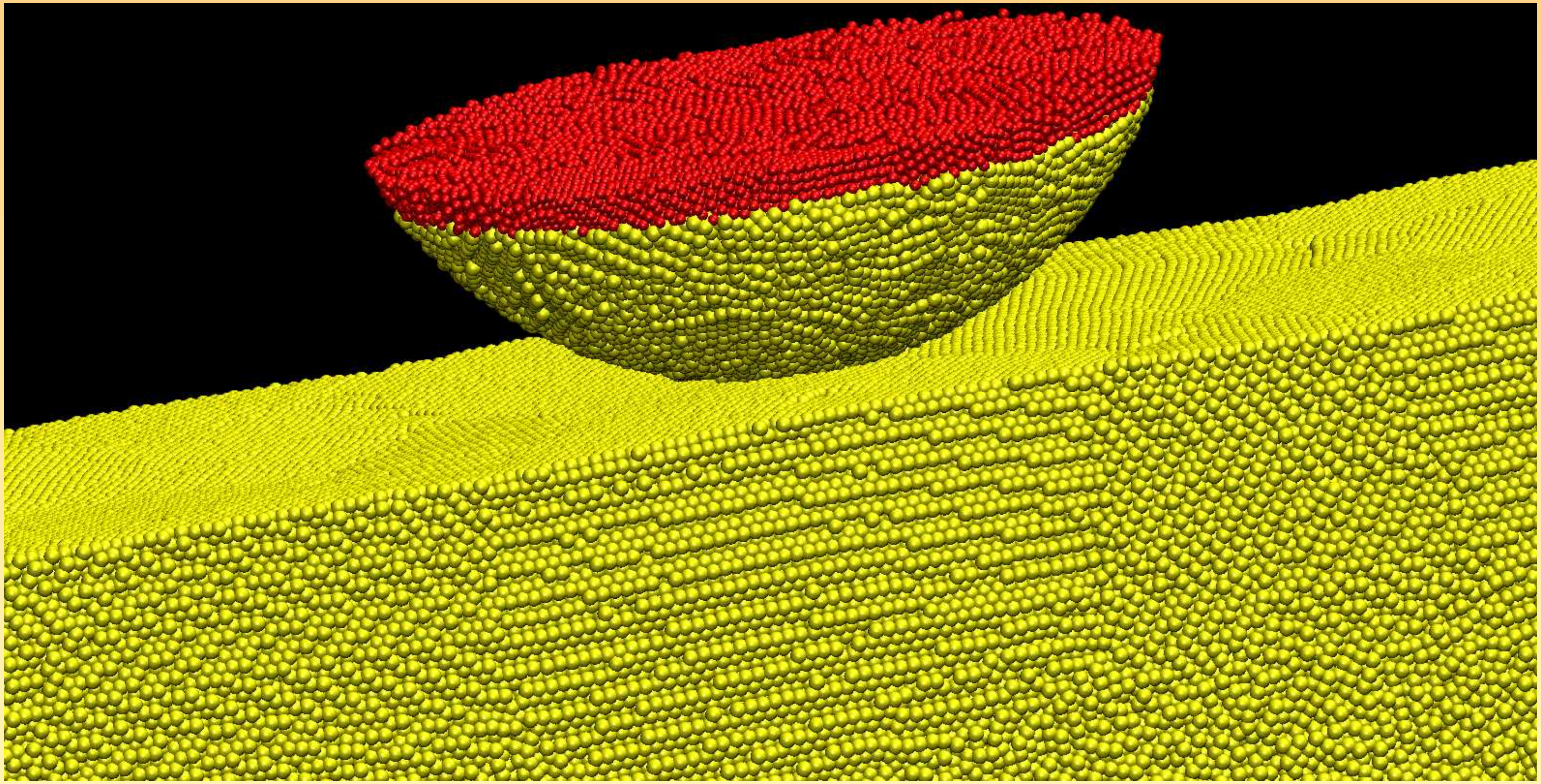
Simulations of Tribology in Nanocrystalline Metallic Films

SAND2011-6388C



M. Chandross and S.F. Cheng
Sandia National Laboratories, Albuquerque NM

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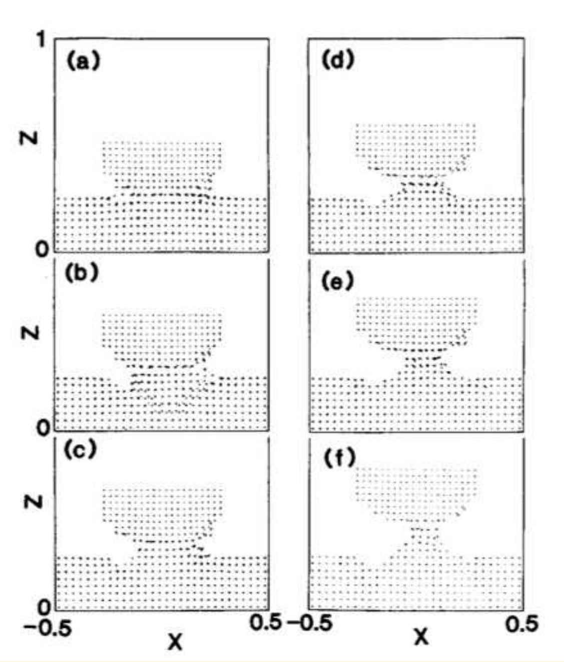
Introduction: Gold

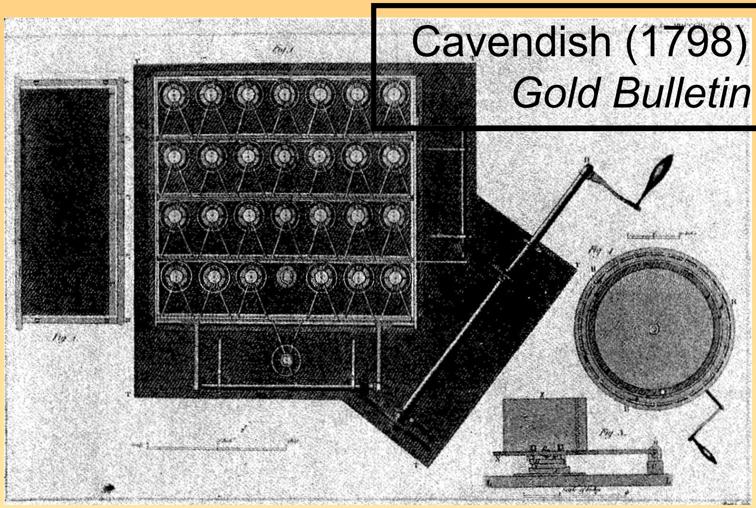
- Gold has desirable properties
  - High conductivity 4.52 x 10^7 S/m
  - Doesn't corrode/oxidize
  - Can be made very thin
- Not everything is shiny..
  - High adhesion (> GPa)
  - High friction ($\mu = 1 - 2$)
- Can we get the best of both worlds?



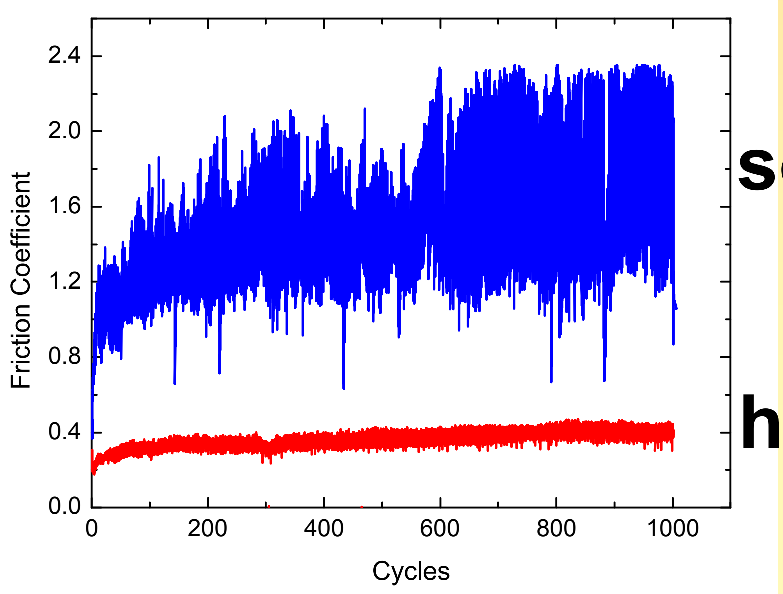
Luedtke and Landman, Comp. Mat. Sci. (1992).

Are Composites the Answer?

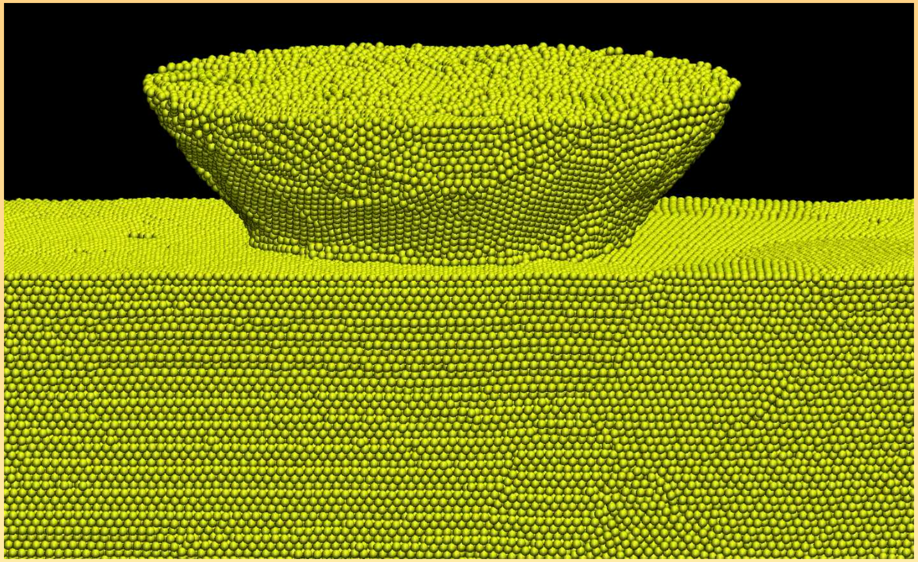
- Alloys investigated in 1798 to reduce wear in coins
  - 11 alloys (including Cu), ~ 8.3 %
  - Cavendish designed testing machine
  - None really worked
- Our goals:
  - Maintain electrical properties
  - Reduce adhesion and friction
- Questions:
  - Why do composites change μ?
  - What is the optimal composition?

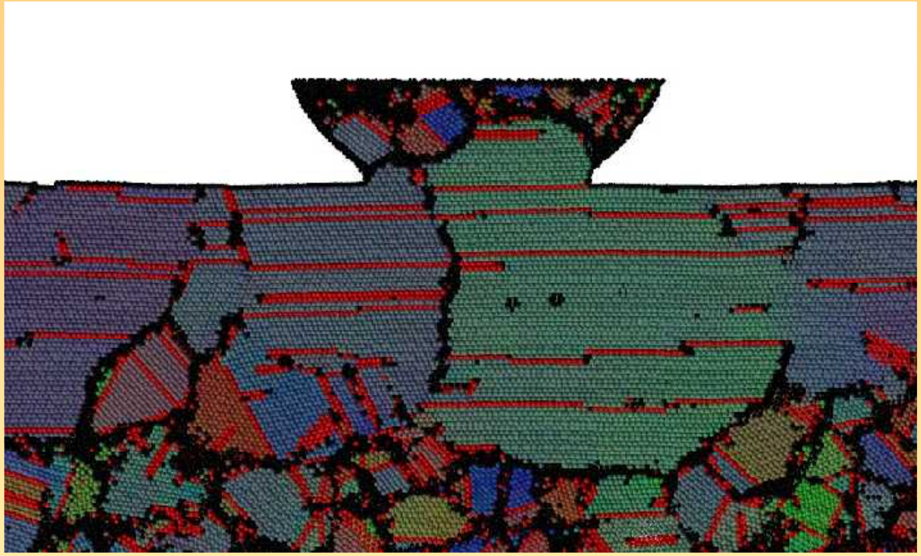


Cavendish (1798) via Chaston, *Gold Bulletin* (1974).



