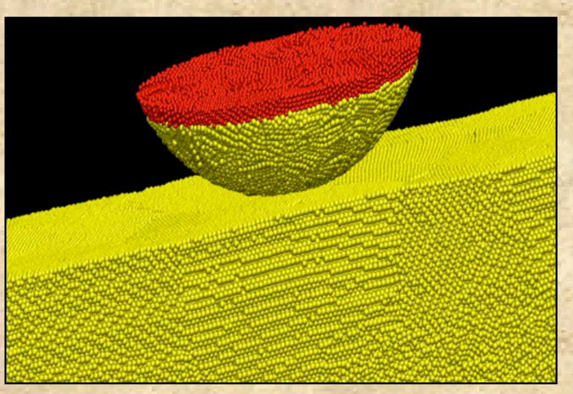
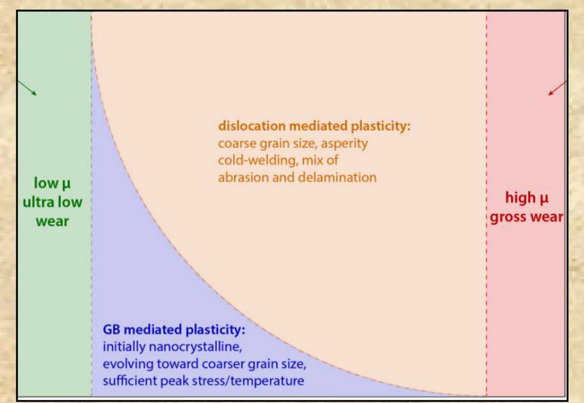
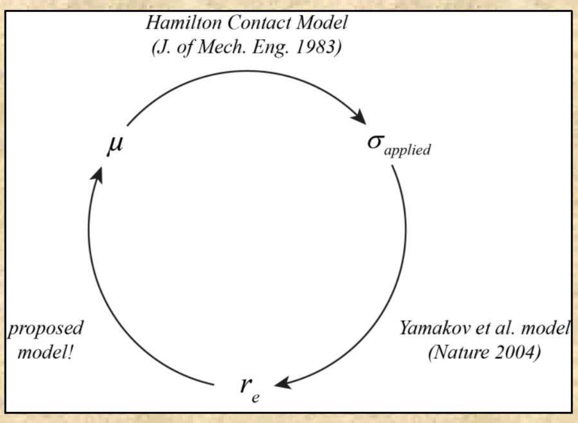
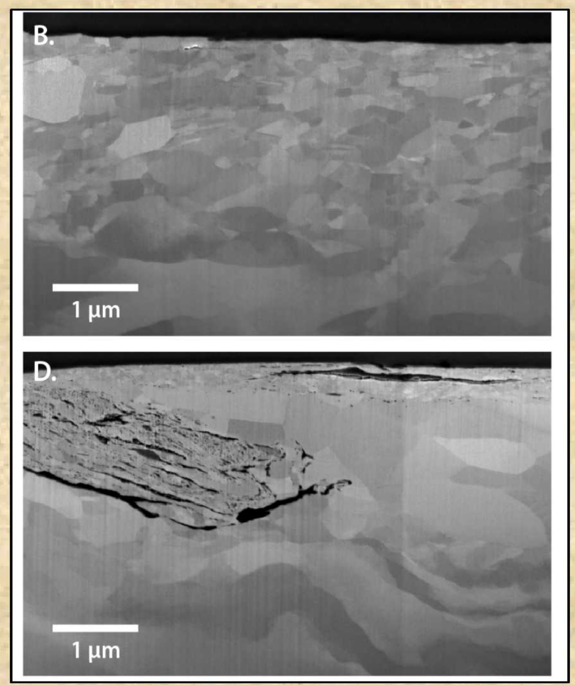
SAND2018-7284C

A General, Predictive Model of Friction in Metallic Contacts









Michael Chandross[1], Shengfeng Cheng[2], and Nicolas Argibay[1]
[1]Sandia National Laboratories, Albuquerque, NM
[2]Virginia Polytechnic Institute and State University, Blacksburg, VA

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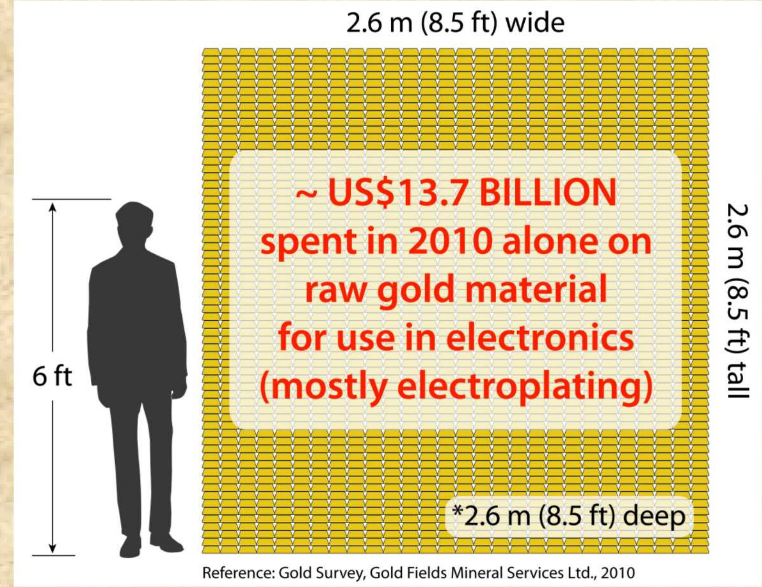
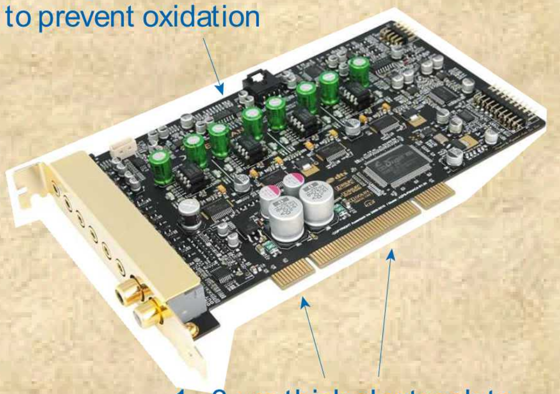
Metals as Tribological Materials

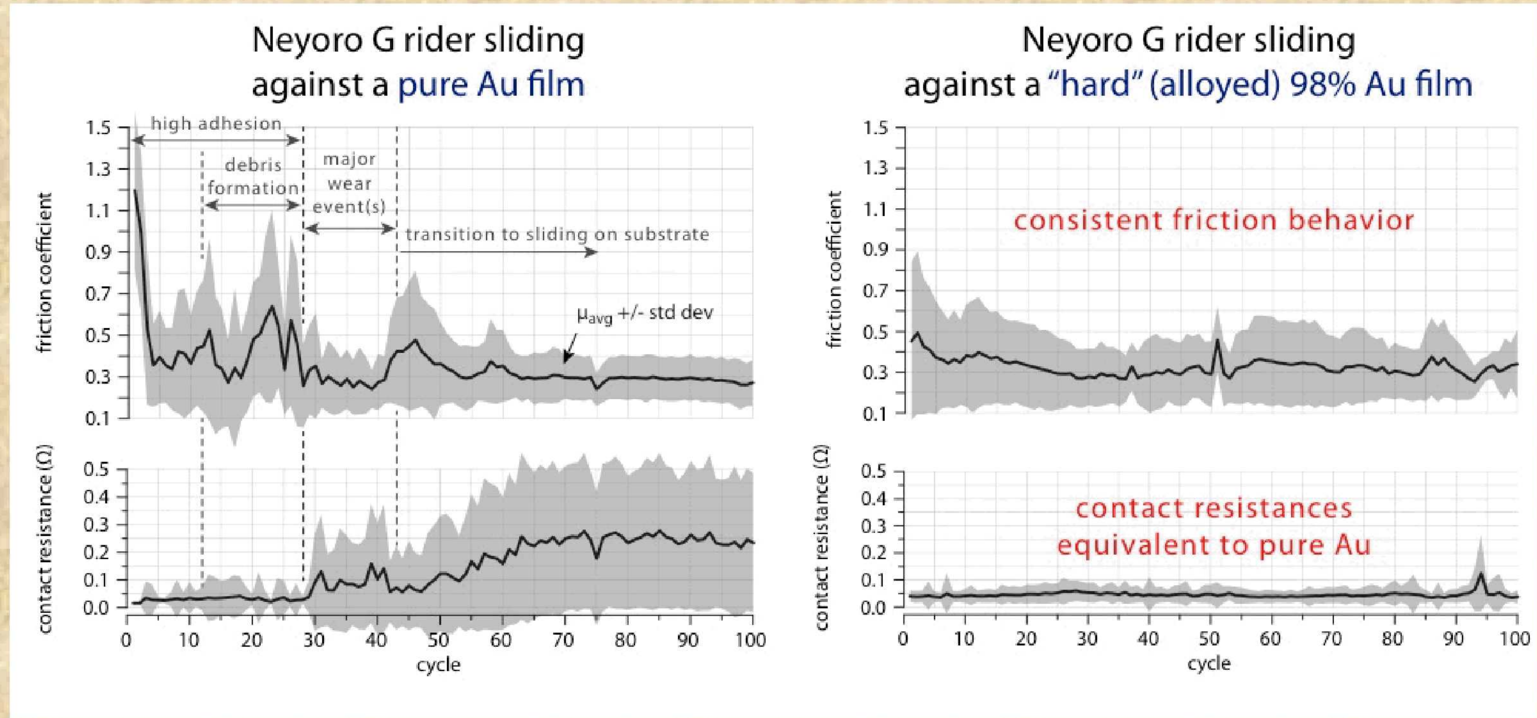


- 300 metric tons of gold used in 2010
  - 11% of yearly extracted amount
  - Cube of ~25,000 gold bars
  - Clad Eiffel Tower with 70 µm of pure gold *every year*
- Protection of PCBs with <2% Ni, Co hardened Au
  - Oxidation prevention
  - Electrical edge connectors

