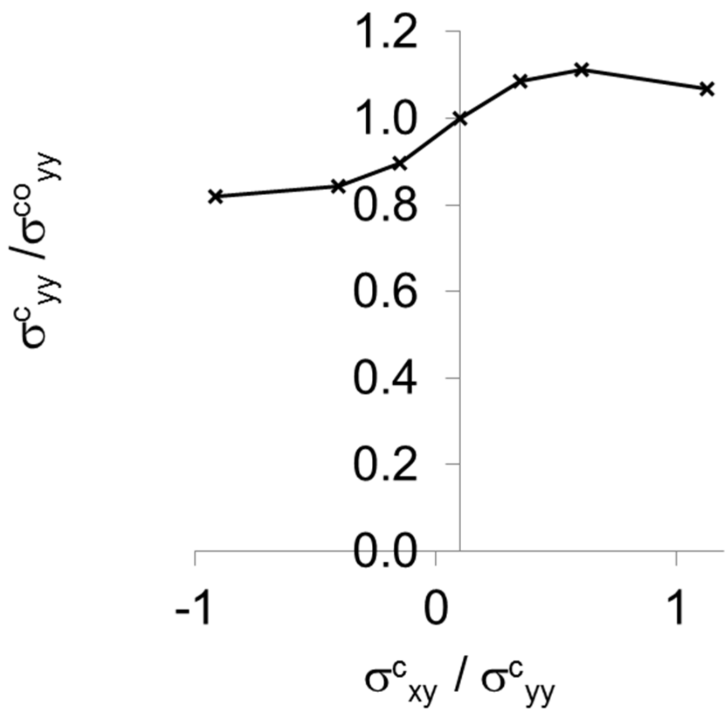
Crack tip at point where T_n=σ^*,
Adhesive zone: where T_n decrease with increasing δ_n.
Frictional zone: where T_t = τ^*.

Test calculations to examine convergence

Vary	Values	% change in Γ_e
Characteristic element size Δ (μm)	0.00125 0.00250	1.0
Upper material's Young's modulus (GPa)	10 100	0.1
Mass damping (μs^{-1})	200 5000	0.1

- Results for $\sigma^c_{xy}/\sigma^c_{yy} = 0.25$ and $\tau^*/\sigma^* = 0.5$.
- Length of the fully formed adhesive zone L_a ~ 10 elements long at initiation of crack propagation $\Delta = 0.0025$ μm.