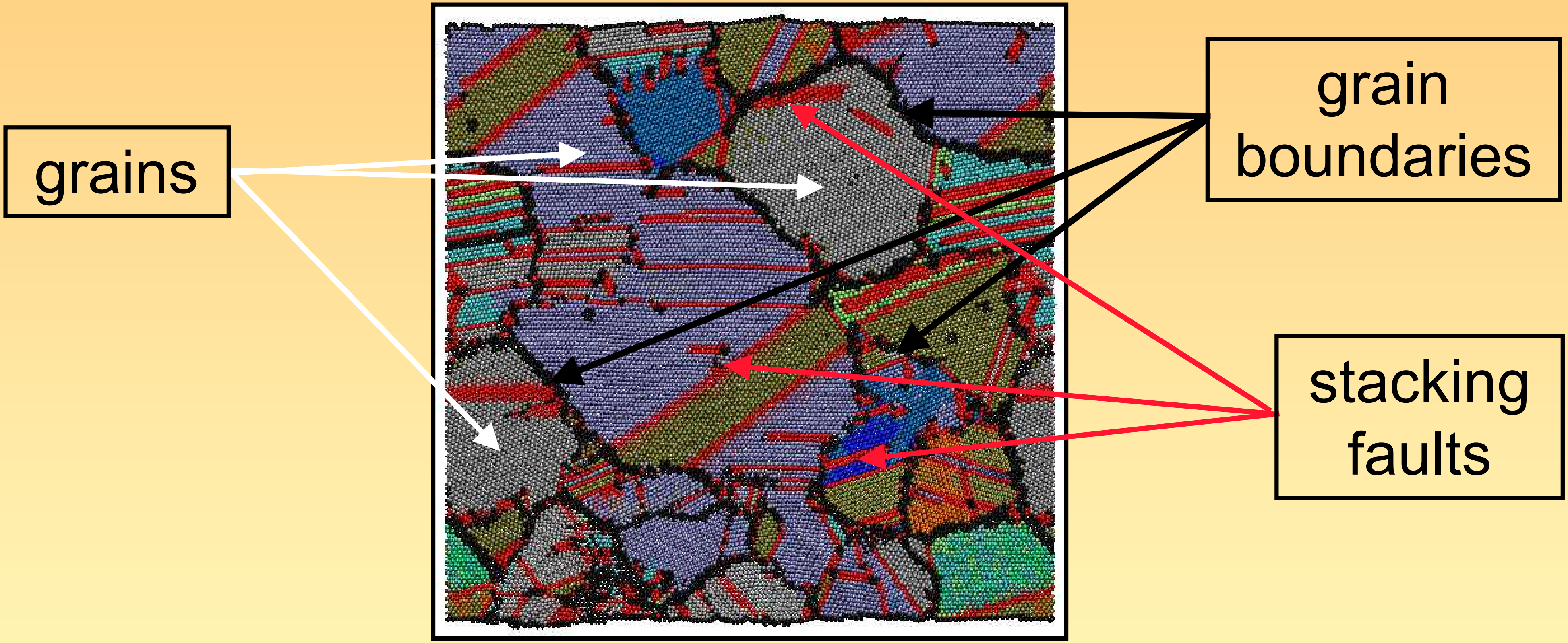
Simulation Methods





- Large scale Molecular Dynamics
  - Can track location, velocity, forces of individual atoms
  - Constraints on length and time scales
- Embedded Atom Method
  - Very accurate for mechanical properties
  - Can’t easily mix without reparameterizing – switch to Ag

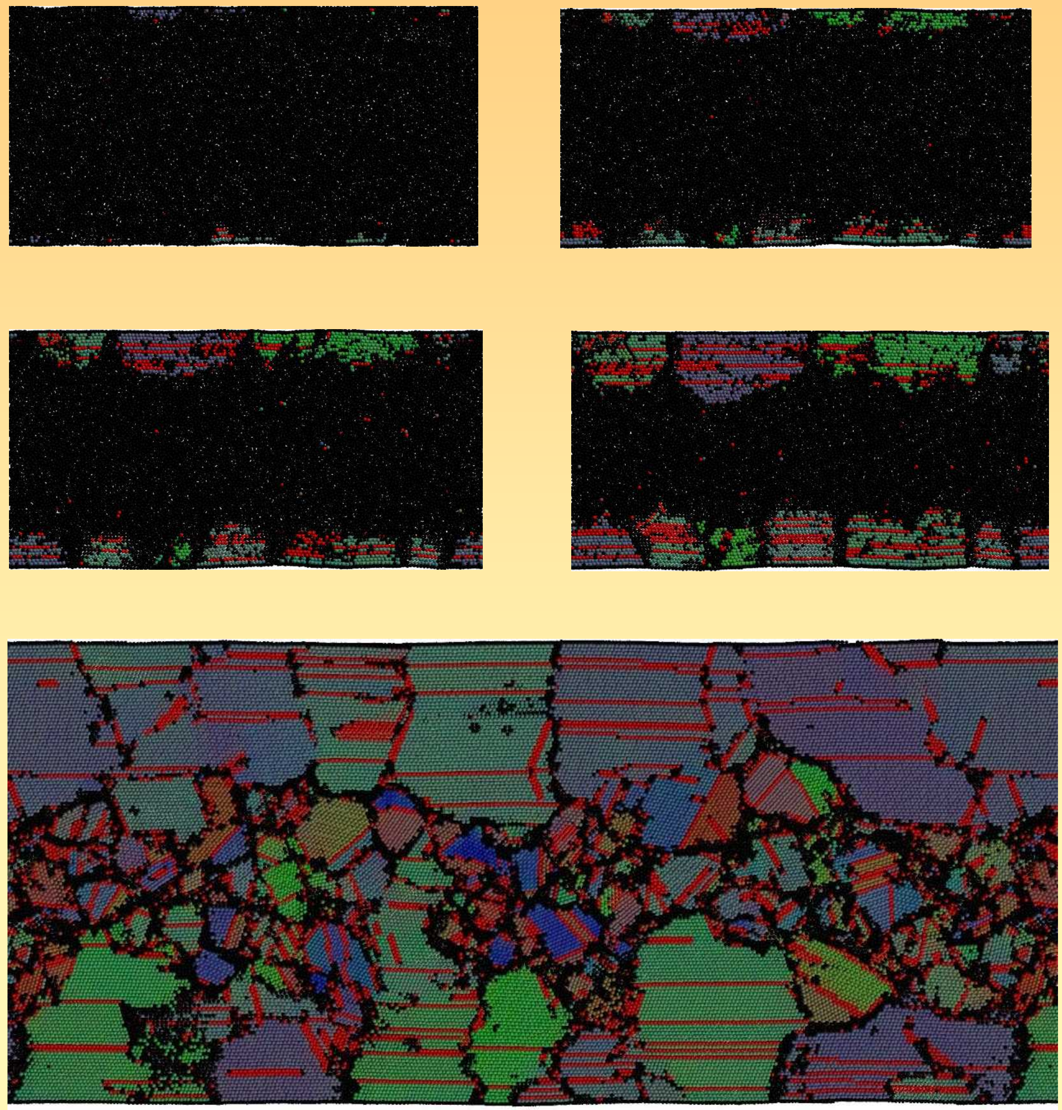
Grain Analysis



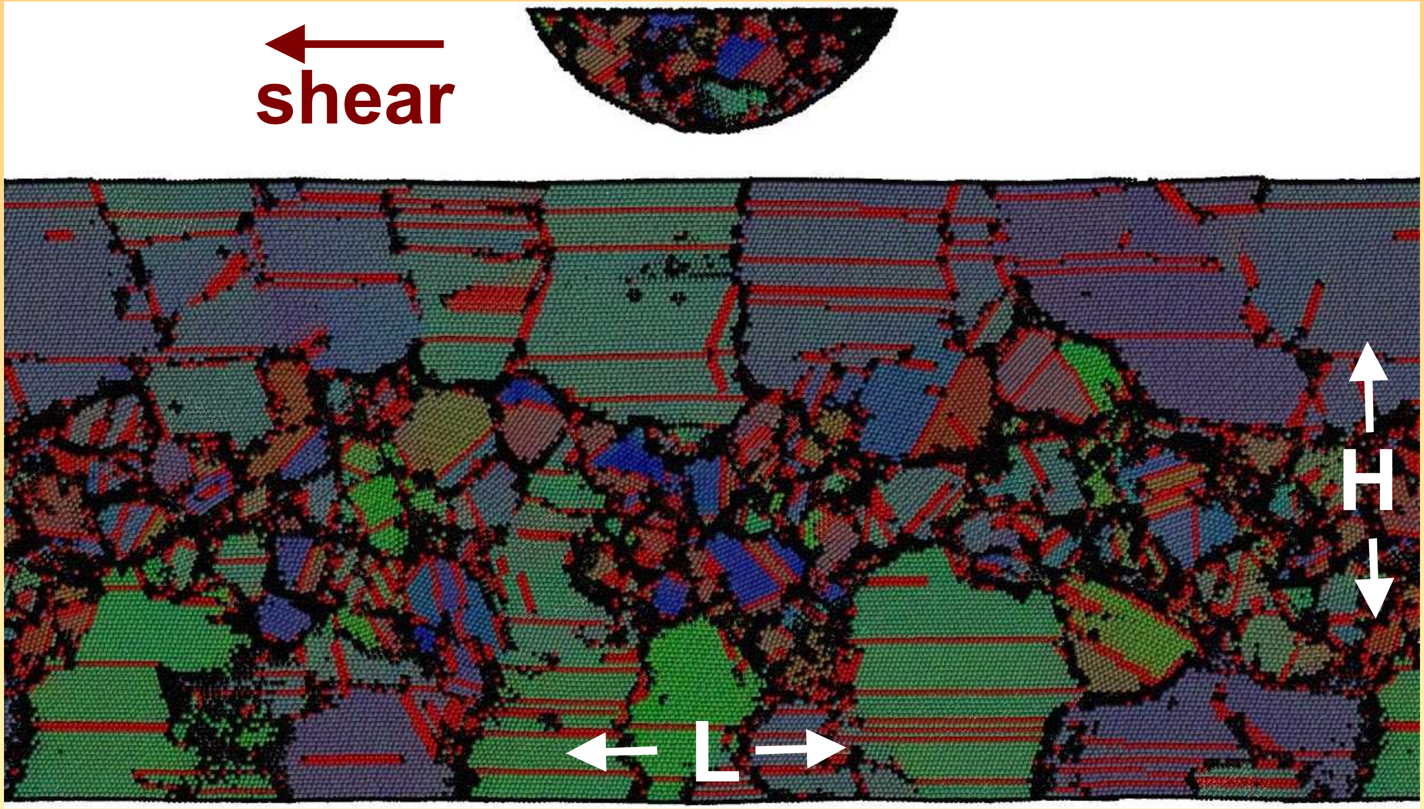
- Locally FCC atoms colored according to Euler angle
- Locally HCP atoms colored red – twins & stacking faults
- Otherwise colored black – grain boundaries

Nanocrystalline Ag

- Melt & quench
  - Start with bulk FCC
  - Melt at 1800 K (20 ps)
  - Rapidly quench (100ps)
  - Grains ~ 5 nm
  - Can grow grains easily
- Metallurgy aside
  - Twins indicate that surface is aligned with {111}
  - Growth pictures indicate that {111} growth direction preferentially nucleates at surface

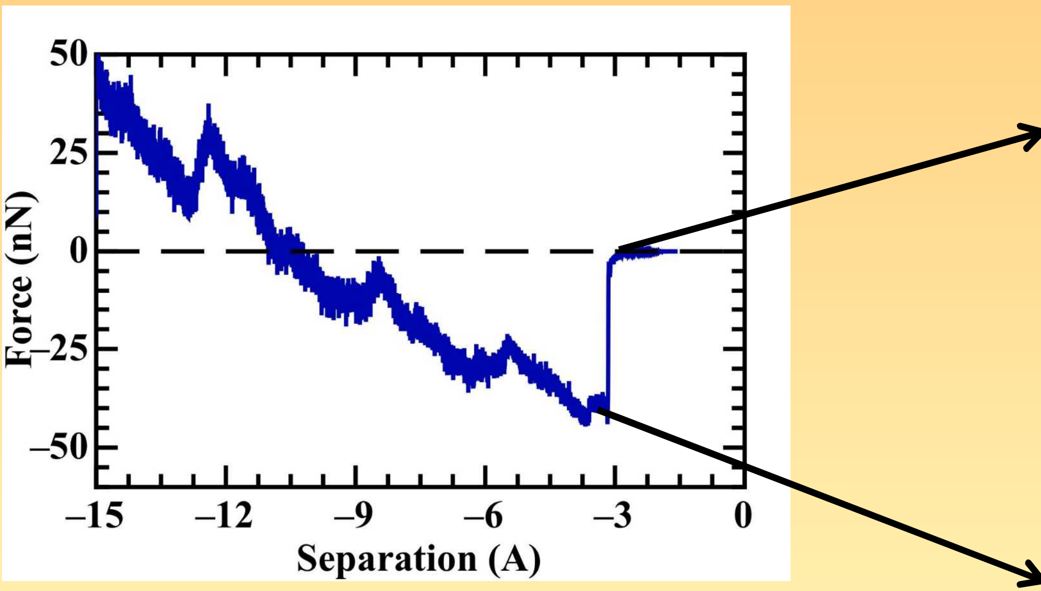


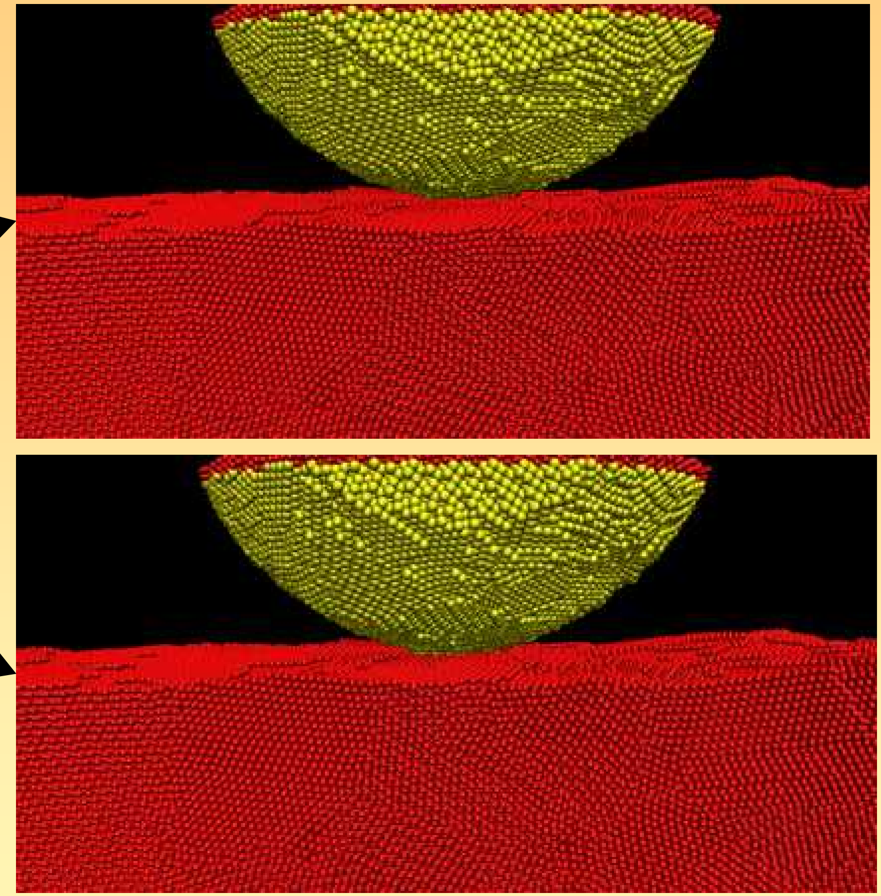
Tip-based Friction Simulations



- Substrate: nanocrystalline Ag, 17 nm (W) x 34 nm (H) x 67 nm (L)
- Tip: 10 nm radius
- Shear velocity: 2 m/s (constant velocity, and separation *or* force)