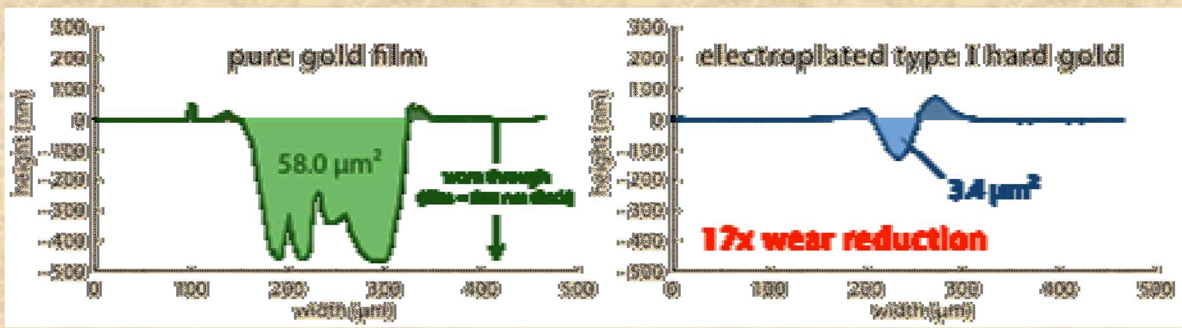
- The good:
  - High conductivity
  - Doesn't corrode/oxidize
  - Can be made very thin
- The bad:
  - High adhesion (> GPa)
  - High friction (µ = 1 – 2)

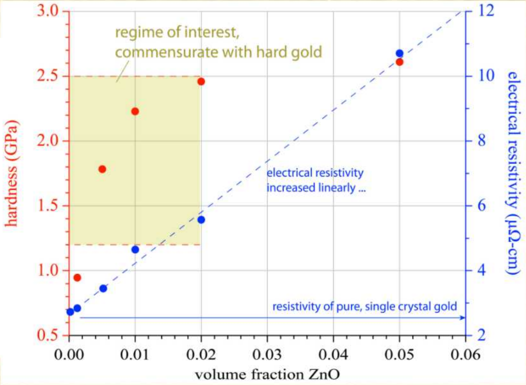


Why Use Hard Gold?



Alloying produces more consistently "low" friction, wear and contact resistance

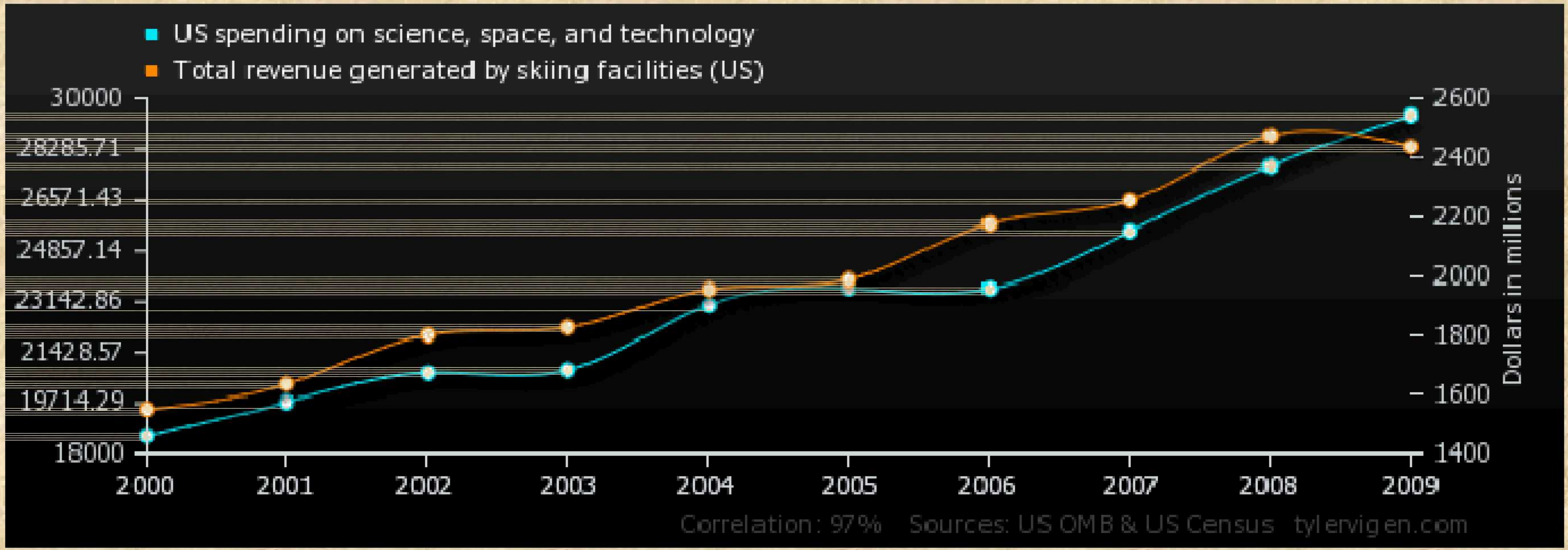




Gross wear/delamination

Wear rate (vs. sapphire): 10^{-6}

Correlation is not Causation

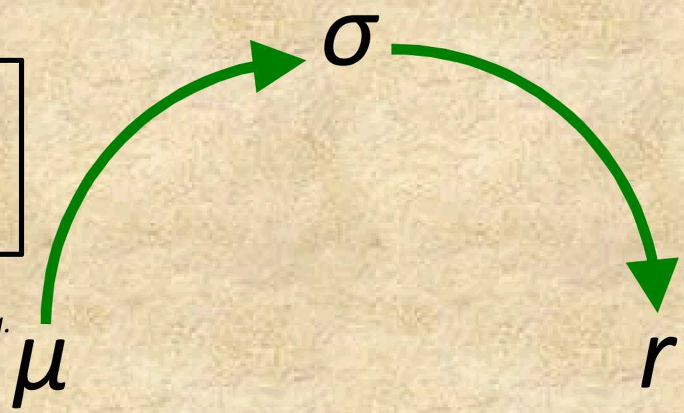


Hardness is not the answer!

Part of the Story

Hamilton's contact mechanics

Hamilton, 1983,
Proc. Inst. of Mech. Eng.



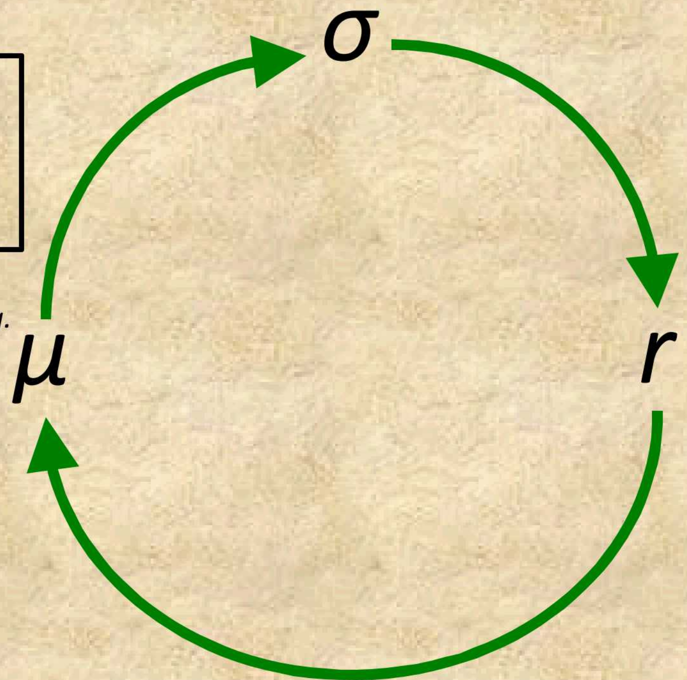
Yamakov, *et al.*'s nanocrystalline deformation mechanism

Yamakov et al.,2004,
Nat. Mat.

The Full Story

Hamilton's contact mechanics

Hamilton, 1983,
Proc. Inst. of Mech. Eng.