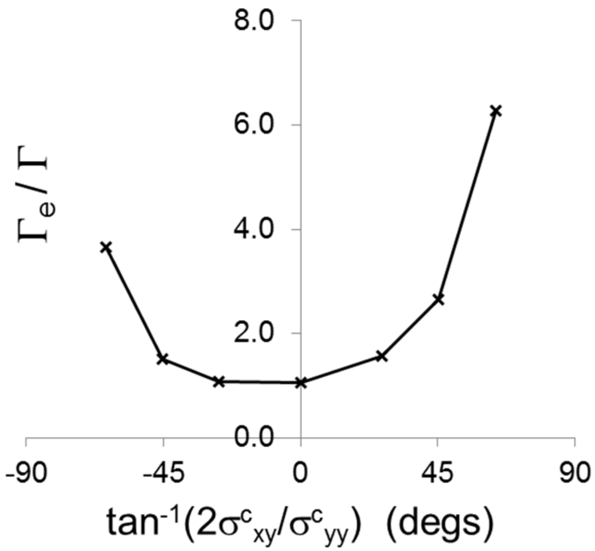
Effect of applied mode mixity

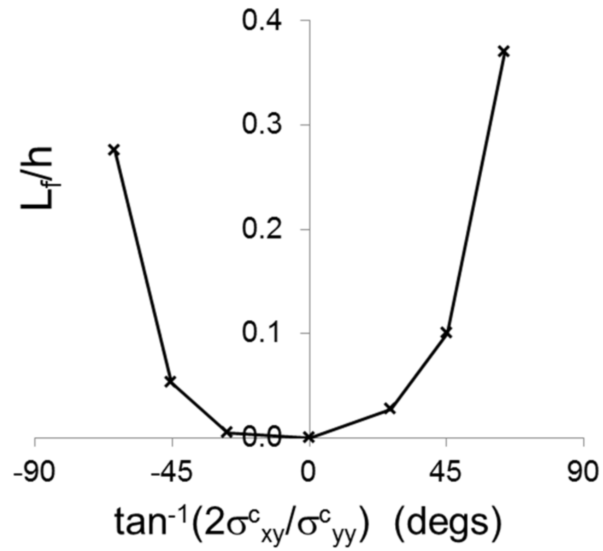


Note: σ^{co}_{yy} is value of σ^{c}_{yy} when $\sigma^{c}_{xy} = 0$

- The value of σ^c_{yy} depends on the level of applied shear.
- The LEFM solution for this problem indicates that δ_n depends on the sign of $\sigma^c_{xy}/\sigma^c_{yy}$.
  - at a distance Δ behind the crack tip, the value of δ_n for $\sigma^c_{xy}/\sigma^c_{yy} = -0.25$ is 1.45 larger than that for $\sigma^c_{xy}/\sigma^c_{yy} = 0.25$.

Effect of applied mode mixity



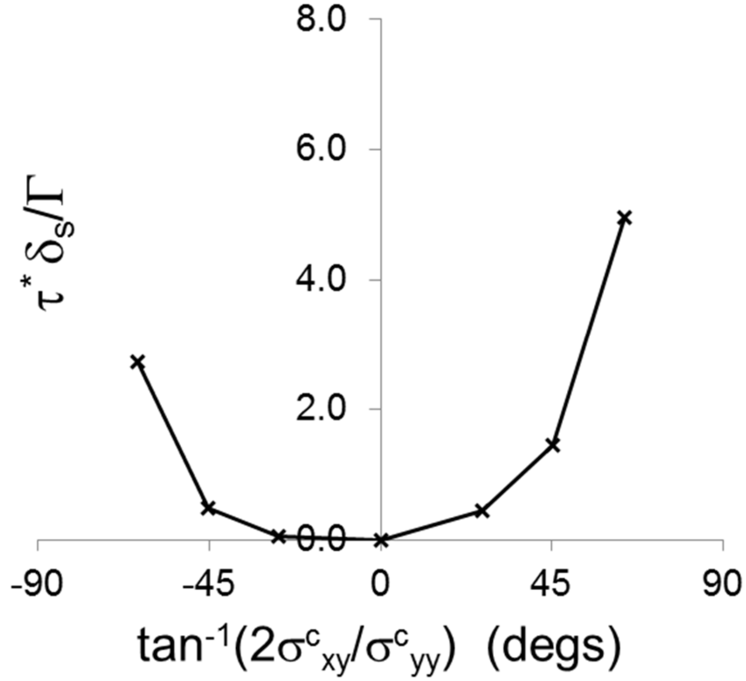


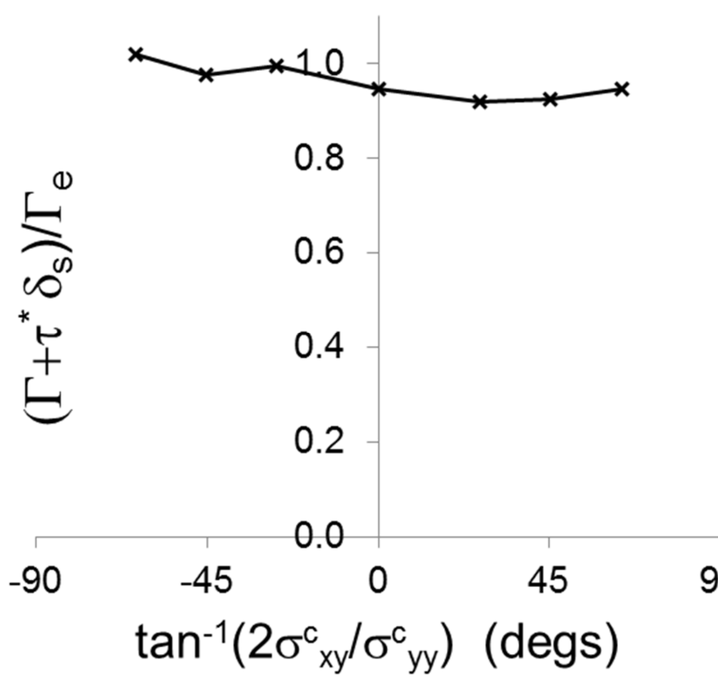
- Calculated effective toughness displays a significant dependence on applied mode mixity $\psi_a \equiv \tan^{-1}(2\sigma^c{}_{xy} / \sigma^c{}_{yy})$.
  - The crack tip mode mixity at a distance l_o in front of a long interfacial crack in a elastic bimaterial strip where the upper material is rigid (Hutchinson and Suo,1992) is