Force vs. Separation

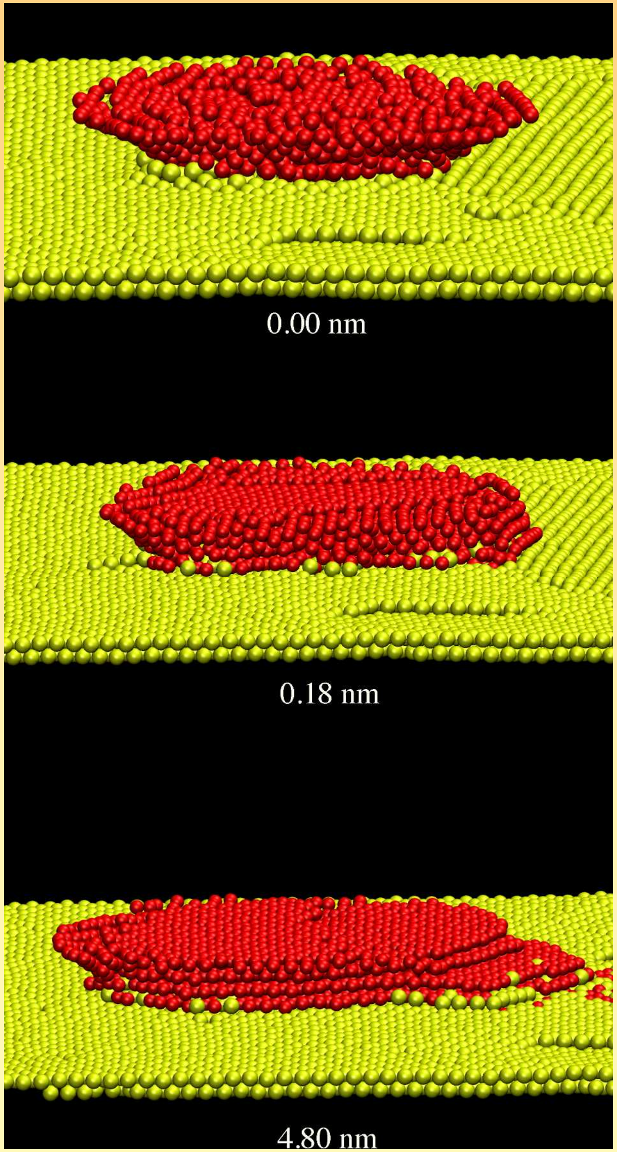


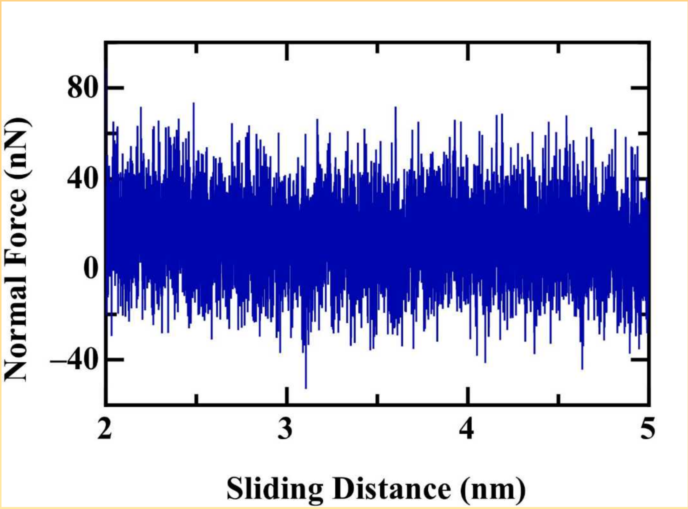


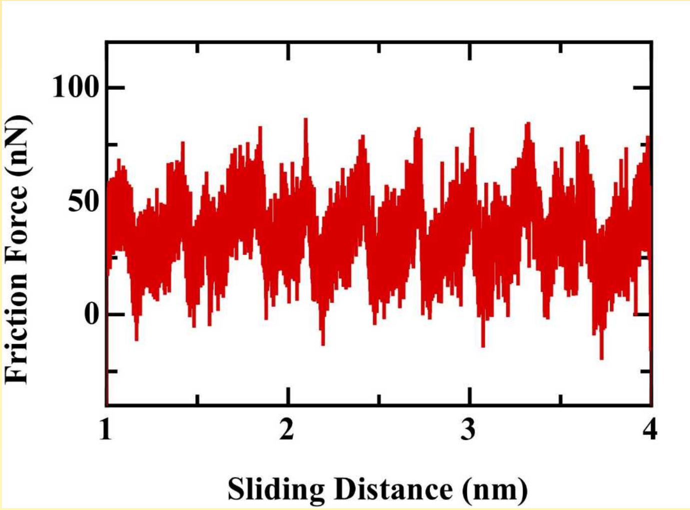
- Separation is arbitrarily defined
- Initial adhesion: ~ 40 nN / 4 Gpa
- Pressures in line with Israelachvili, *Acta Mat.* (2003).

Behavior Under Shear

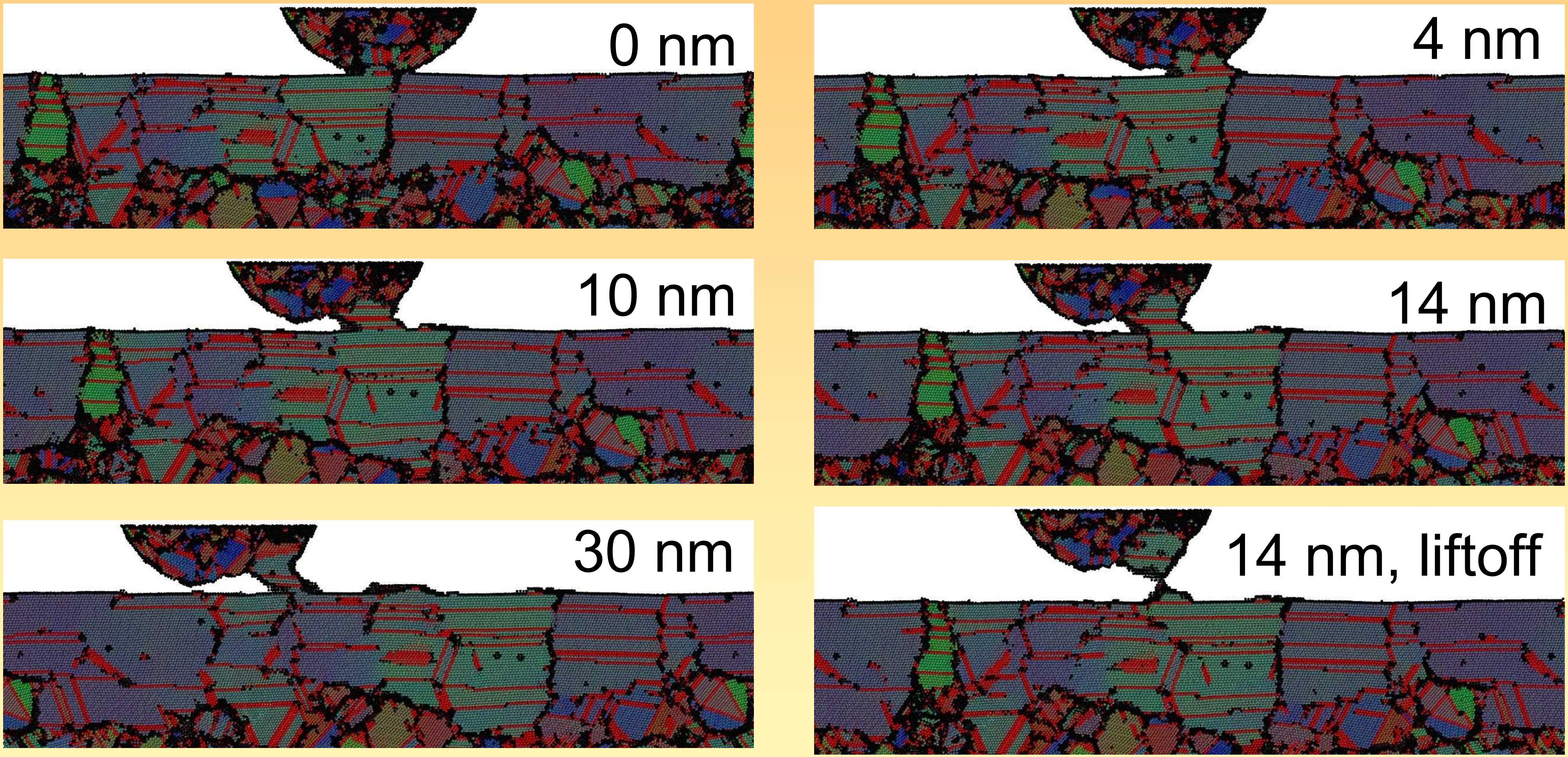
- Layering of tip atoms
- Stick-slip in friction signal
- Shear induces commensurate contact
- Commensurabilit y => high friction
- Do composites suppress this?





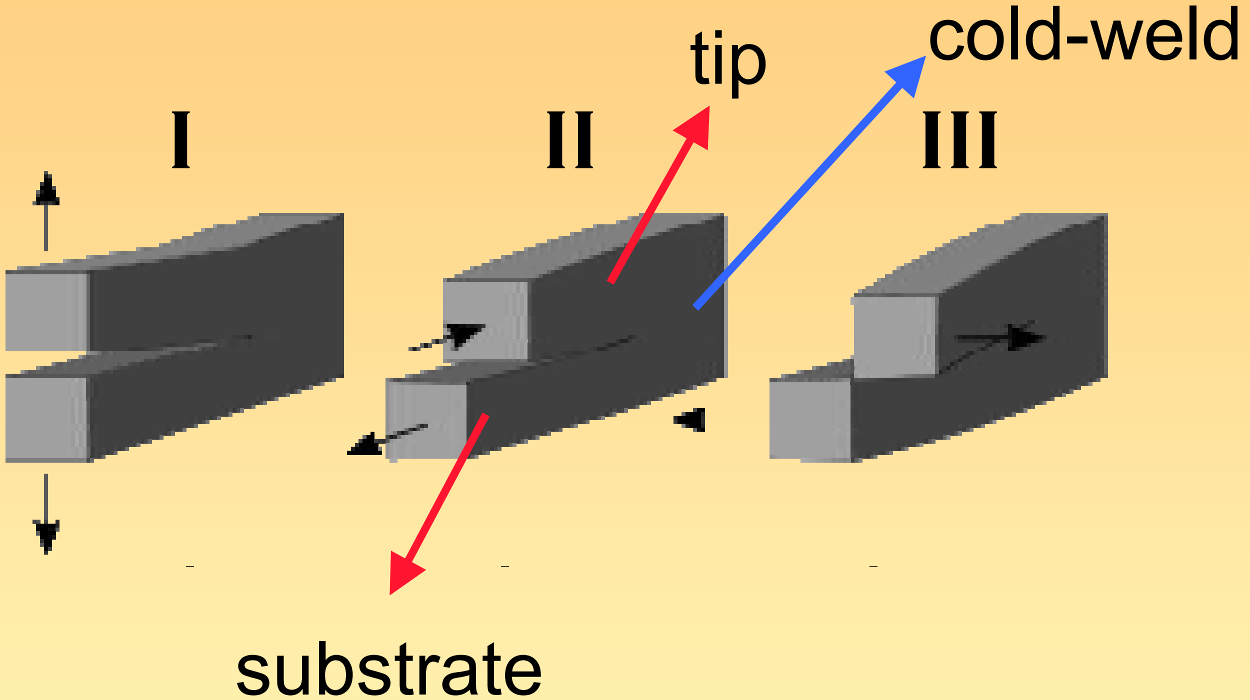


Grain Level Snapshots



- Initially distinct grains
- After shear (adhesive load), coalescence – now a mode II crack
- Single grain forms across interface – stress induced grain growth