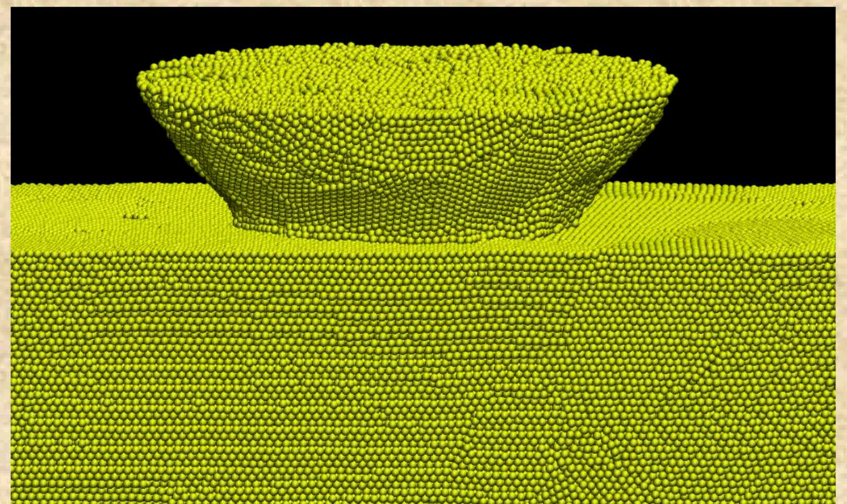
Yamakov, *et al.*'s nanocrystalline deformation mechanism

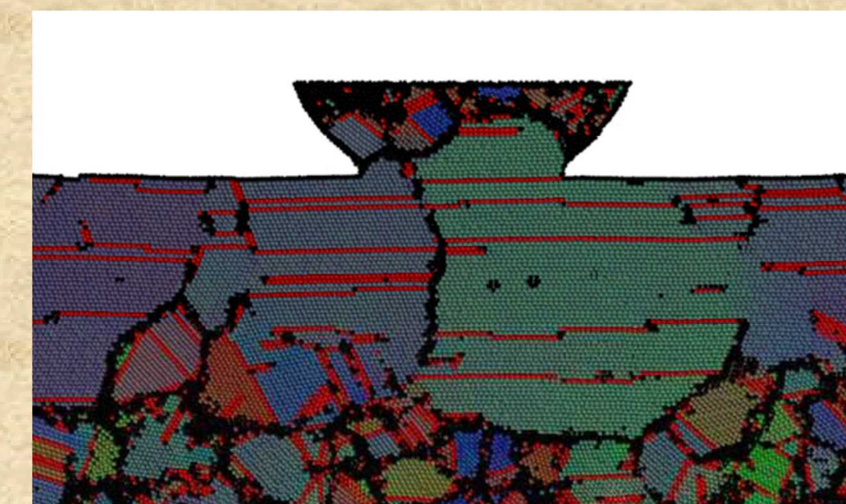
Yamakov et al.,2004,
Nat. Mat.

Our proposed model

Submitted to Science

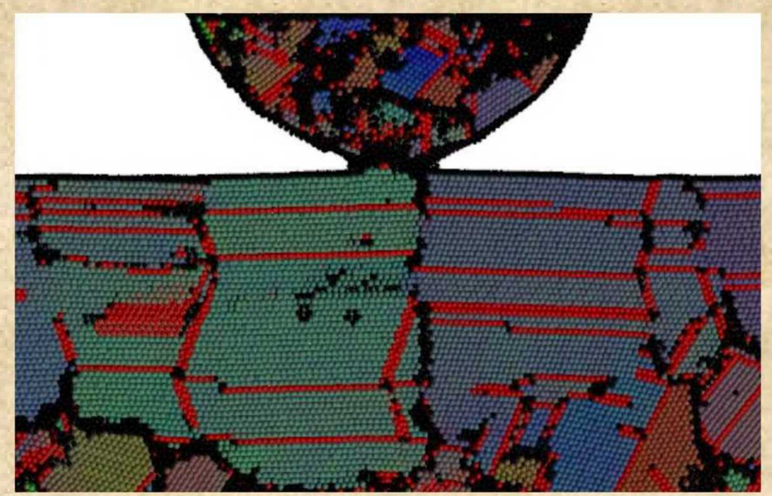
What is the Origin of Reduced Friction?





- 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

Microstructural evolution is the key



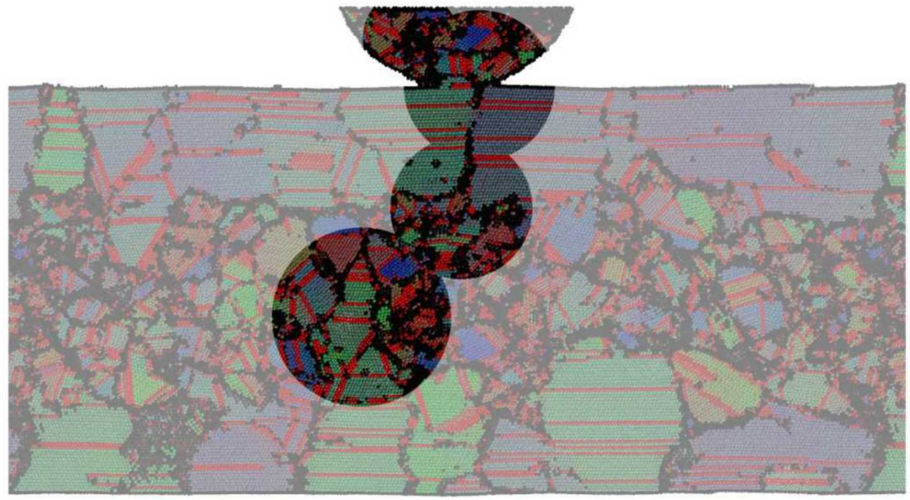
Pure Silver

Silver-Copper Alloy

- Cold welding at the contact point
- Different microstructures
- Competition between grain growth and refinement

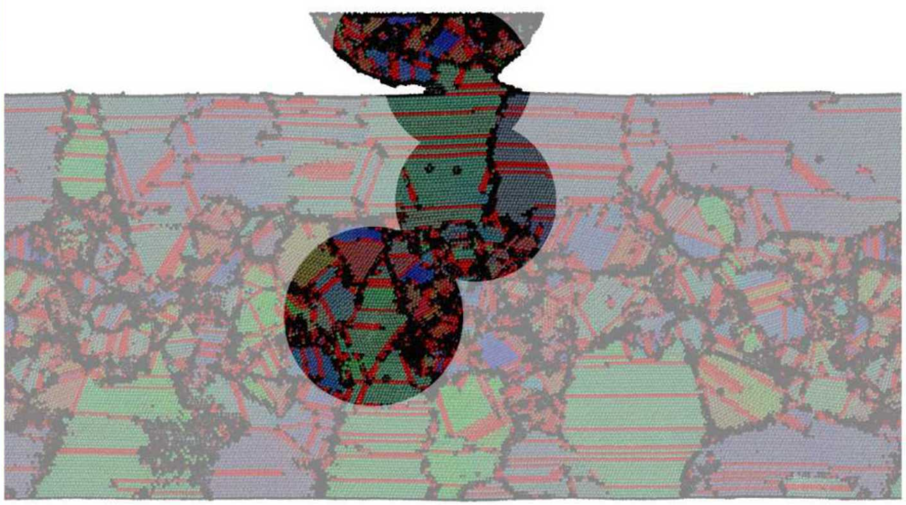
Alloying stabilizes grain boundaries

initial microstructure
of Ag and Ag-Cu alloy
(no sliding yet)