$$\psi_{r=l_o} = \gamma + \omega + \varepsilon \ln(l_o / h)$$

  - when α= 1.0 and β= 0.25 (i.e., ν= 1/3), ω= -17^o and γ= ψ_a.
  - In these calculations, ε = -0.081. If l_o/h=0.01, $\omega + \varepsilon \ln(l_o / h) = 4.5^o$.
  - note, L_f/h relatively large for high ψ_a, violate small-scale yielding assumption.

Work of adhesion and frictional dissipation





- Dissipation due to frictional slip is primary source of the dependence of Γ_e on ψ_a.
  - frictional dissipation = $\tau^*\delta_s$, where δ_s is the maximum frictional slip (found at the tip of the adhesive zone where the normal interfacial stress $\sigma=\sigma^*$).
  - δ_s/Δ ~4 when $\tan^{-1}(2\sigma^c_{xy}/\sigma^c_{yy})=64^o$; implementation of Ad/AF as a surface interaction model allows relatively large slips to occur.
- Dissipation associated with the stress waves (vibrations) generated by the abrupt release of frictional stress as adhesion zone forms is relatively small (< 10%).

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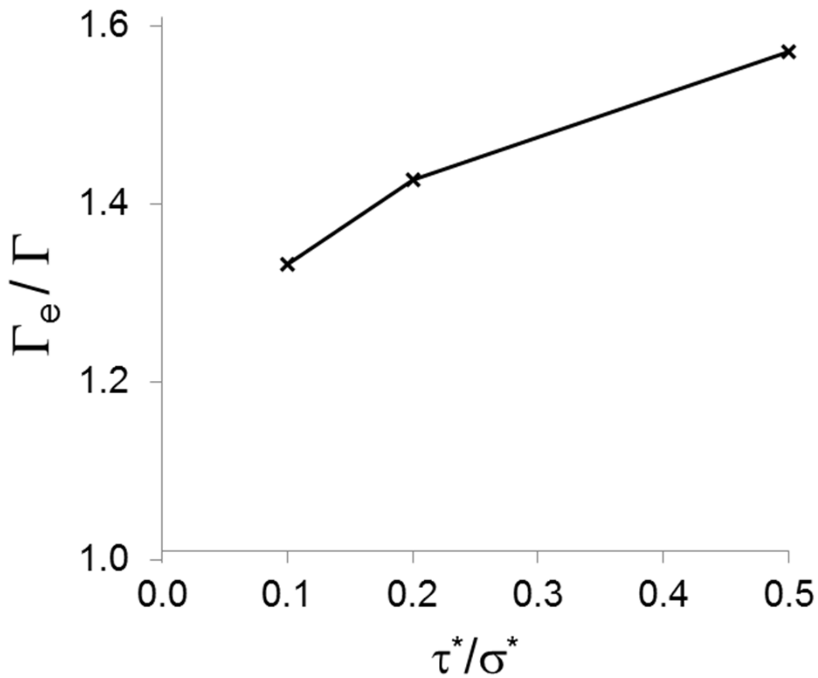
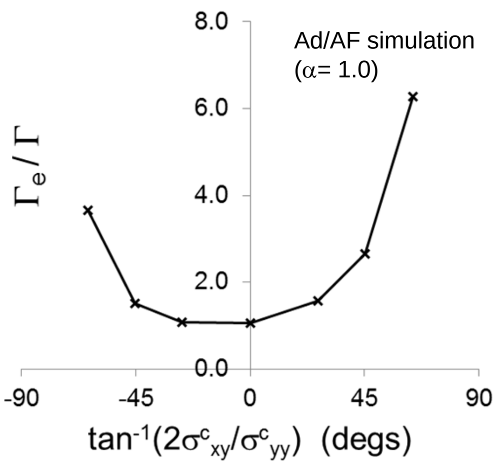
Dependence on τ^*/σ^*