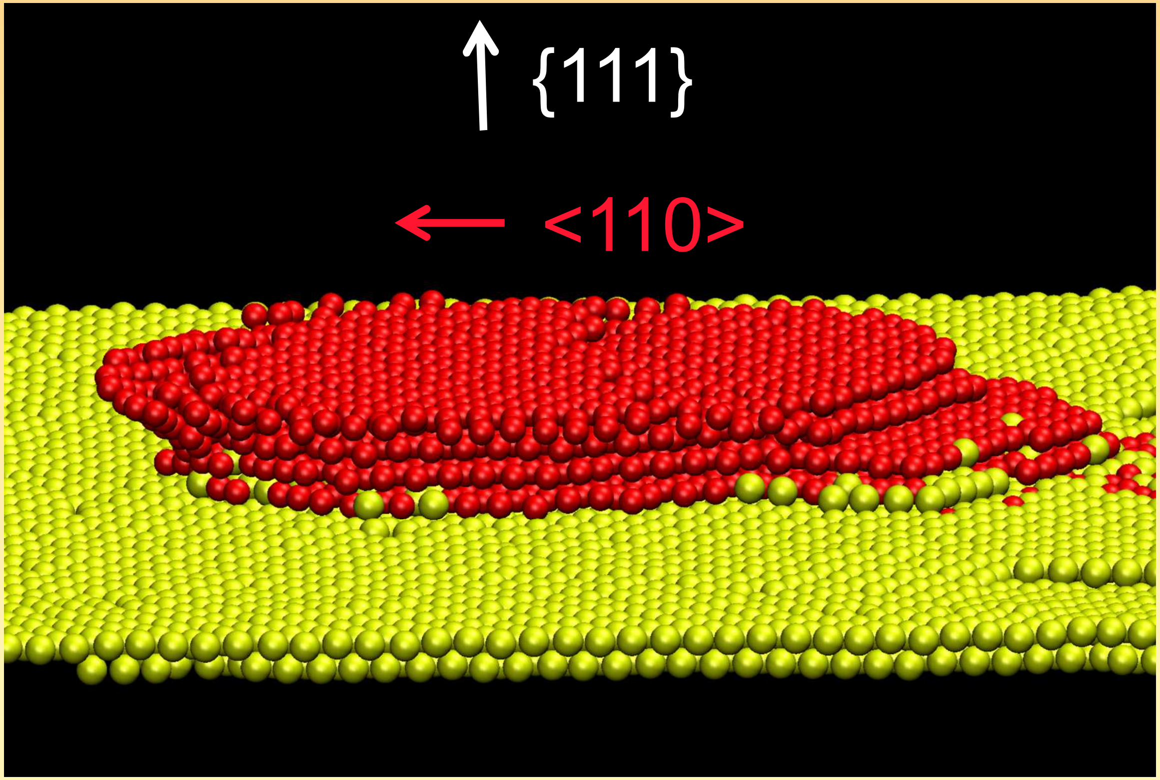
Types of Cracks



- Mode **I**: Tensile Shear
- Mode **II**: In-plane Shear
- Mode **III**: Out-of-plane Shear

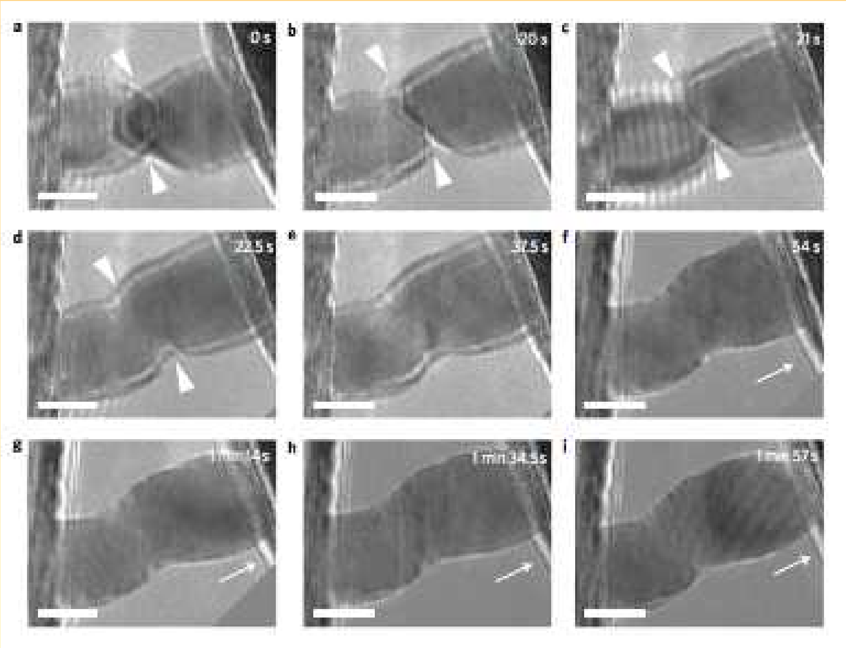
FCC Slip Systems

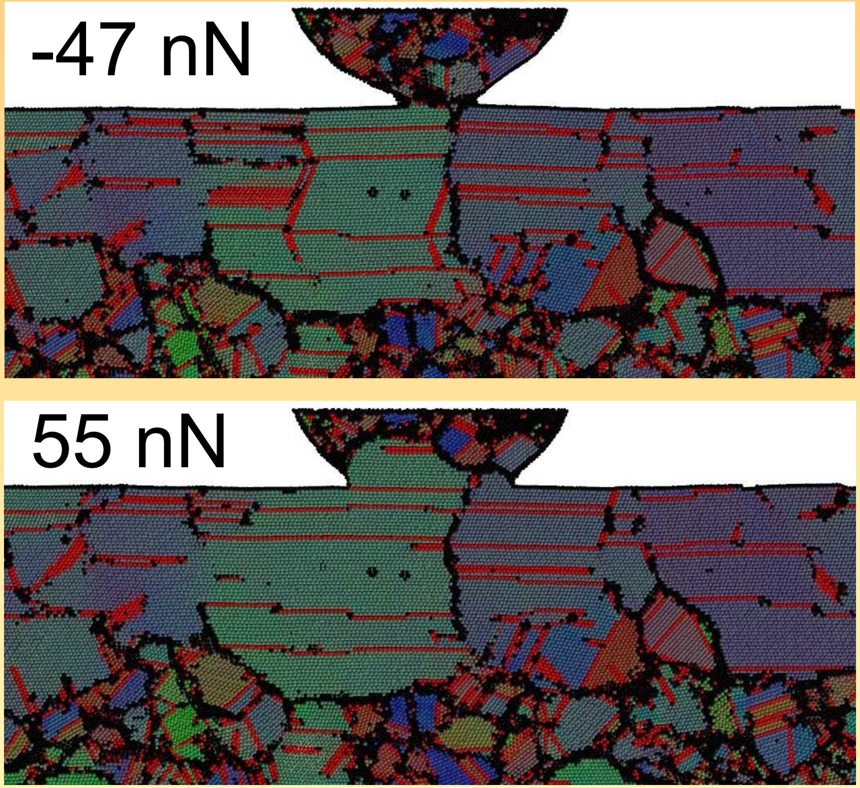
- Along {111} plane
- In <110> direction
- Ductility
- Plastic deformation
- *Not* fracture



Experimental Verification

Lu, *Nature Nanotech*, 2010

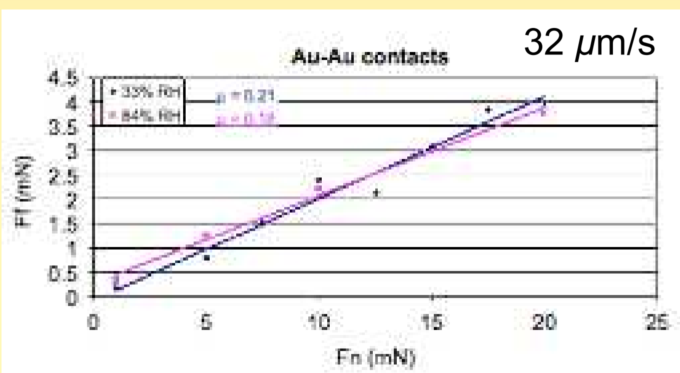




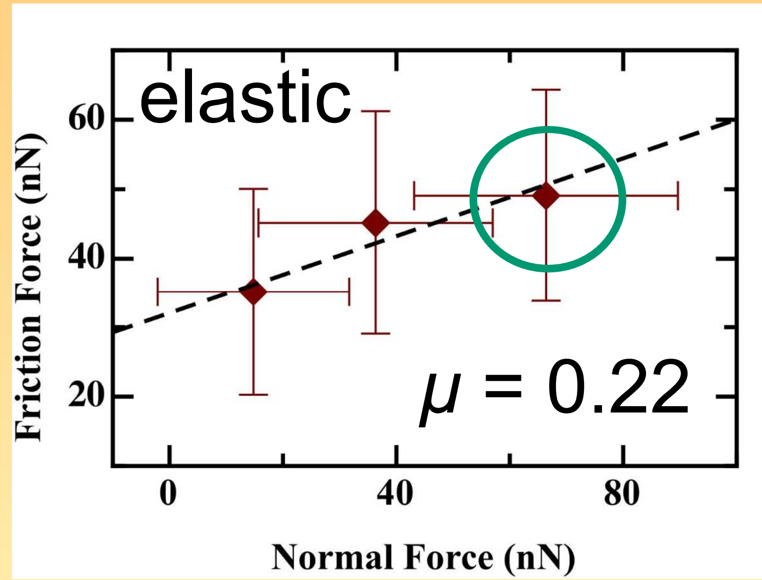
- Cold welding of single crystals with substructure evolution
- 1.5 s of contact time with little external force (exp)
- Simulations show growth with 2 ps contact under compressive load

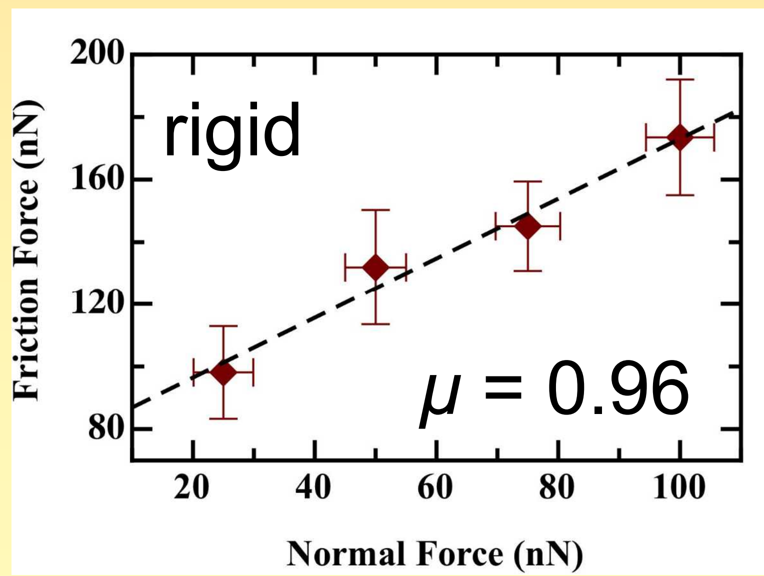
Friction Coefficient

- For pure metals, expect μ = 0.5-2.0
- What is the issue?
  - Elastic tip?
  - Multiasperity contacts?
  - Transfer films?
  - Third bodies?
  - Data for last point not great…