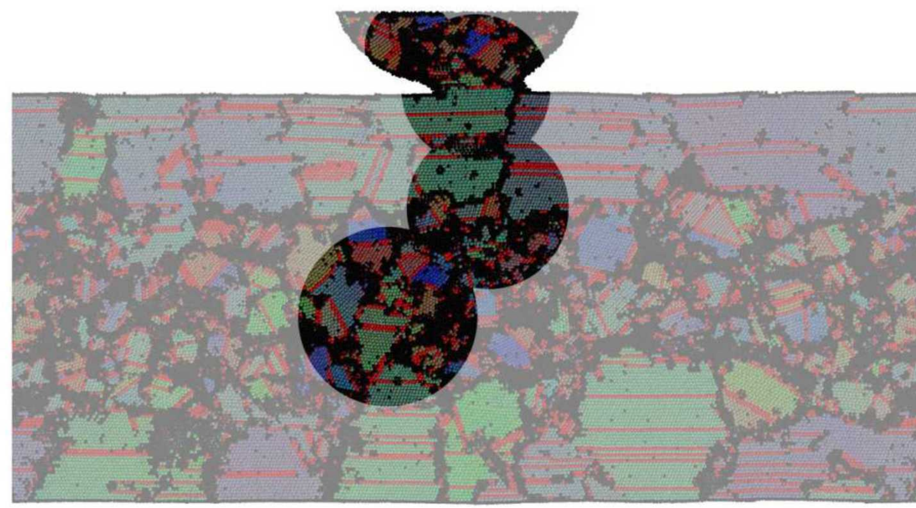


300 MPa contact stress
300 K temperature
2 m/s sliding speed

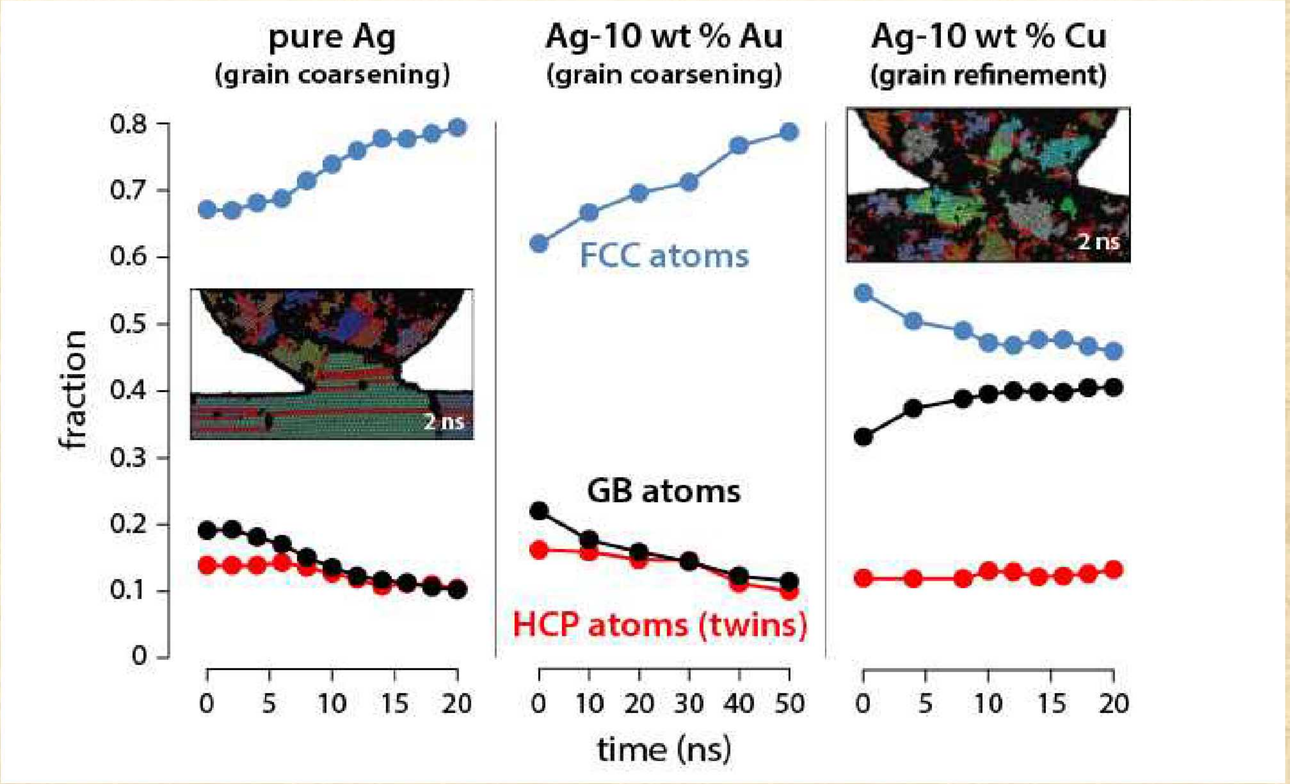
pure Ag after 4 nm of sliding



Ag-10% Cu alloy after 4 nm of sliding



Quanitative Measure of Stabilization

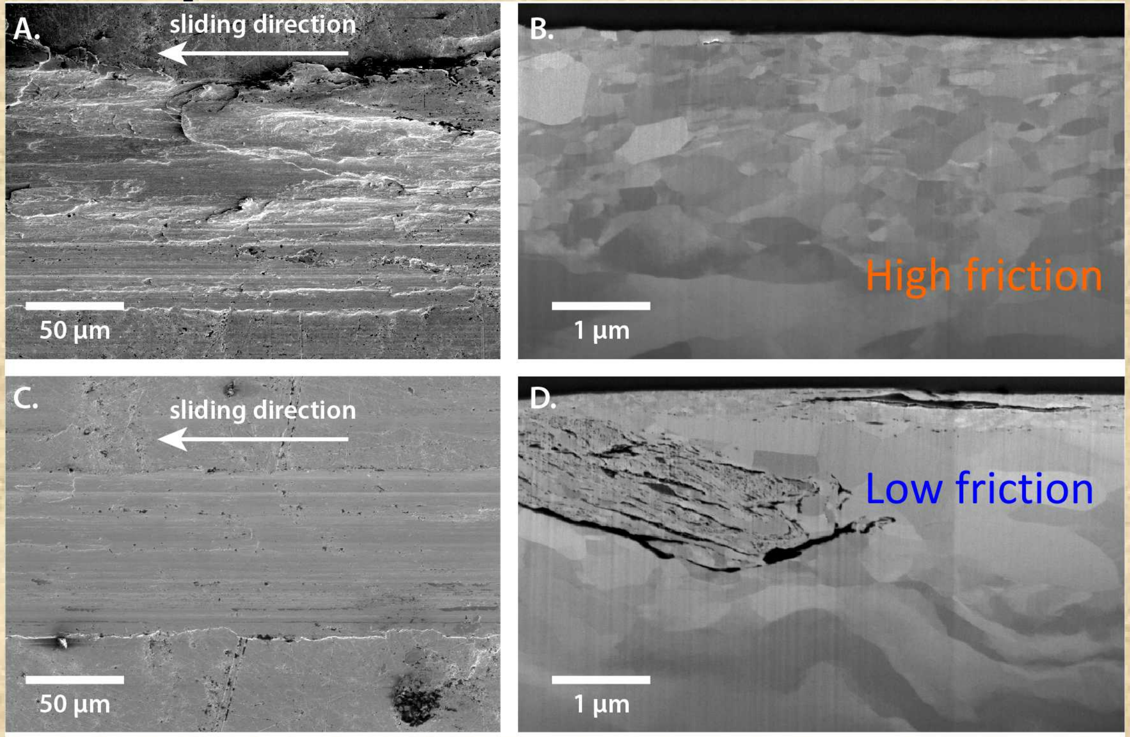


- Experiments: alloys stabilize grain boundaries, prevent grain growth
- Simulations: alloys prevent grain growth through lattice mismatch
- Both: Lack of grain growth avoids formation of commensurate interface, lowering friction

MD also reveals that GB mediated plasticity prevails when friction is low, and dislocation mediated plasticity prevails when friction is high