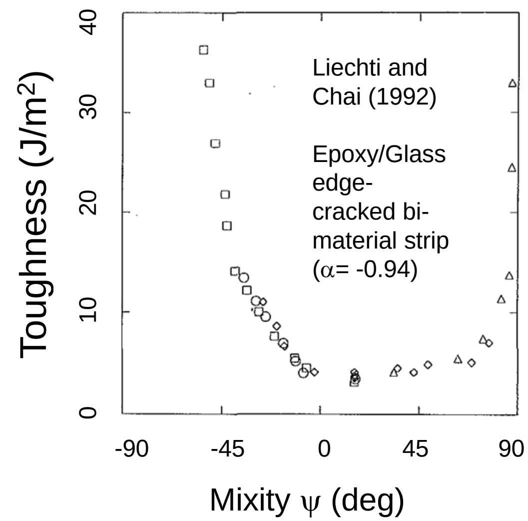


- Results for
  - $\sigma^c_{xy}/\sigma^c_{yy}$= 0.25.
  - Γ = 0.05 J/m^2
  - σ^*=50 MPa

- Γ_e/Γ increases as τ^*/σ^* increases.
  - the rate of increase in Γ_e/Γ with τ^*/σ^* decreases as τ^*/σ^* increases.
  - expect that there might be a maximum value of Γ_e/Γ as τ^*/σ^* increases.

Discussion





Liechti, K. M. and Y. S. Chai (1992). "Asymmetric Shielding in Interfacial Fracture Under In-Plane Shear." Journal of Applied Mechanics 59: 295-304.

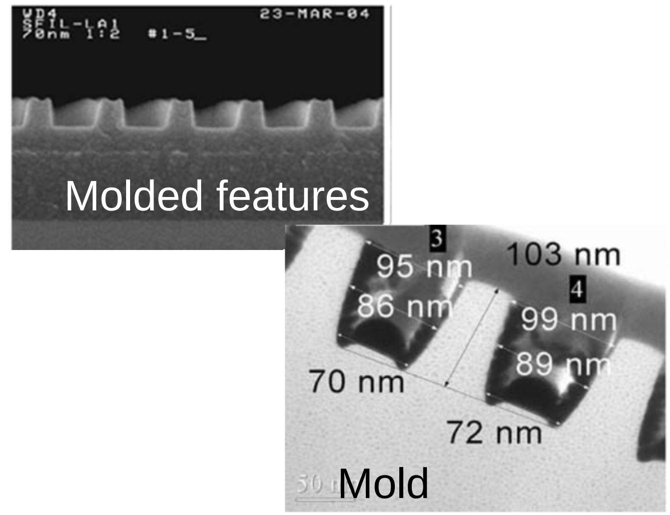
- The calculated dependence of Γ_e on ψ_a is qualitatively similar to that observed experimentally.
  - e.g. Liechti and Chai (1992) for an epoxy/glass interface where epoxy yielding is the dominate source of mode-dependent energy dissipation.
- The dependence of Γ_e on ψ_a is a direct outcome of Ad/AF model.
  - Γ_e vs. ψ_a is not an input to FEA, but rather Ad/AF model parameters define Γ_e vs. ψ_a.
- The two primary parameters that define the Ad/AF model (Γ and τ^*) can be measured using AFM friction force microscopy techniques.

Imprint

FEA simulation of imprint step in a nano-fabrication process

Imprint step

- rubbery polymer (low modulus, nearly incompressible).
- large deformations as polymer pushed into mold.