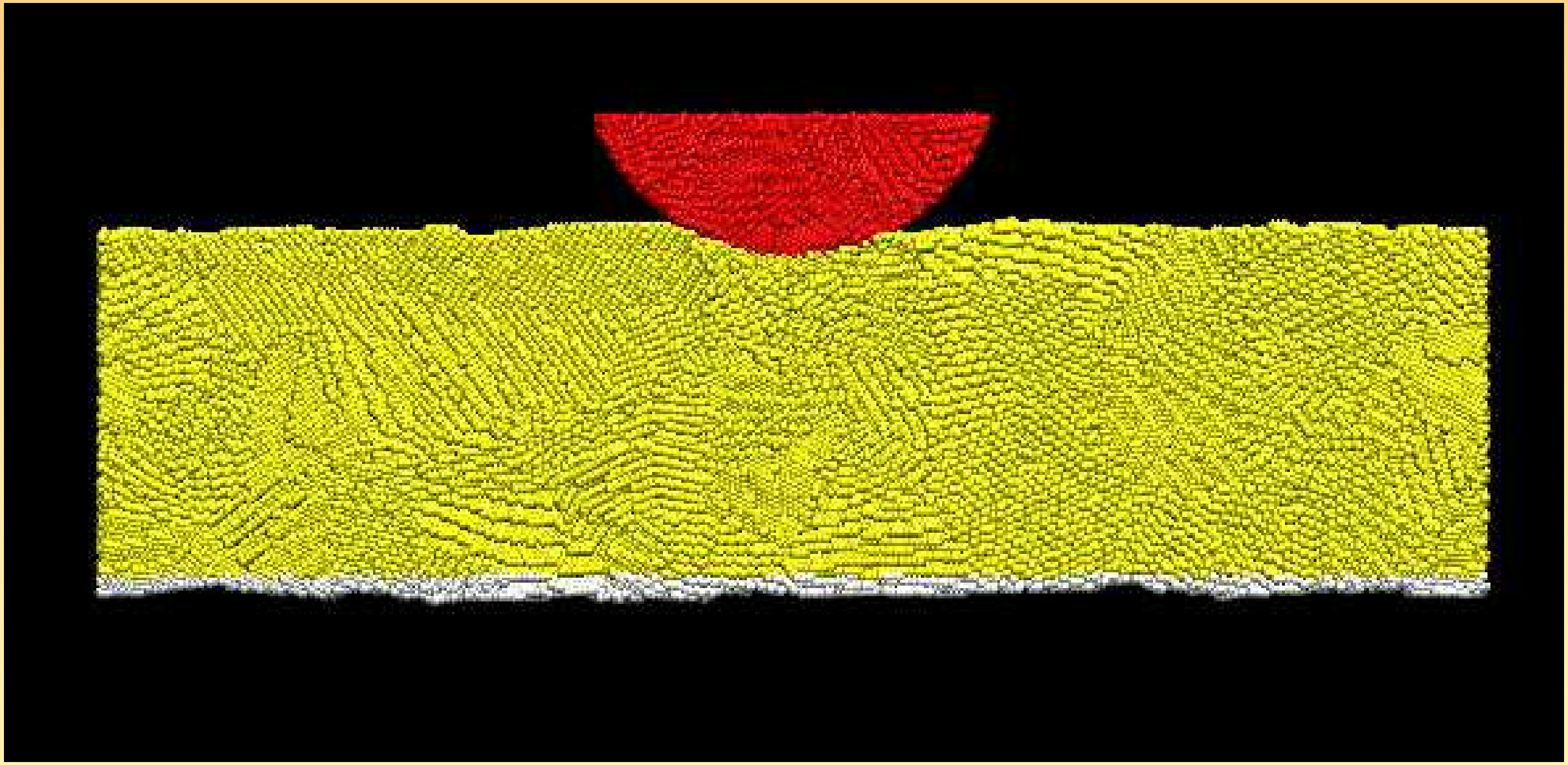


Barriga, *Tribology International*, 2007





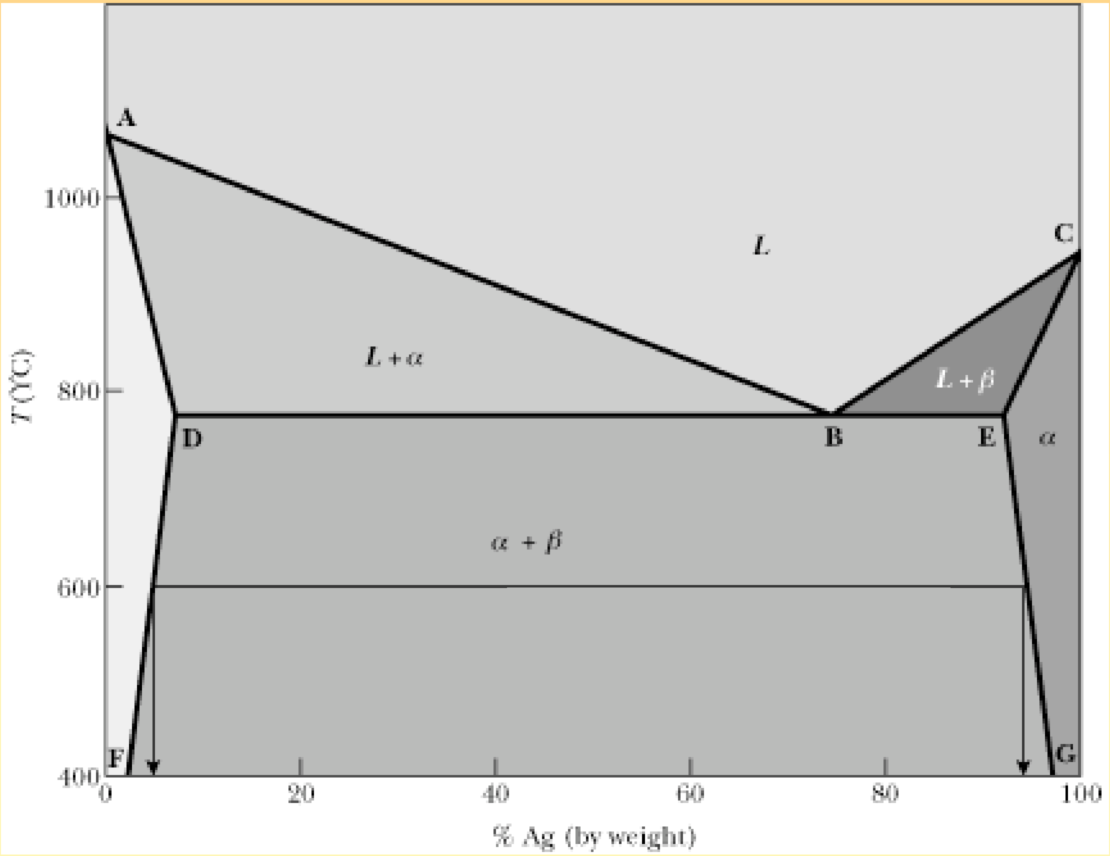
Plowing Movie



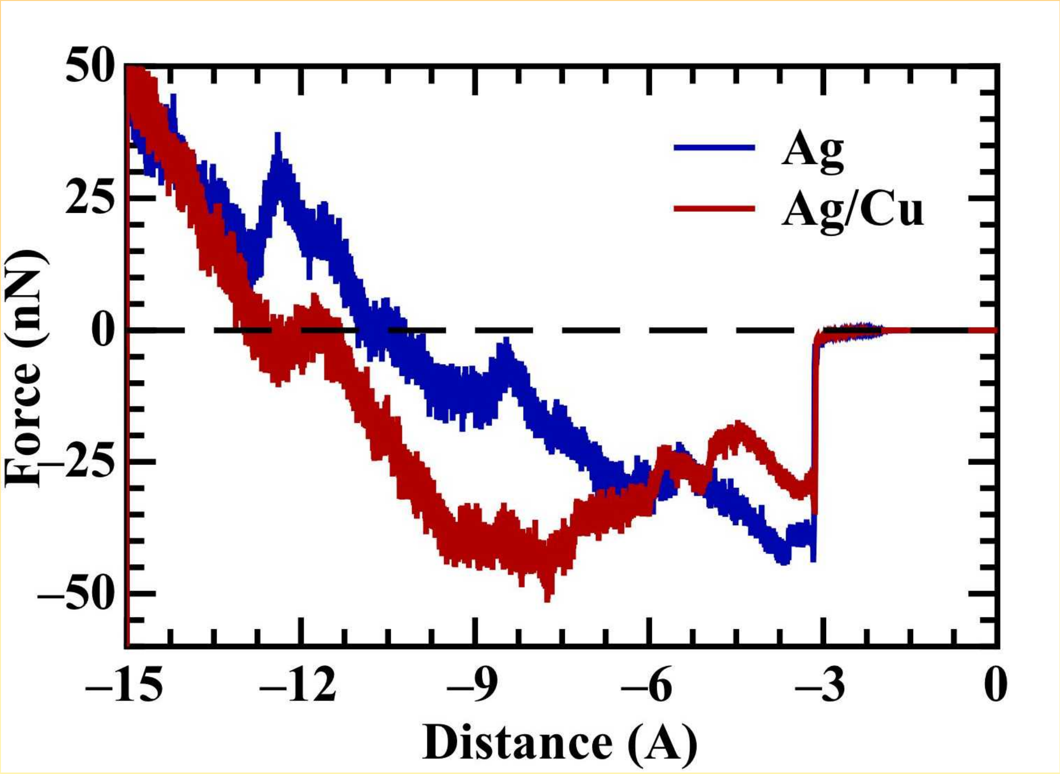
- Constant applied load of 100 nN
- Constant tip velocity of 2 m/s
- Movie shows plowing of substrate from rigid tip

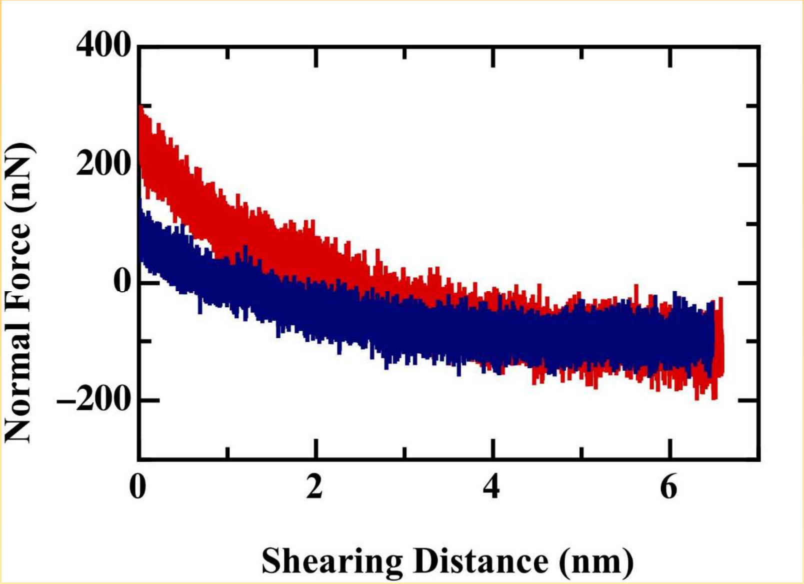
Alloys: Ag/Cu

- Not many alloy potentials with Au or Ag
- Cu is not very soluble in Ag
- Sterling silver is 7.5% Cu by weight (~12% atomic)
- Our method is unorthodox, but fine on our timescales



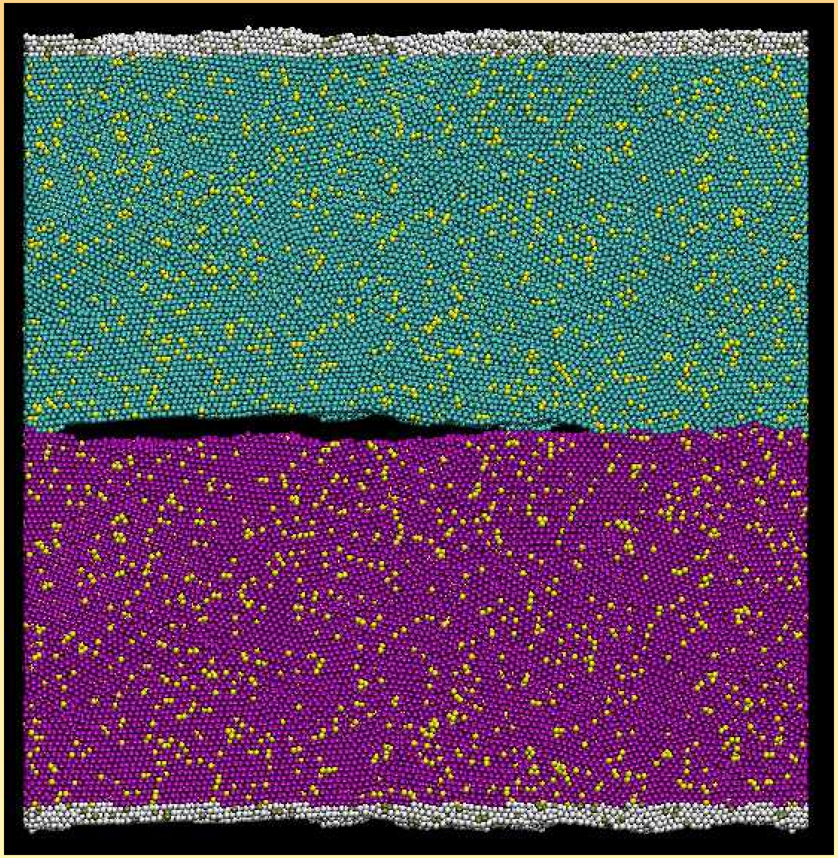
Tip/Slab with Ag/Cu

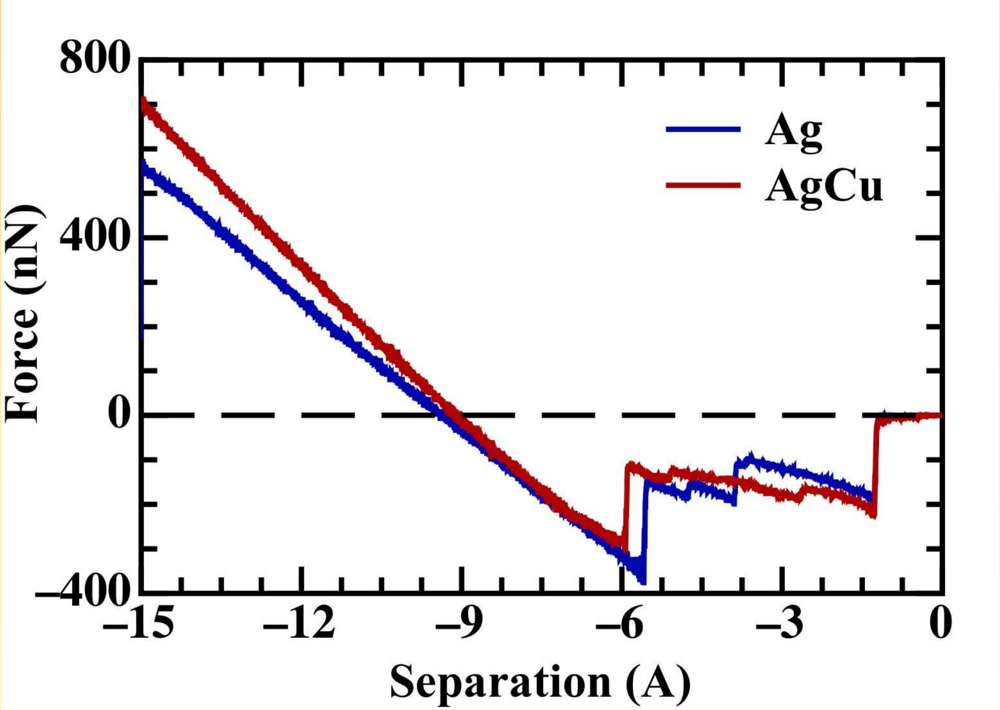




- Alloy is more adhesive (work of adhesion twice that of Ag)
- Can't measure friction with tip/slab geometry
- Alloys suppress commensurate contacts