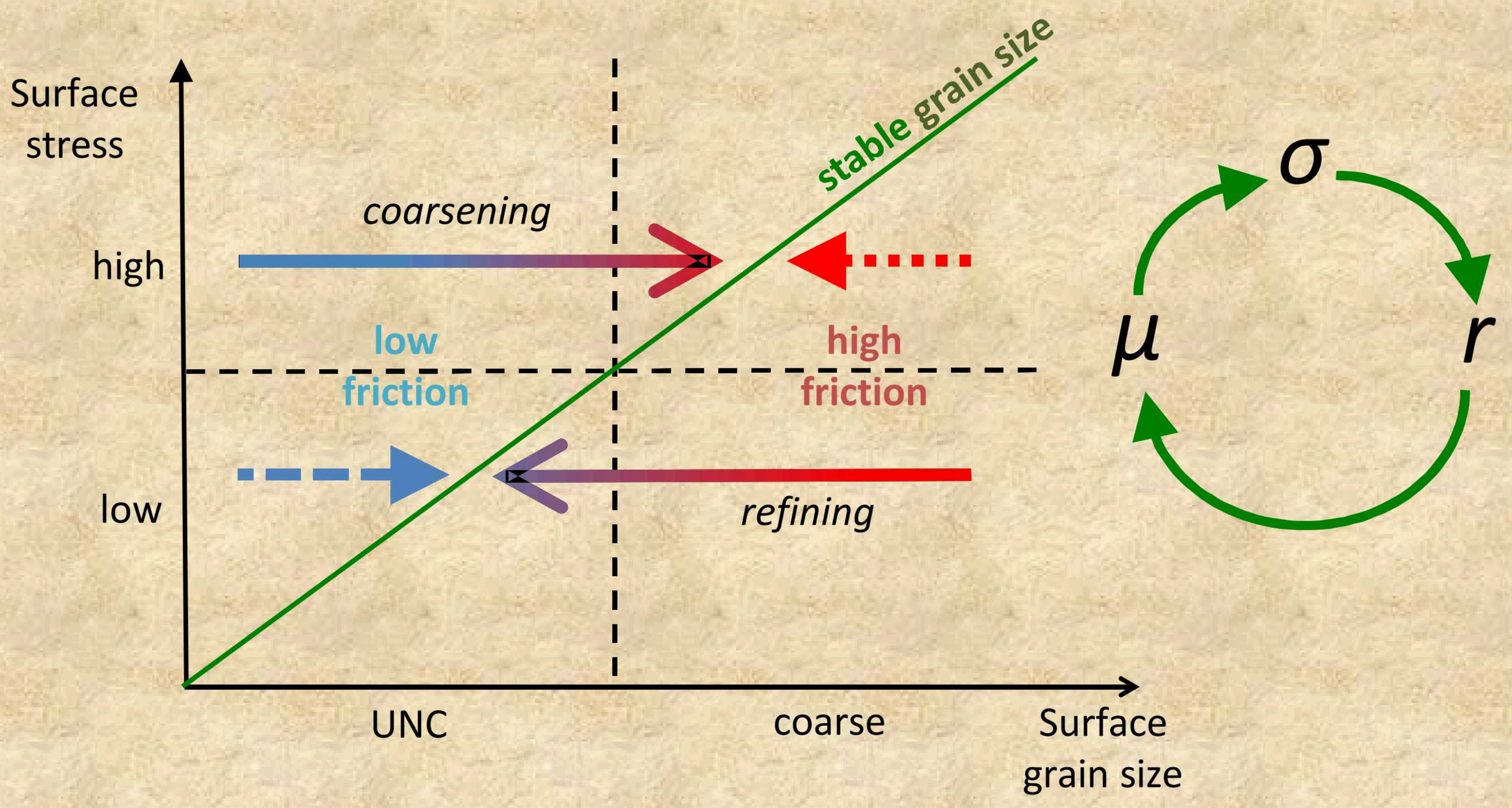
Experimental Results

Gold pin on gold substrate



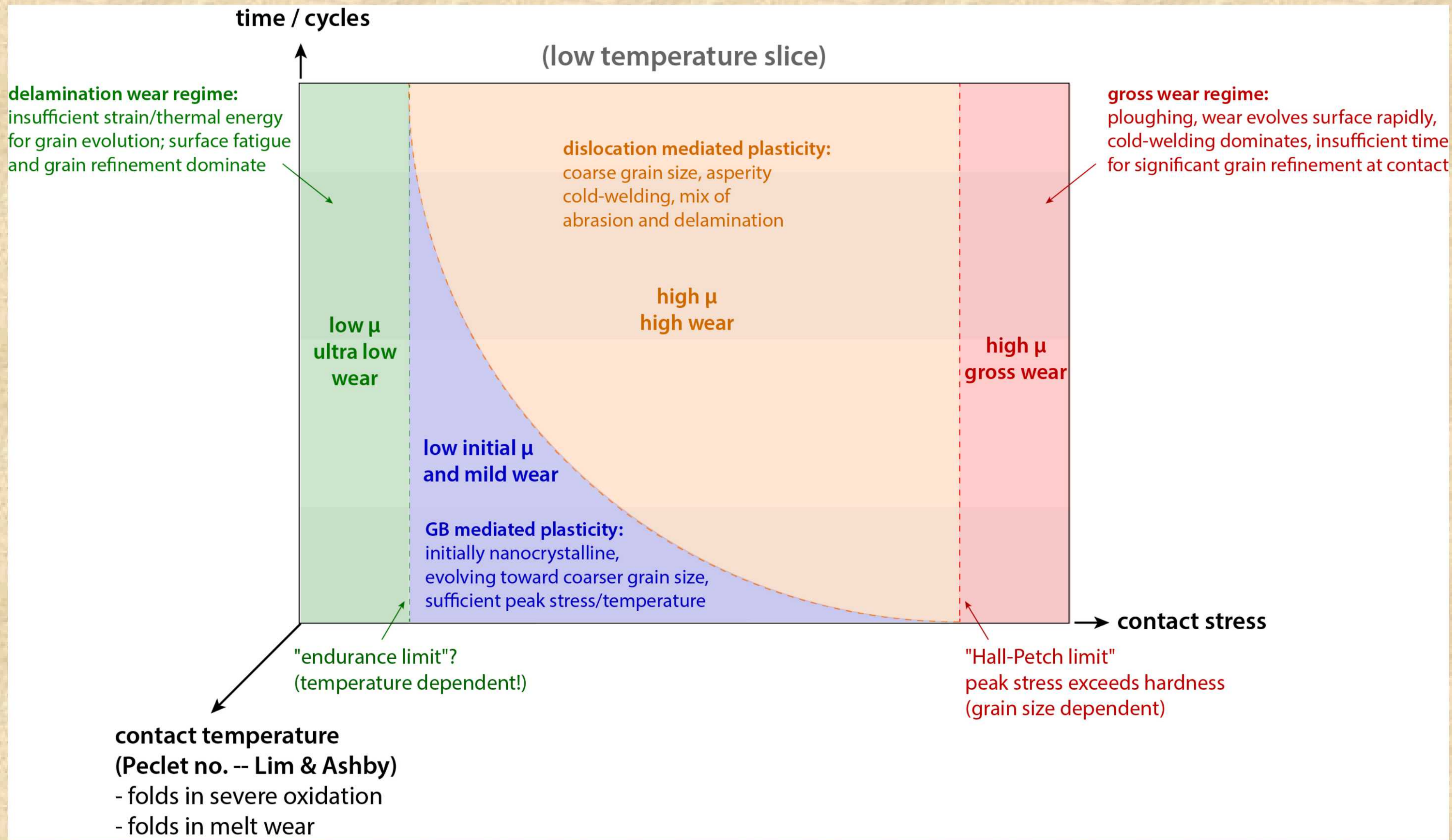
- Low friction accompanied by UNC layer
- High friction shows coarse grained structure
- Seen by many people
- Implies relationship between grain size and friction

Cartoon of the Evolution



- Stress drives grain size to the green line
- The location of the line (UNC or coarse grained) determines μ
- Stability of μ over time is determined by initial quadrant

Conceptual Friction Map



- Different stress regimes
- Time evolution only at intermediate stresses

Now Things Get Hairy…

- The management would like to apologize for the following slides…

How do you make it predictive?

Average grain size: d

Splitting distance at zero stress:

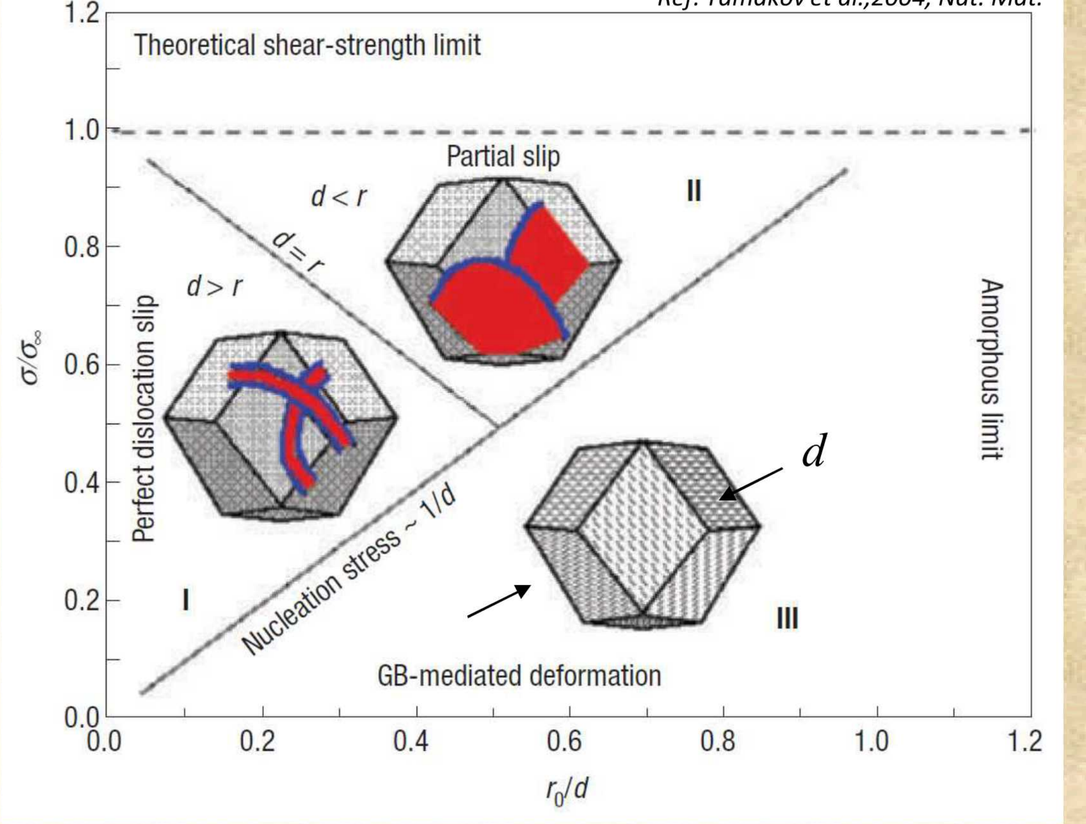
$$r_0 = \frac{(2+\nu)Gb^2}{4\pi(1-\nu)\gamma_{sf}}$$

Stress at which splitting distance is infinite (theoretical shear strength):

$$\sigma_\infty = \frac{2\gamma_{sf}}{b}$$

Ref: Froseth et al. (Acta Mat. 2004)

Ref: Yamakov et al.,2004, Nat. Mat.

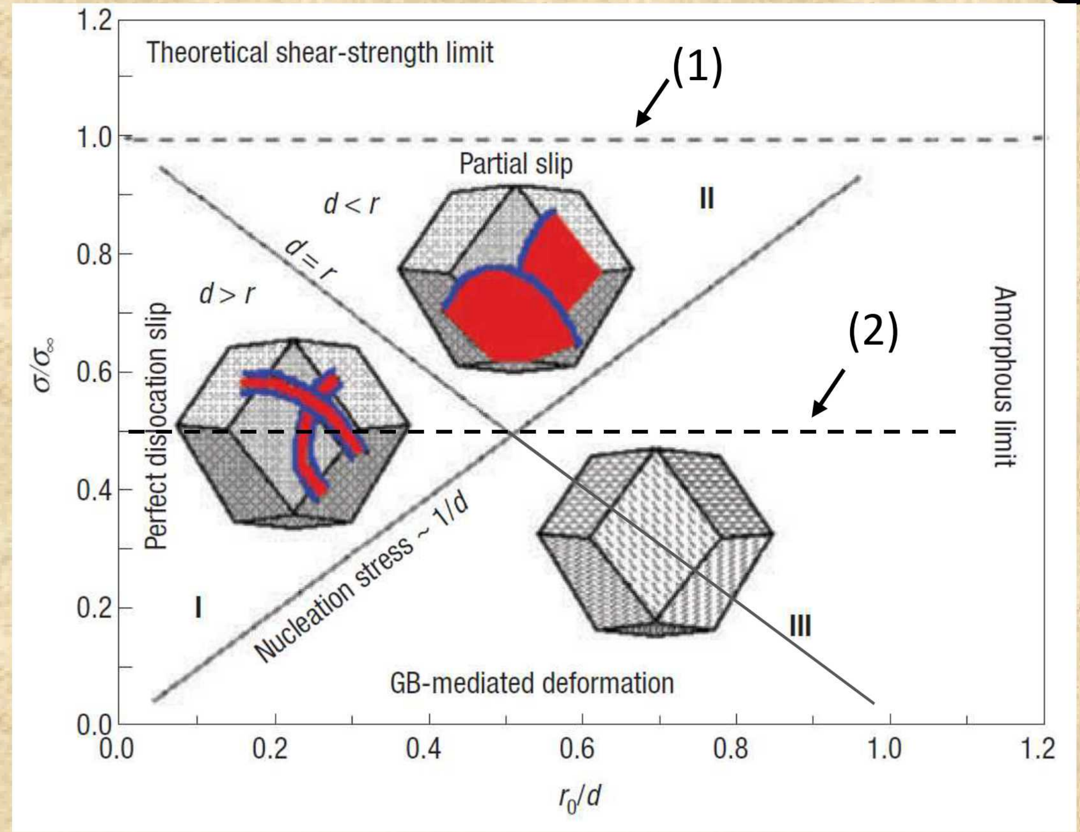


Equilibrium splitting distance (size of a stacking fault):