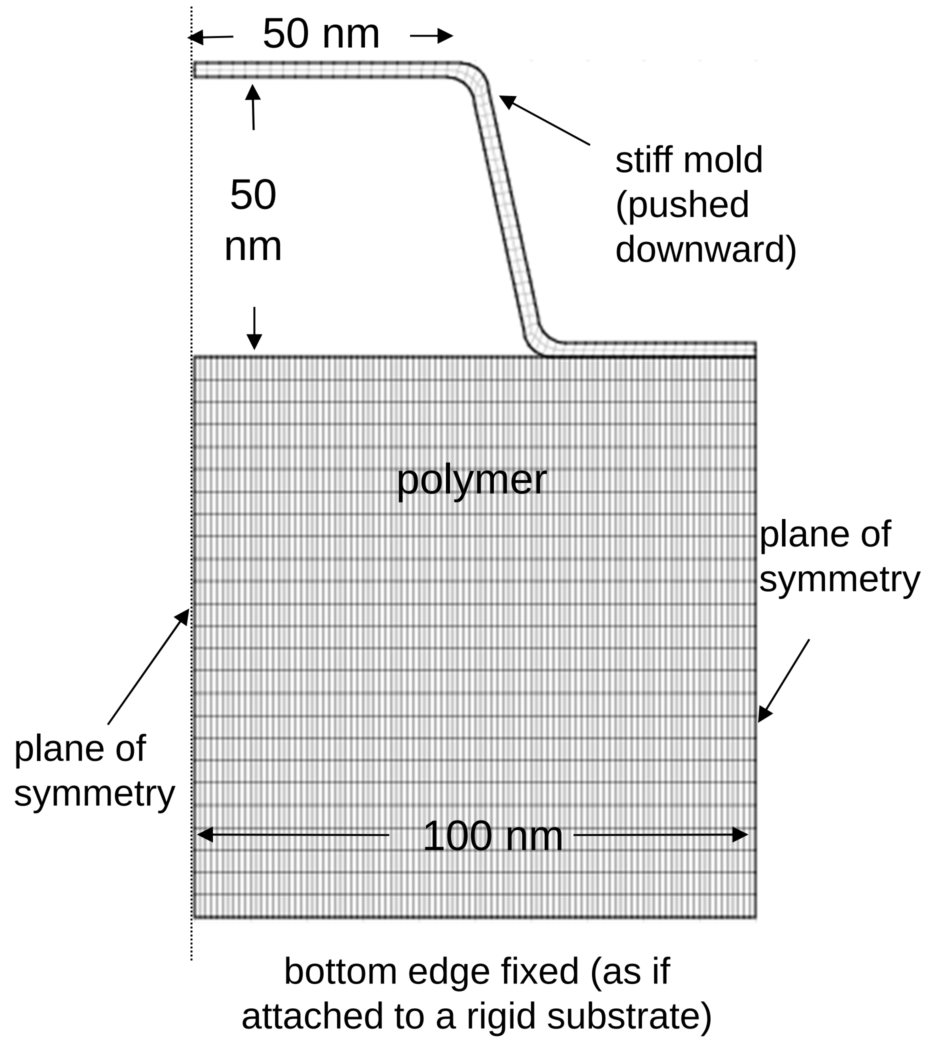


From: Effects of etch barrier densification on step and flash imprint lithography, S. Johnson, et. al. J. Vac. Sci. Technol. B V23, Nov/Dec 2005.

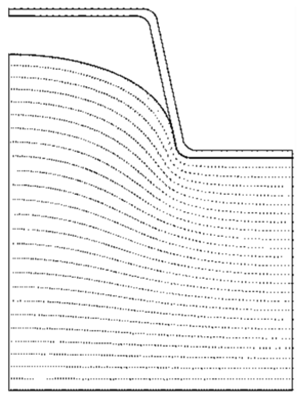
Modeling parallel channel pattern

Nano-fabrication imprint step

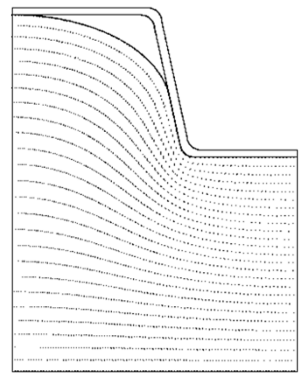
- Considering the idealized case of molding a long feature (plane strain).
  - ~100 x 50 nm mold cavity.
  - ~12^o taper, 5 nm radii.
- Use a Moody-Rivlin material model for polymer.
  - nominal, small strain Young's modulus is 1 MPa and Poisson's ratio is 0.499.
- Mold pushed into polymer at a rate of 0.2 m/s.