Slab on Slab Geometry

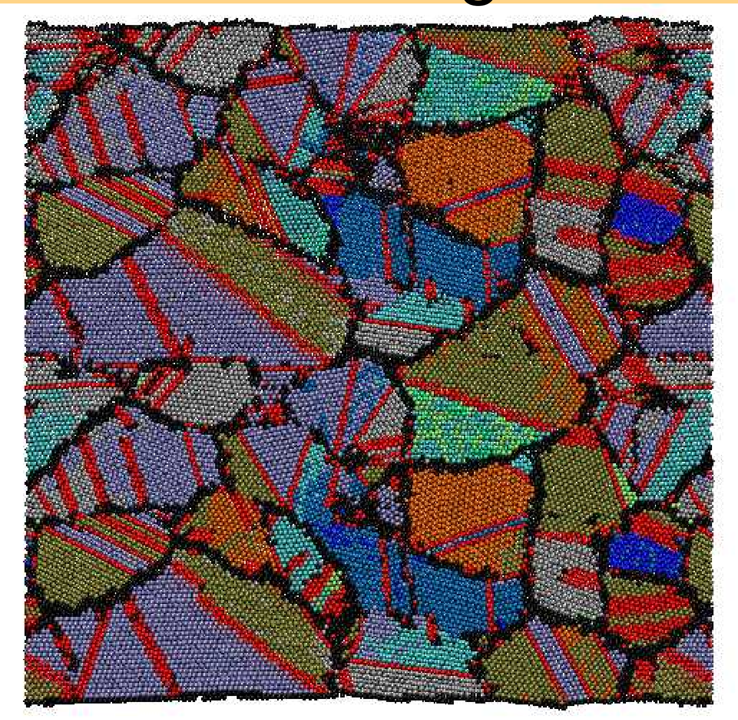




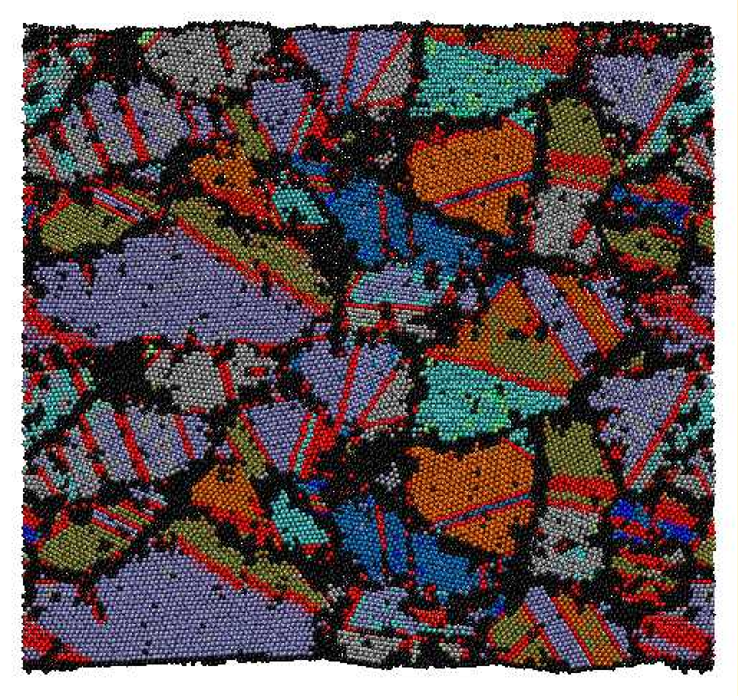
- Duplicate slab & rotate
- Bring into contact (two snap-ins from roughness)
- Adhesion is similar for Ag and Ag/Cu

Slab on Slab Geometry

Pure Ag

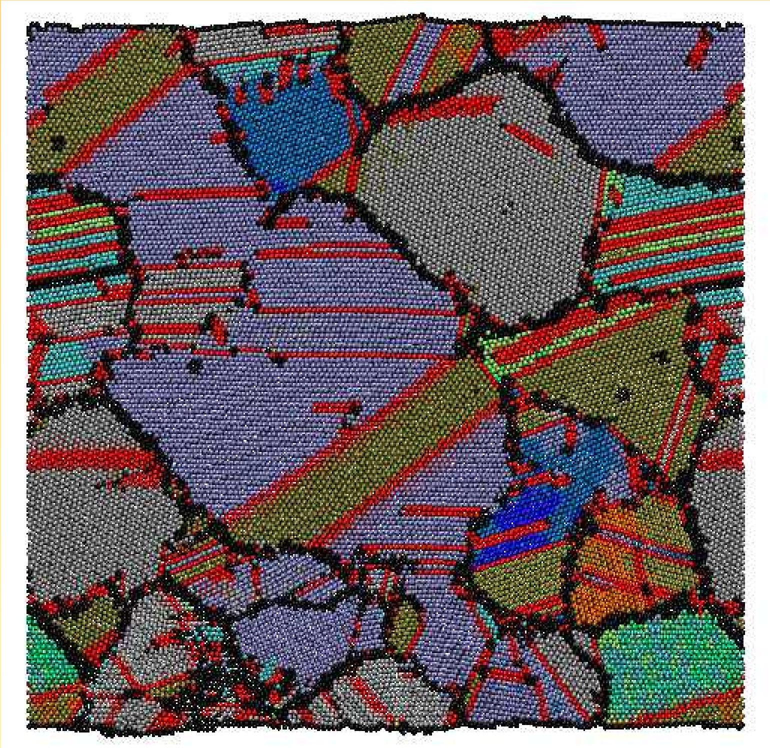


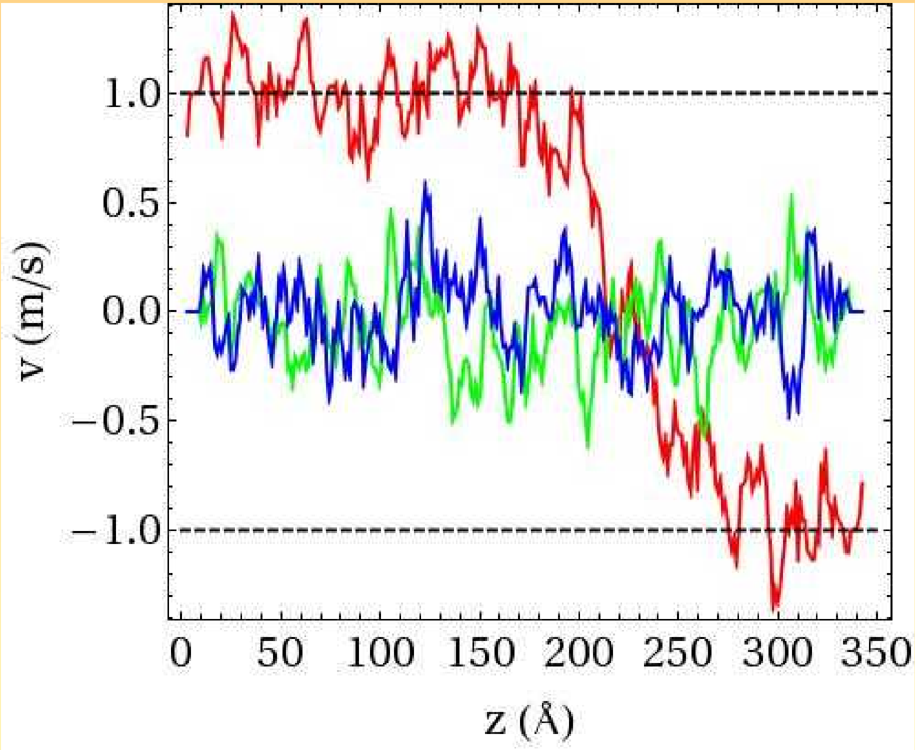
Ag/Cu alloy



- Hold in contact – some grain growth
- More disorder in alloy
- Shear using fixed atoms at top, similar to tip

Ag Slabs Fail

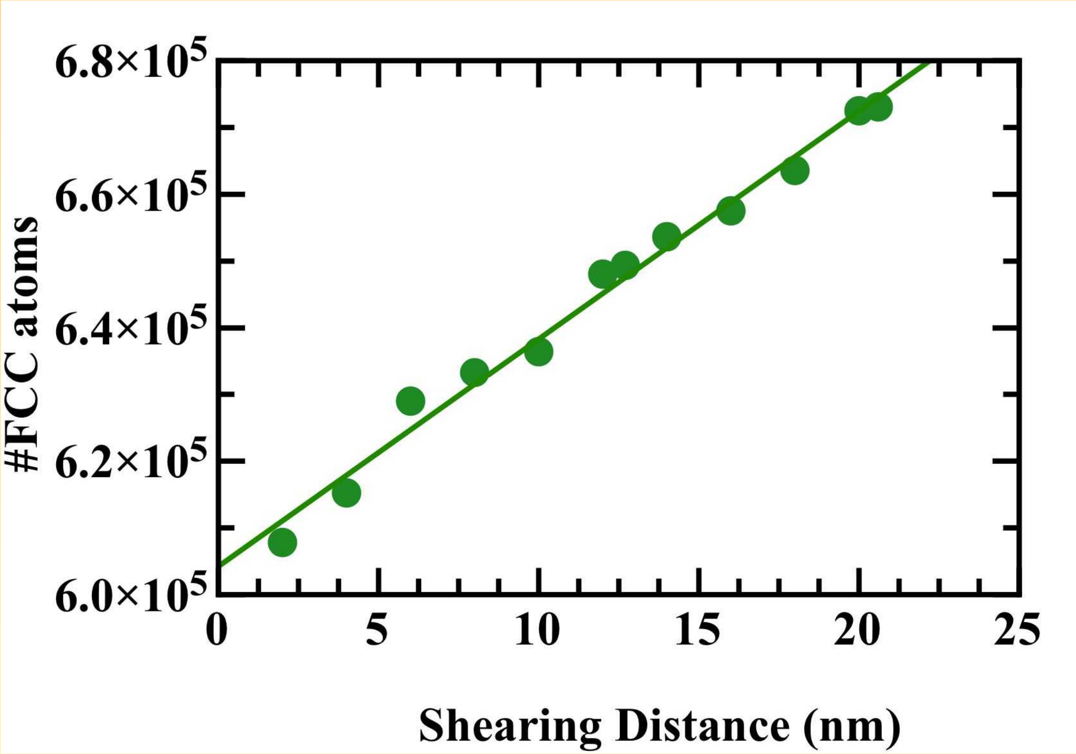




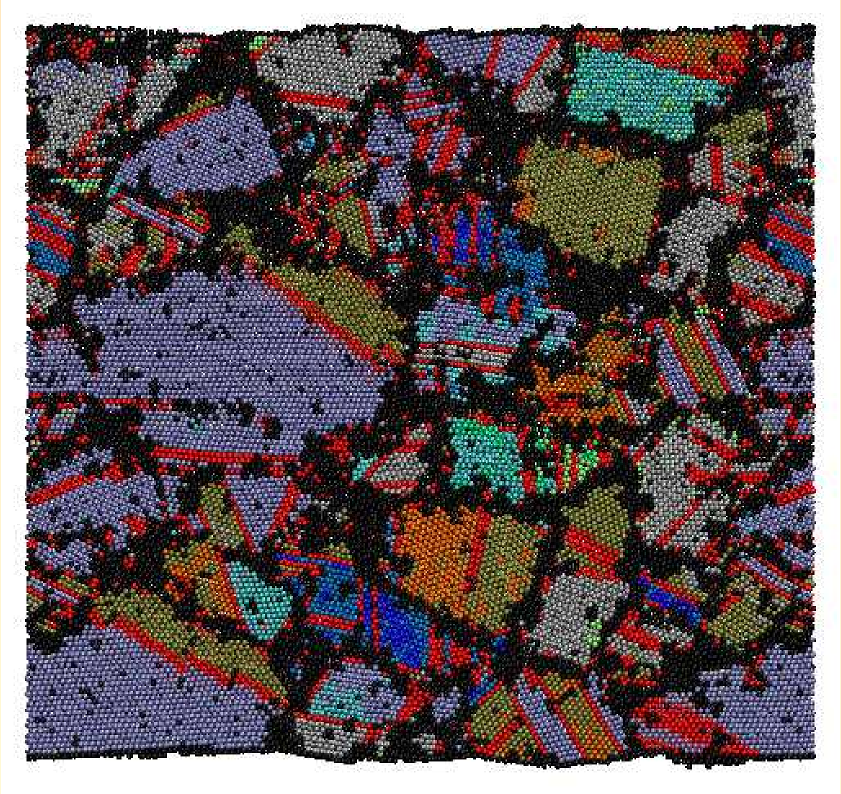
- Coalescence
- Stress induced grain growth
- Shear occurs at stacking faults, not junction -- not shearing distinct slabs

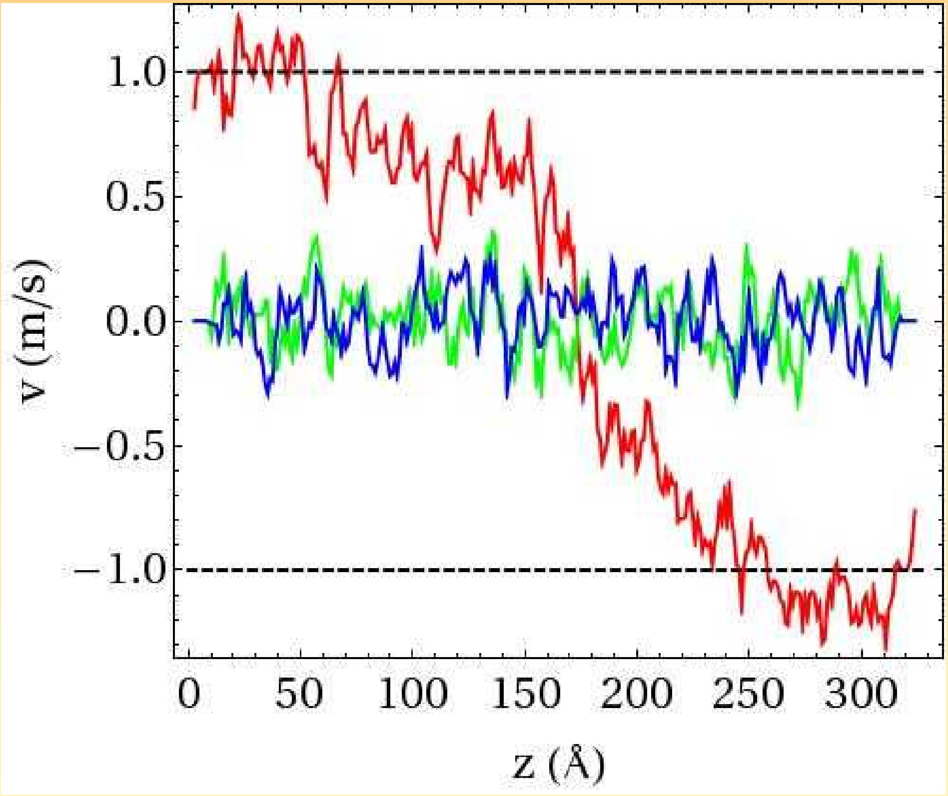
Grain Growth vs. Time

- Rigid top slab
- #FCC atoms correlates to grain size
- Effects:
  - Increasing
  - decreasing system size
  - tensile stress @ fixed separation