All materials parameters

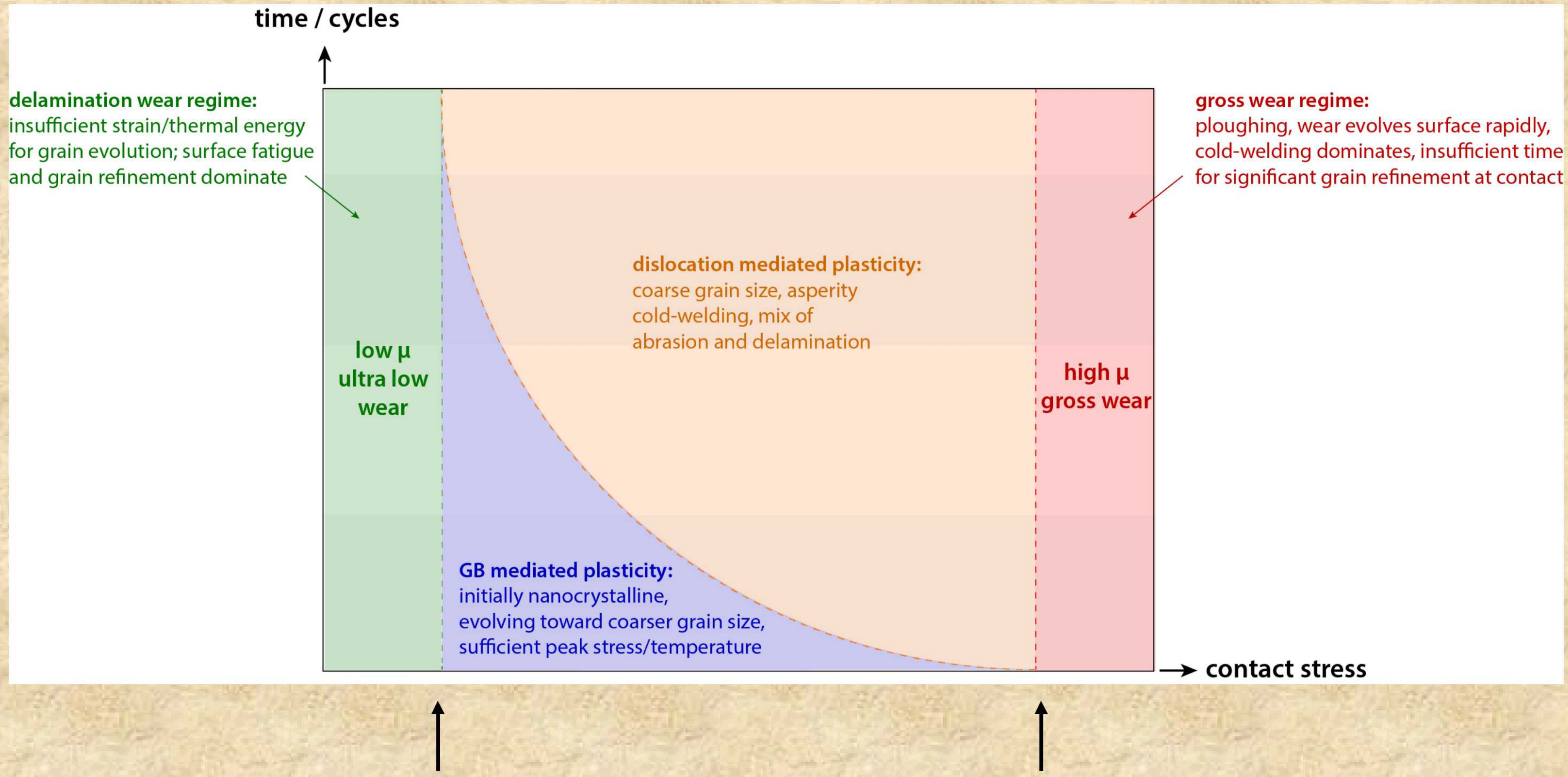
$$r = \frac{r_0}{1-\sigma/\sigma_\infty}$$

Connection to Tribology



- Two limiting conditions:
  - Applied stress = theoretical strength = σ_∞
  - Applied stress = $\sigma_\infty / 2$, implies a grain radius
  - Below *2r_o*, GBMP. Above *2r_o*, DMP

Two Limits Defined



stress limit below which GBMP will always occur

stress limit above which DMP will occur immediately

What About Grain Evolution?

$$v_{gb} = \frac{2\gamma_{GB}}{b} M_0 e^{(-Q/kT)} e^{[(\sigma - \sigma_\infty/2)V^*/kT]}$$

γ_{GB} = grain boundary energy

b = Burger's vector

M_0 = grain boundary mobility

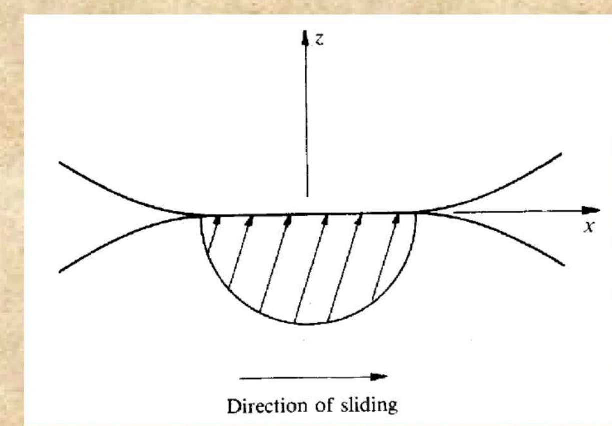
Q = activation energy

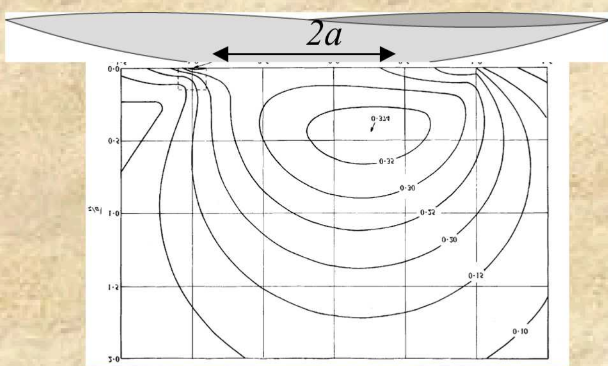
V^* = activation volume

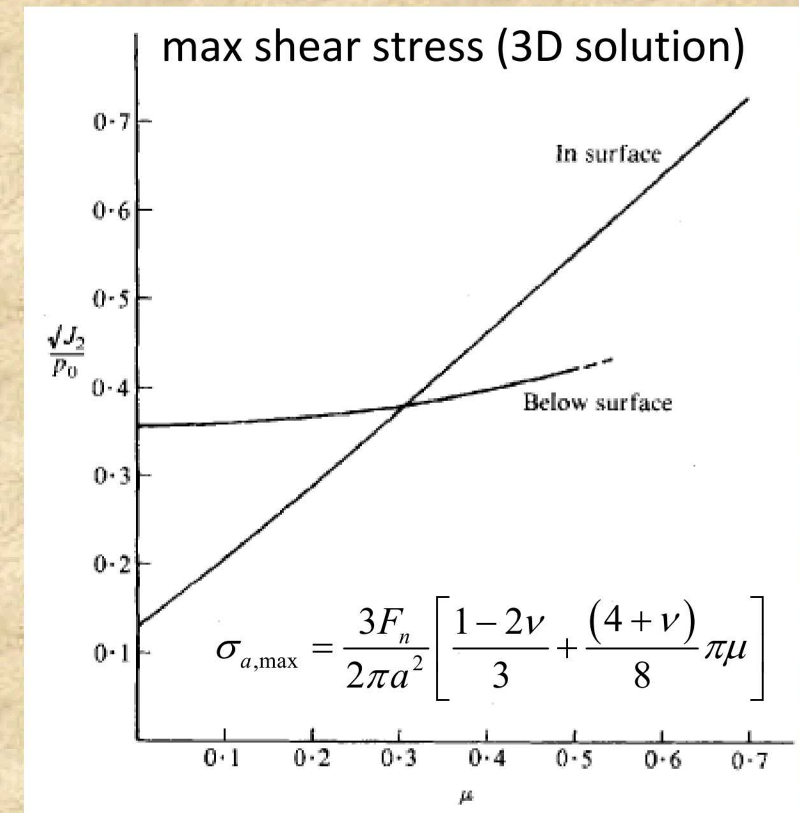
- Standard grain growth equation
- Extra term depends on applied stress
- Use this to see how long it takes to evolve grains to $2r_o$