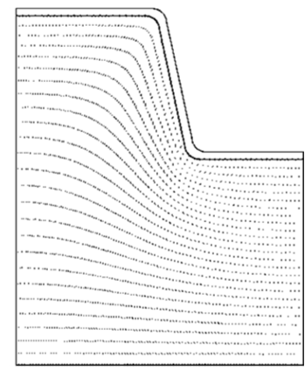
Nano-fabrication imprint step: no adhesion and no friction



U= 18.0 nm

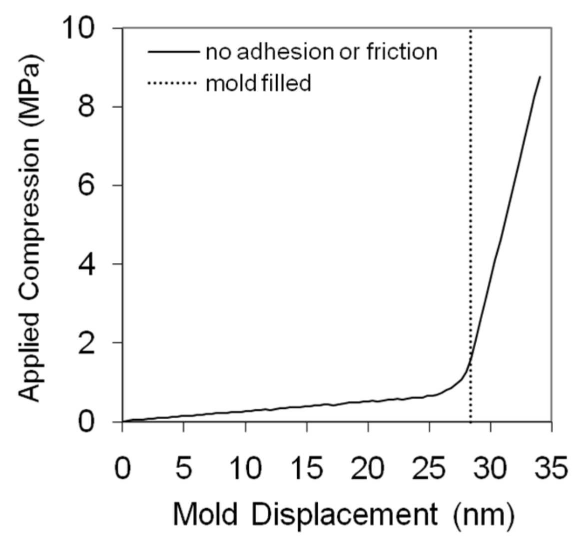


U= 24.8 nm



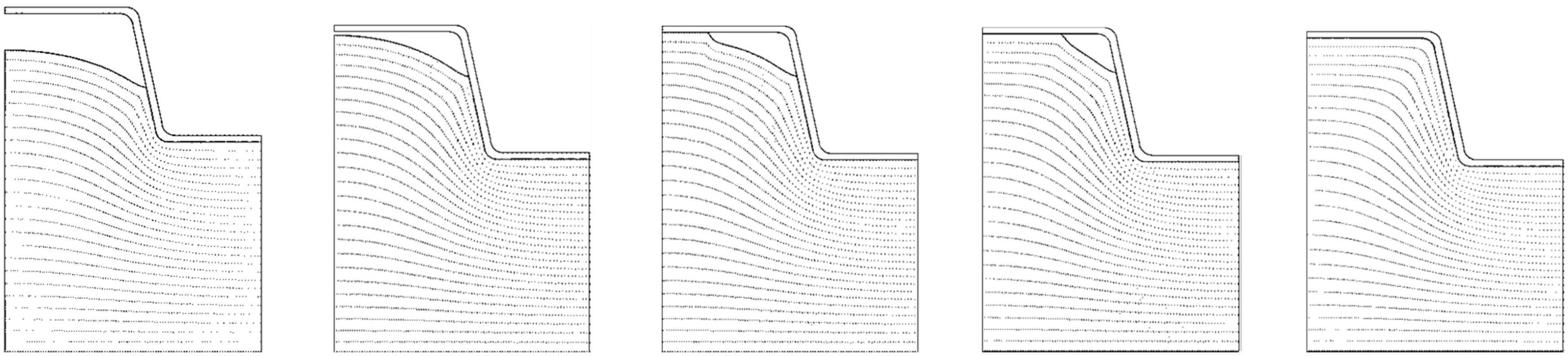
U= 28.4 nm

- Applied compression *C* (i.e., load/base area) to fill mold is 1.6 MPa.
- Load increases rapidly once filled.



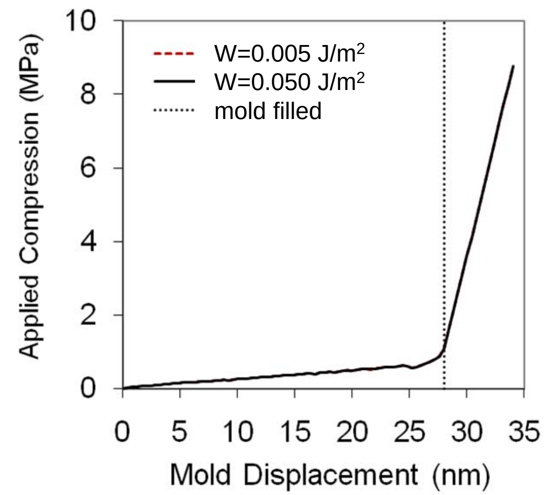
Nano-fabrication imprint step: adhesion but no friction