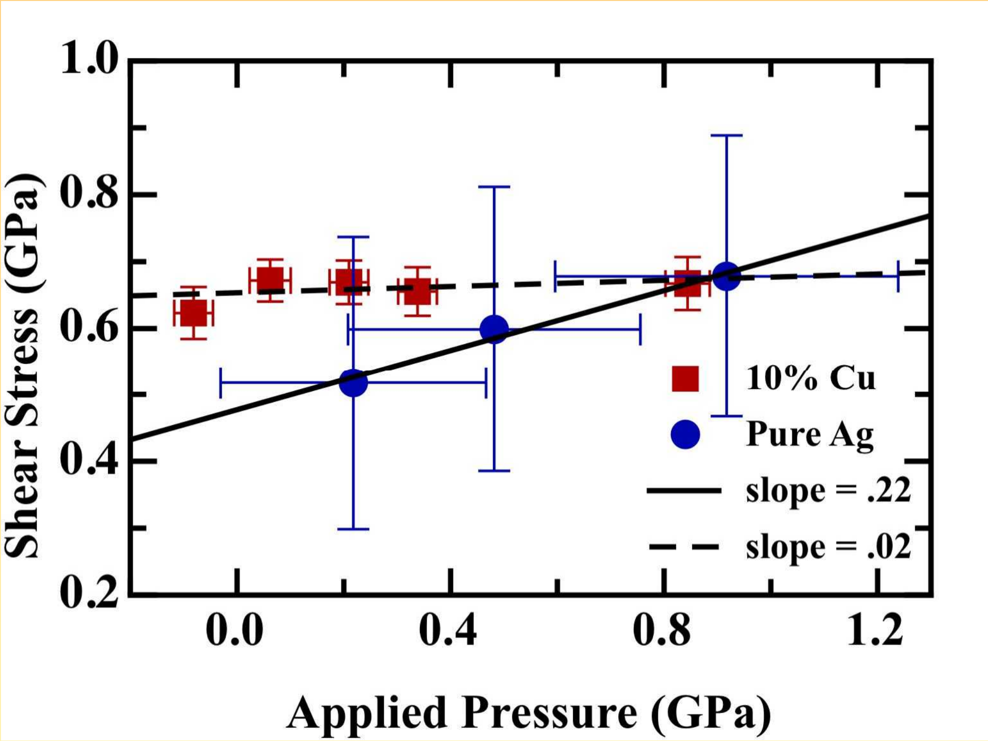
Alloy Slabs Slide

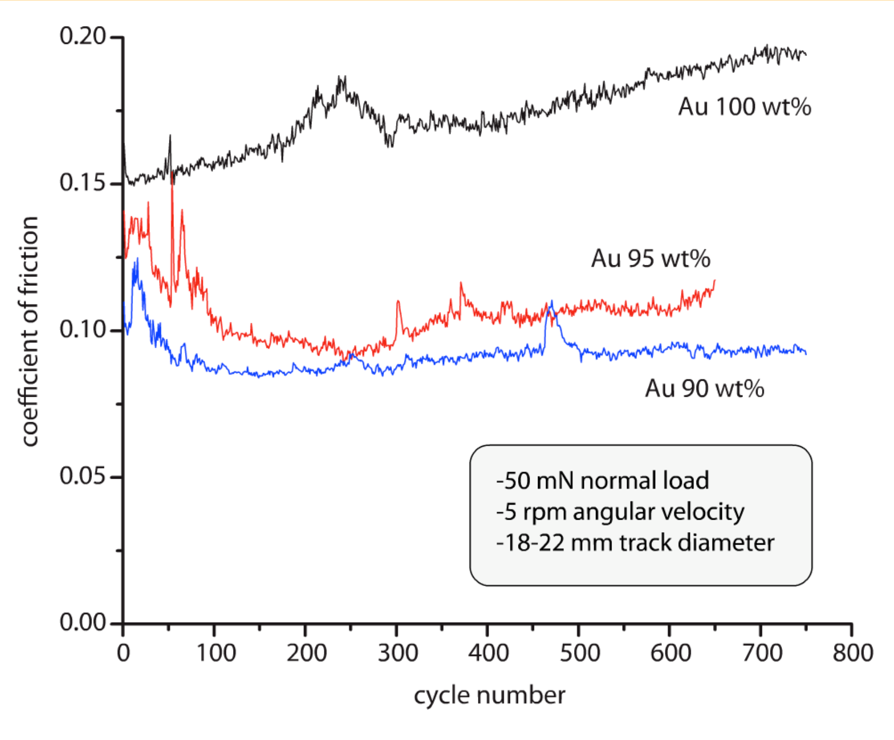




- Mechanism preventing grain coalescence allows sliding
- Shear occurs primarily at junction

Comparison of Friction





Courtesy: WG Sawyer, U. Florida

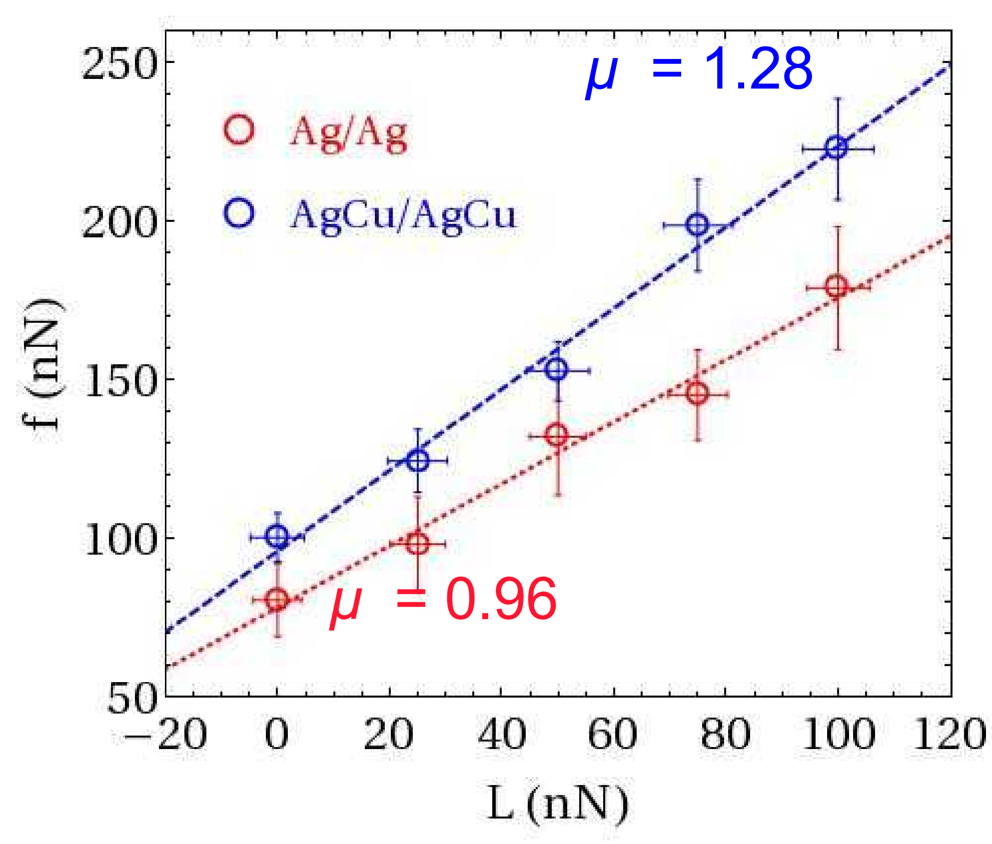
- Alloy has lower friction
- Qualitative agreement with experiment
- No commensurate interface formed

What is the Mechanism in Alloys?

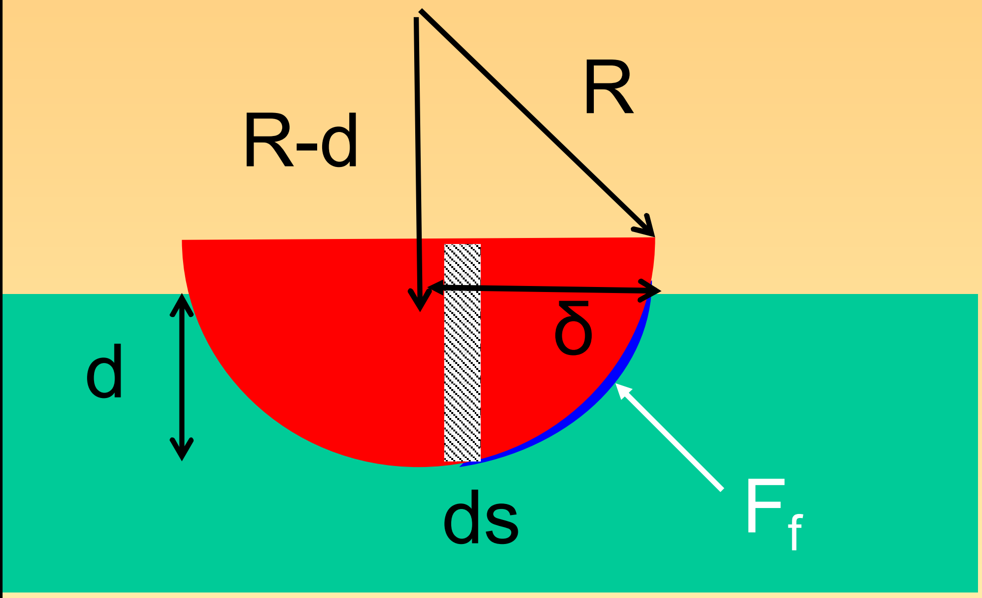
- Friction comparison slightly unsatisfying
  - Comparing tip friction to slab friction
  - Factor of 4 (not 10) seen by us, Harrison
- Ideal comparison:
  - Same system (tip/slab or slab/slab)
  - Remove grain growth mechanism
  - Determine what reduces friction in alloys

Rigid Tips

- Rigid tips => no grain growth
- *μ* slightly ***higher*** for alloy
- Shear strength essentially identical
- Materials properties have little effect
- All friction is plowing!
- Is this because of flow stress?