All materials parameters

Finally, Applied Stress



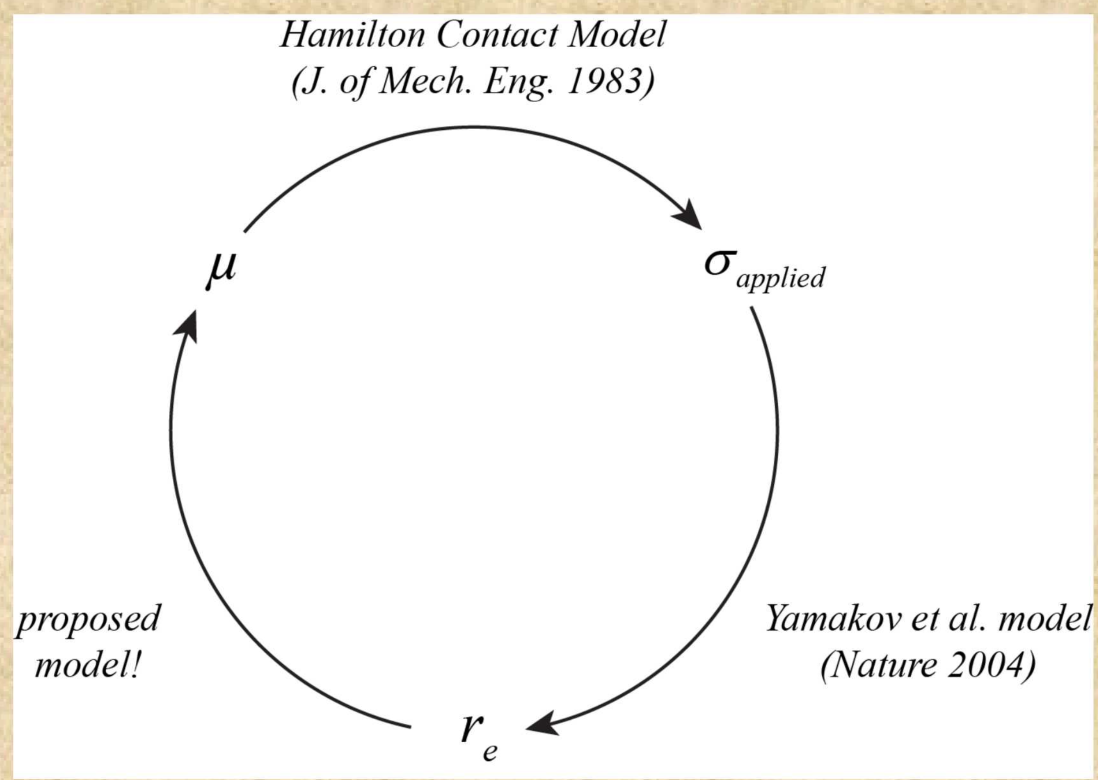




friction coefficient

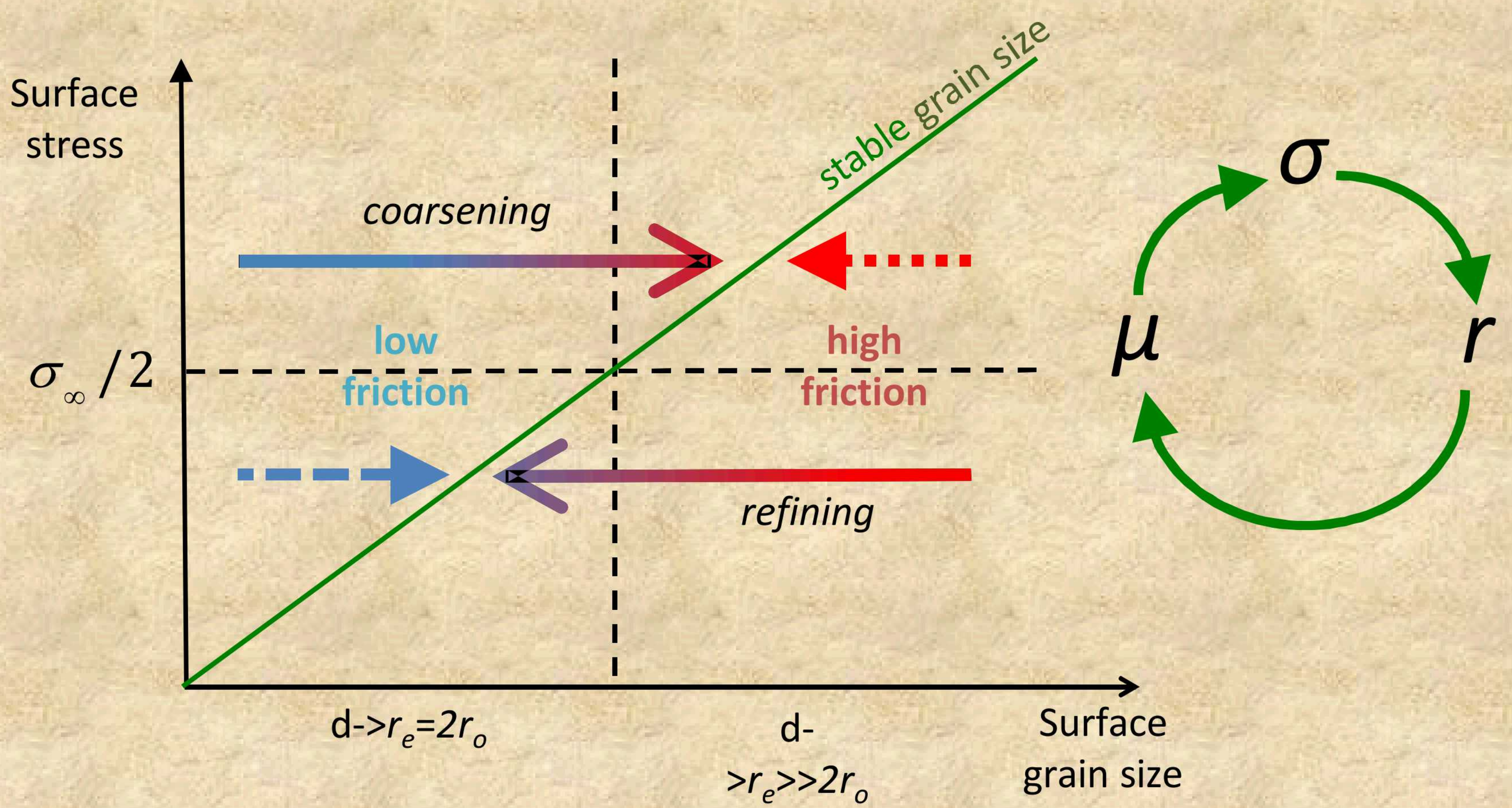
- Hamilton's model: *G. Hamilton, Proc. Inst. of Mech. Eng. Part C (1983)*
- Like Hertz, but with friction
- Uses Hertz solution for contact radius

Can Now Complete the Circle



- Numerical correlation between applied stress, grain size and friction coefficient.
- All based on materials parameters.

Update the Cartoon



- Stress drives grain size to the green line
- The location of the line (UNC or coarse grained) determines μ