Γ=0.05 J/m^2 with σ^*=100 MPa, δ_c=1 nm



U= 18.0 nm | U= 24.4 nm | U= 24.8 nm | U= 26.0 nm | U= 28.0 nm

- *C* to fill mold is 1.1 MPa vs. 1.6 MPa w/o adhesion.
- Essentially same results for Γ=0.005 and 0.05 J/m^2 (i.e., σ^*=10 or 100 MPa, δ_c=1 nm).
- Adhesion has only a modest effect on polymer deformation, as well as *U* and *C* at fill.



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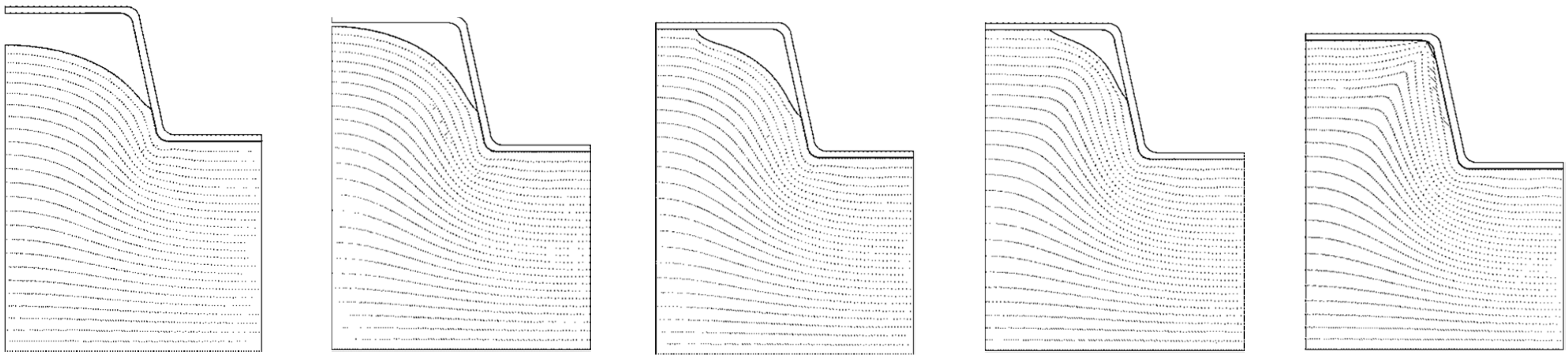
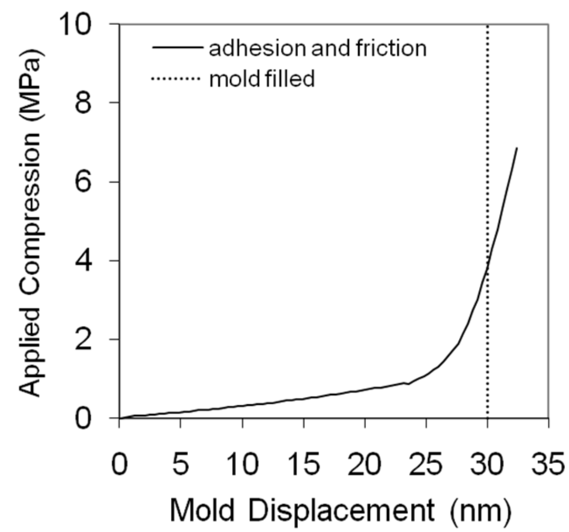
Nano-fabrication imprint step: adhesion and friction