Flow Stress Contributes Little



$R \cos\theta = R - d$

$d \cong \delta^2 / 2R$

$$A = \int_0^{\delta} (d - s^2 / 2R)\, ds$$

$A = 2\,\delta^3 / 3R$

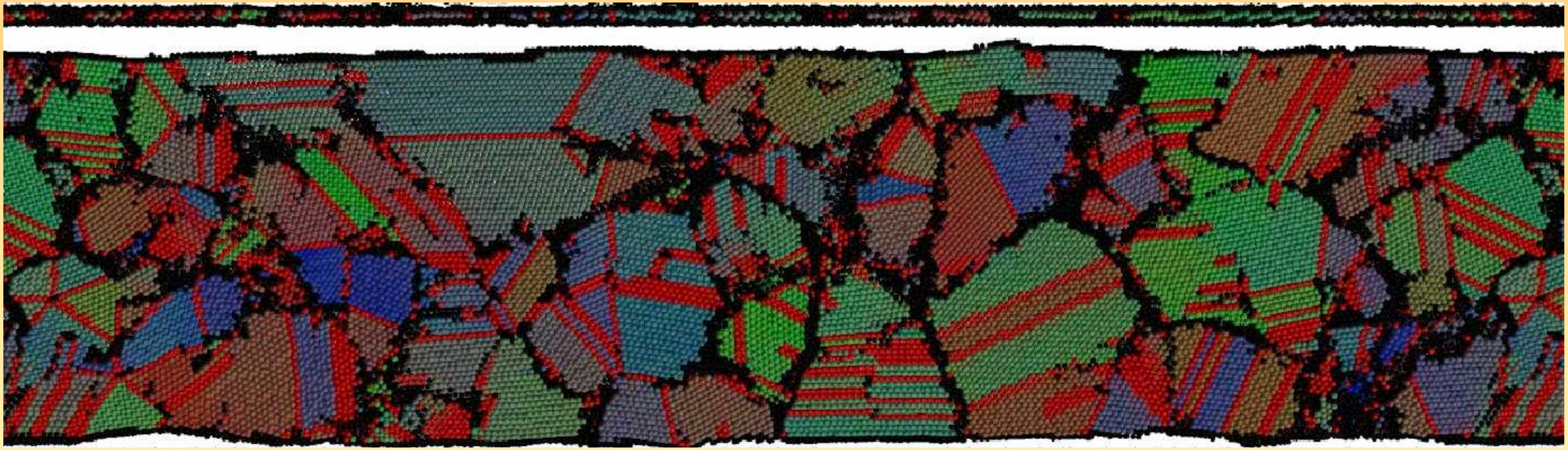
$F_n = \frac{1}{2} \pi \delta^2 H$

$F_f = (2\,\delta^3 / 3R)\, H$

$\mu = F_f / F_n \cong 0.1$

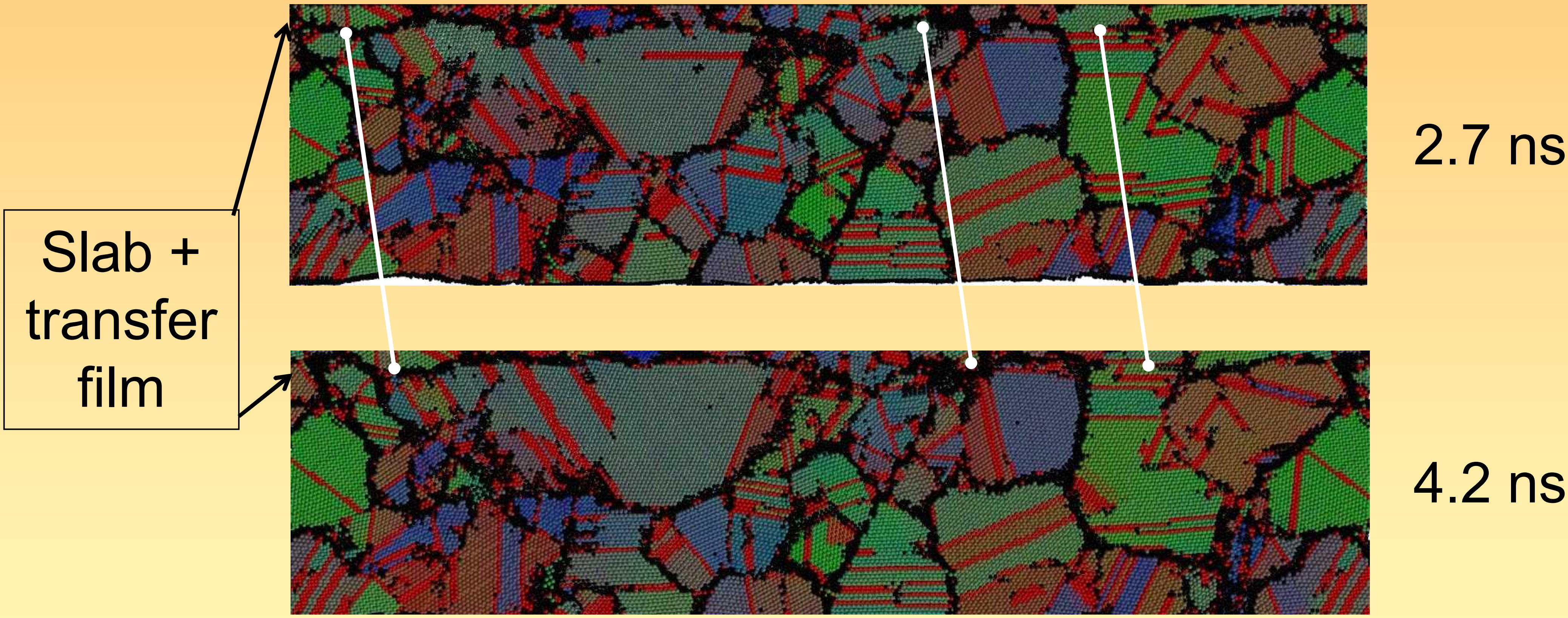
- Flow stress contribution ~.1, independent of hardness

Rigid Slab on Substrate



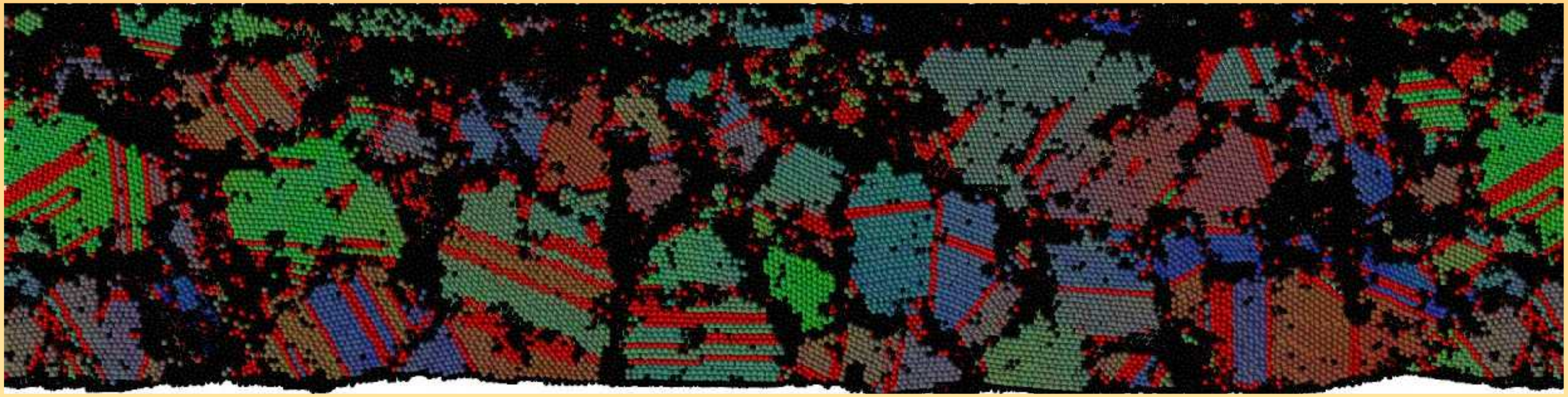
- Rigid slabs suppress grain growth
- No plowing is possible

Rigid Slab – Pure Ag

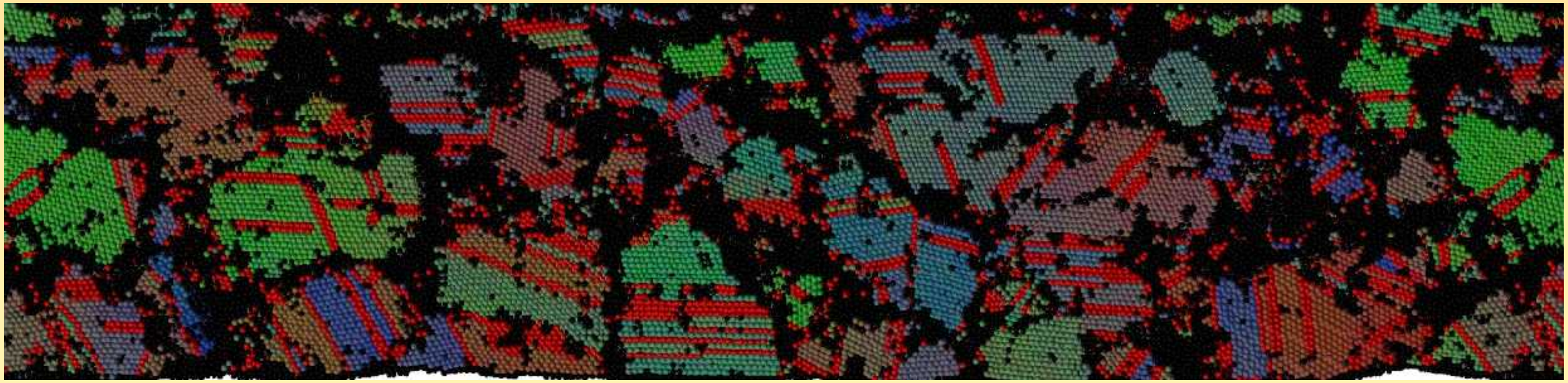


- Slight grain growth, forms transfer film
- Slides along grain boundary (of transfer film) or stacking fault depending on availability

Rigid Slab -- Alloy



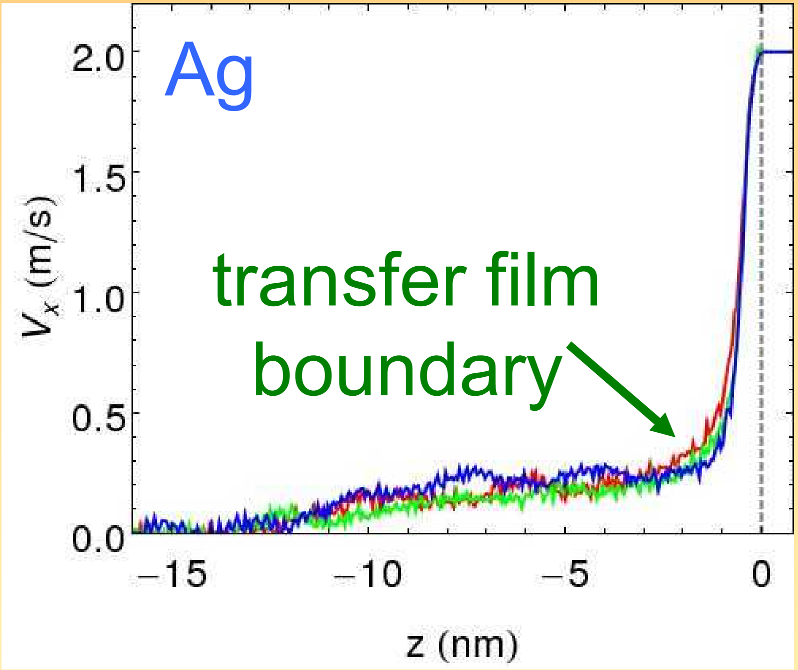
3 ns

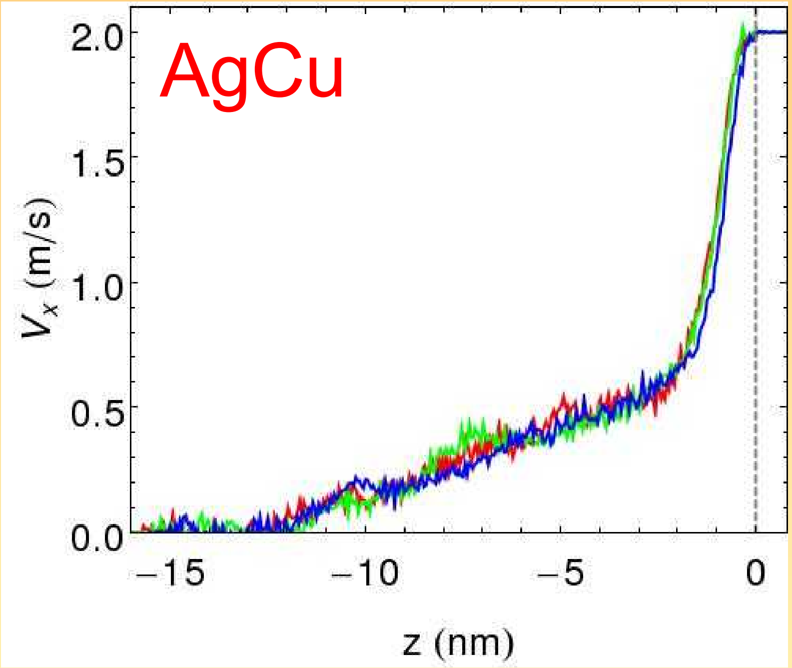


8 ns

- Alloy slides at boundary, but also throughout substrate

Velocity Profiles

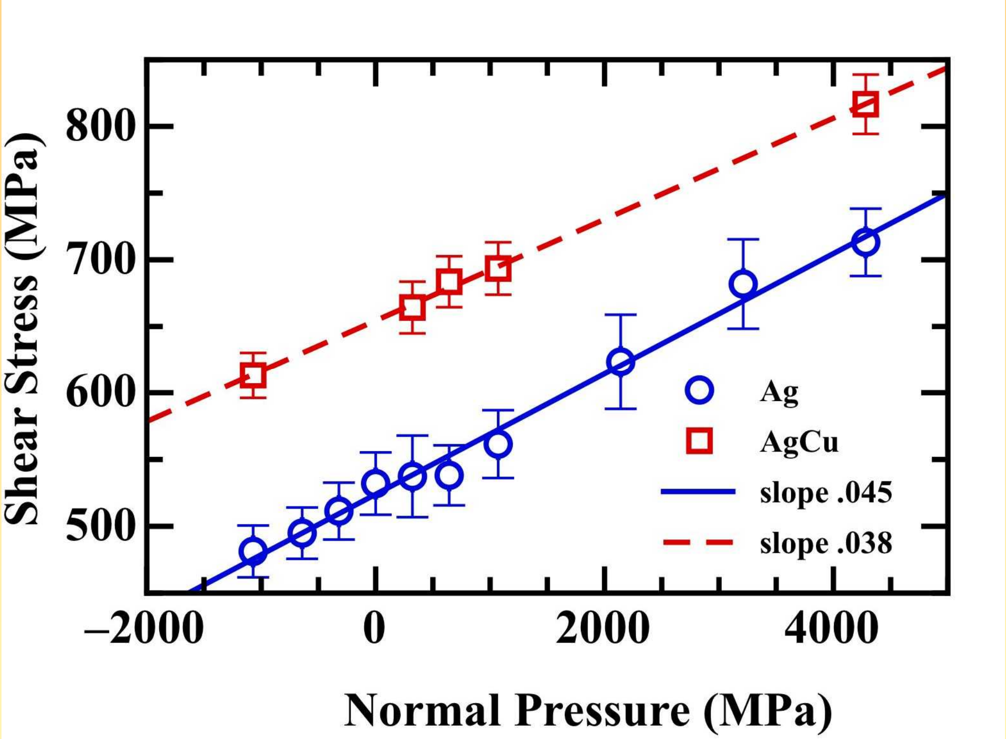




- Velocity profiles indicate liquid-like shearing
- Ag shears at transfer film
- AgCu shears at boundary, also throughout substrate
- Can extract pseudo-viscosities: Ag = 19 Pa·s, AgCu = 10 Pa·s
- Compare to Merkle and Marks, Wear (2008): Au = 2 Pa·s

Rigid Slab Friction

- Alloy shear stress 20% higher (650 MPa vs 530 MPa)
- Liquid Cu viscosity slightly higher than liquid Ag
  - Implies alloy has higher viscosity
  - Does this imply higher shear stress in the alloy?
- *μ* essentially identical – grain growth suppression leads to same friction mechanism



Conclusions

- Metallic friction mechanisms revealed
- Pure metals
  - Cold welding, grain reorientation
  - Shear along slip planes
  - Commensurate interface = high friction
- Alloys/composites (with different lattice constants)
  - Still cold welding, but grain reorientation suppressed
  - Shear along grain boundaries
  - Liquid-like lubrication = lower friction
  - Similar to mechanism proposed in different metal (Ni) at different scales (Prasad, Battaile and Kotula, Scripta Mat. 2011)

Come to Costa Rica!

- Advances in Lubrication: Linking Molecular, Meso, and Machine Scales
- January 8-13, 2012
- http://www.engconfintl.org/12al.html
- Chair: M. Chandross, co-chairs, R. Carpick, M. Dienweibel, M. Dugger, M. Masuko, H. Spikes