Γ=0.05 J/m^2 with σ^*=100 MPa, δ_c=1 nm and τ^*=10 MPa

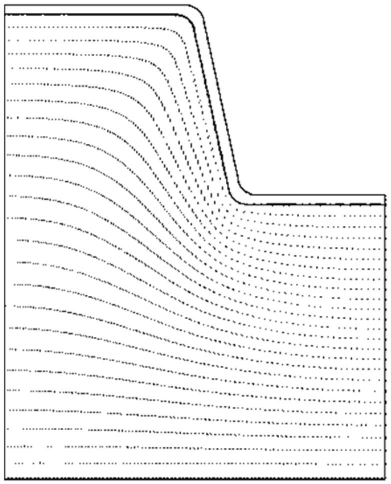


U= 18.0 nm U= 23.2 nm U= 23.6 nm U= 26.0 nm U= 30.0 nm

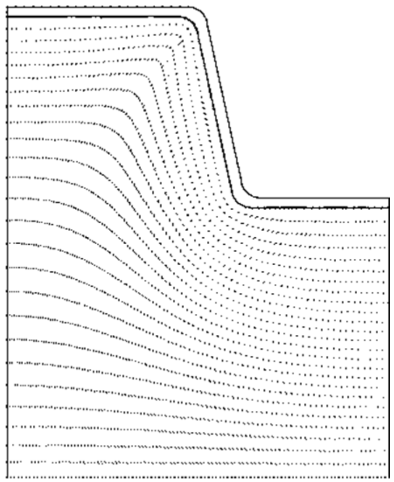
- *C* to fill mold is 3.8 MPa vs. 1.1 MPa when adhesion only.
- Atomistic friction has a significant affect on polymer deformation, as well as *C* at fill.



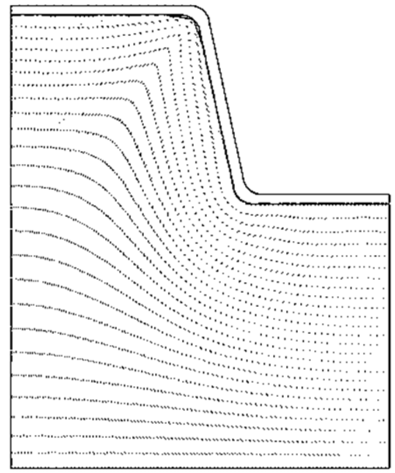
Discussion



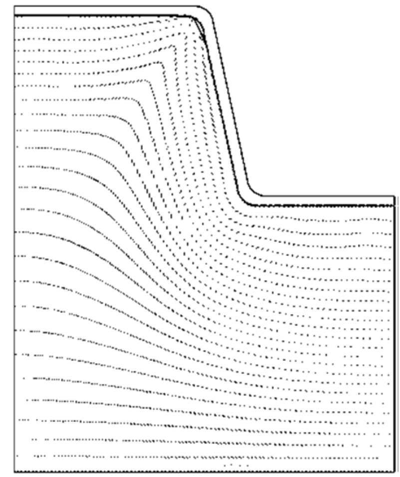
U= 28.0 nm, C=1.1 MPa
τ^*=0 MPa



U= 29.2 nm, C=2.7 MPa
τ^*=1 MPa

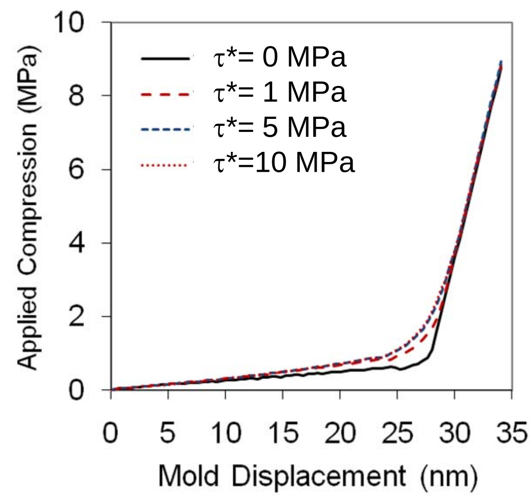


U= 30.0 nm, C=3.8 MPa
τ^*=5 MPa



U= 30.0 nm, C=3.8 MPa
τ^*=10 MPa

- Even low levels of τ^* have an effect.
- Results become insensitive to τ^* value as τ^* increases.
- May be hard to push polymer into corner when feature has a high aspect ratio.



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Summary

1) Demonstrated use of novel Ad/AF surface interaction model for weak interfaces as implemented in an explicit dynamics FE code.

2) Simulated interfacial separation in a long edge-cracked bimaterial strip where the upper material is rigid.

   - Ad/AF model generates a strongly mode-dependent effective interfacial toughness.

3) Simulated a nano-fabrication imprint step.

   - even low levels of adhesion and atomistic friction can have a significant effect on deformations during imprint.