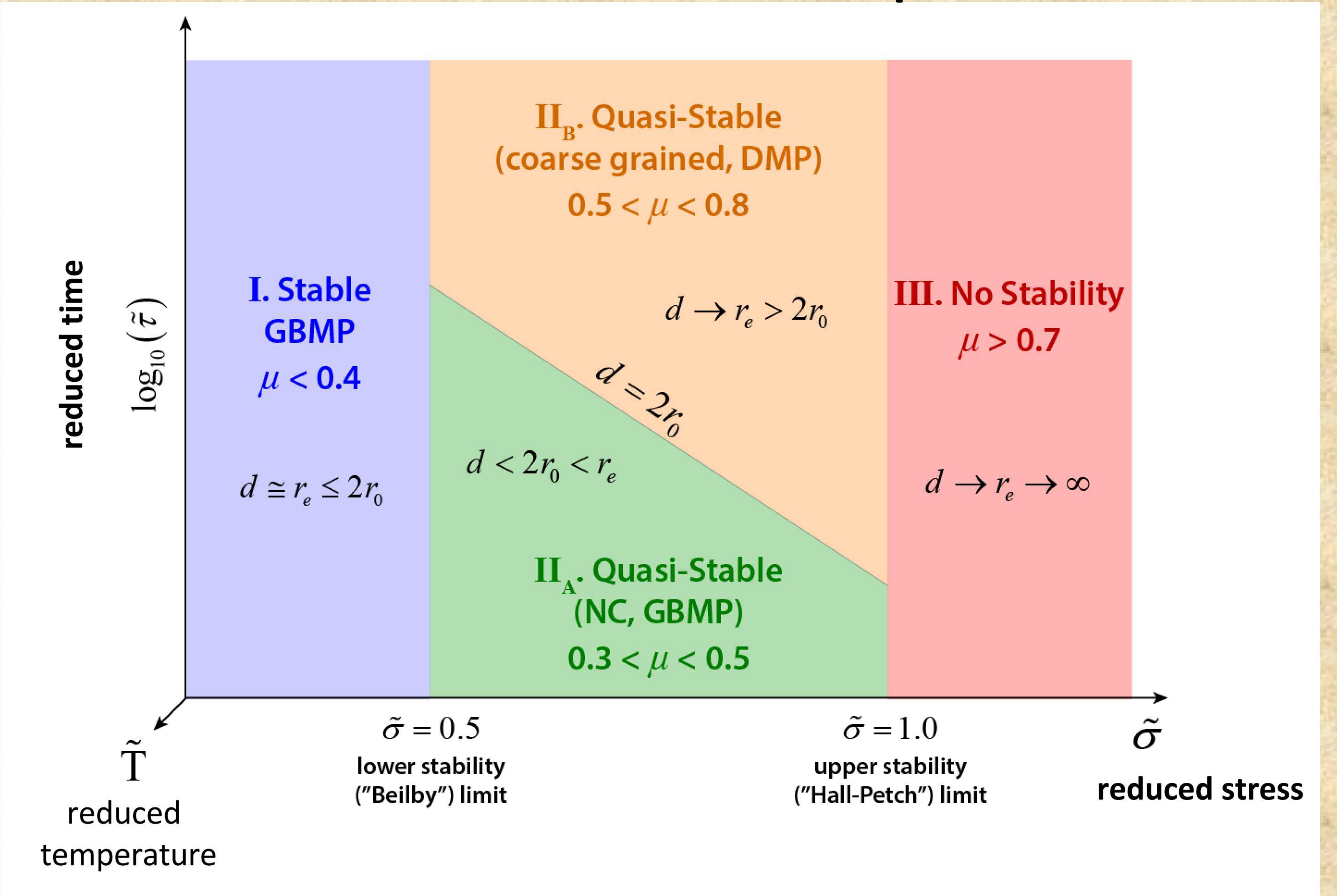
Make it Dimensionless

$$\tilde{\sigma} = \frac{\sigma_{a,\max}}{\sigma_{\infty}}$$

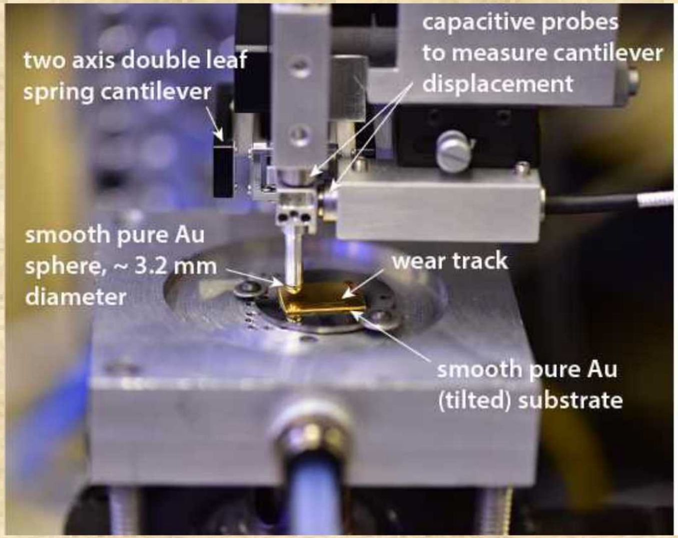
$$\tilde{\tau} = \log_{10}\left[\left(\frac{2\lambda_a}{v_s}\right)\left(\frac{4\gamma_{gb}M_0}{r_0^2}\right)\right]$$

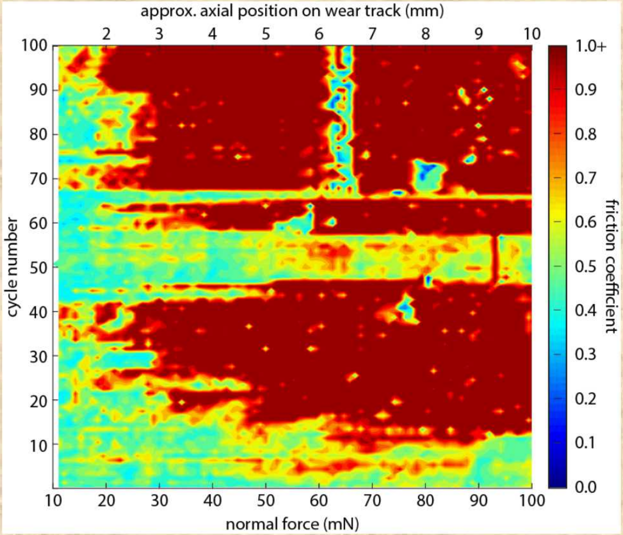
- Normalize stress by a fundamental stress
- Normalize time by the fundamental “grain boundary time”
- Plot semilog

Full Friction Map

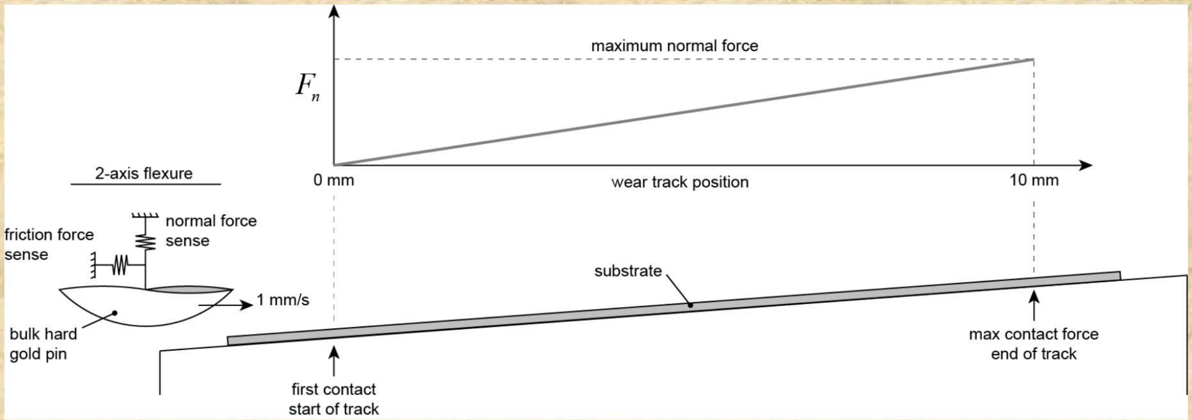


How Can We Test This?





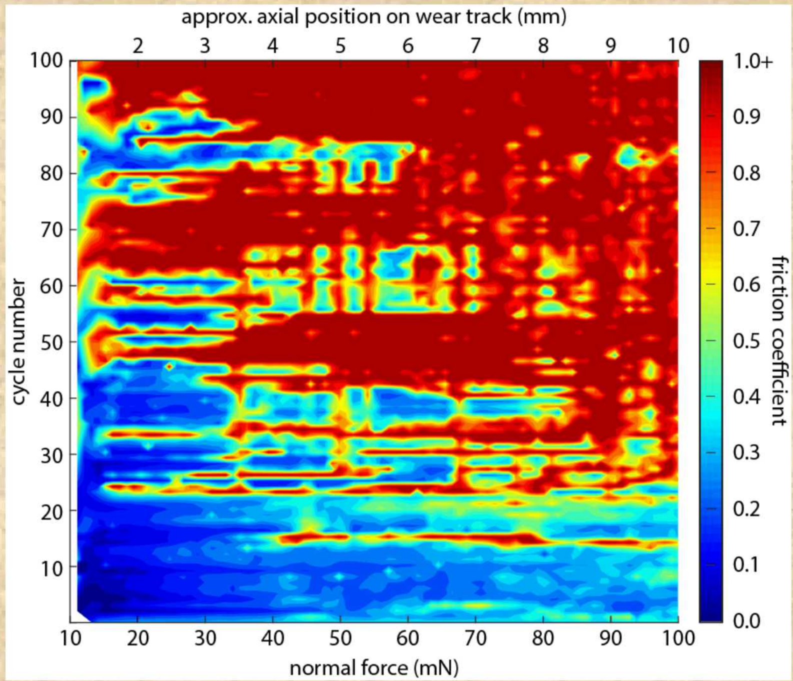
self-mated Au

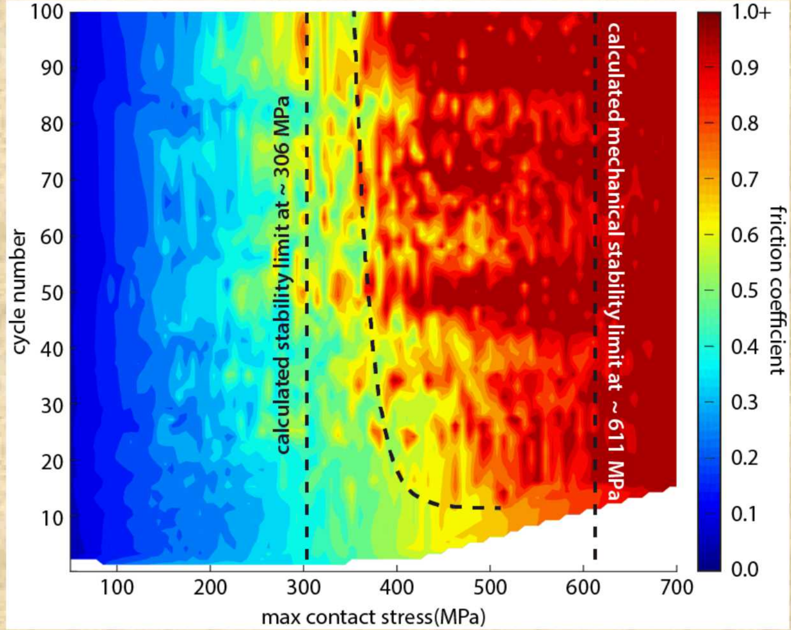


- Ramped load test
- Force increases linearly with distance
- Track friction force vs. load for each cycle

Clean It Up With Hamilton's Model

raw friction data → **applying Hamilton model**





(μ as function of max surface stress)

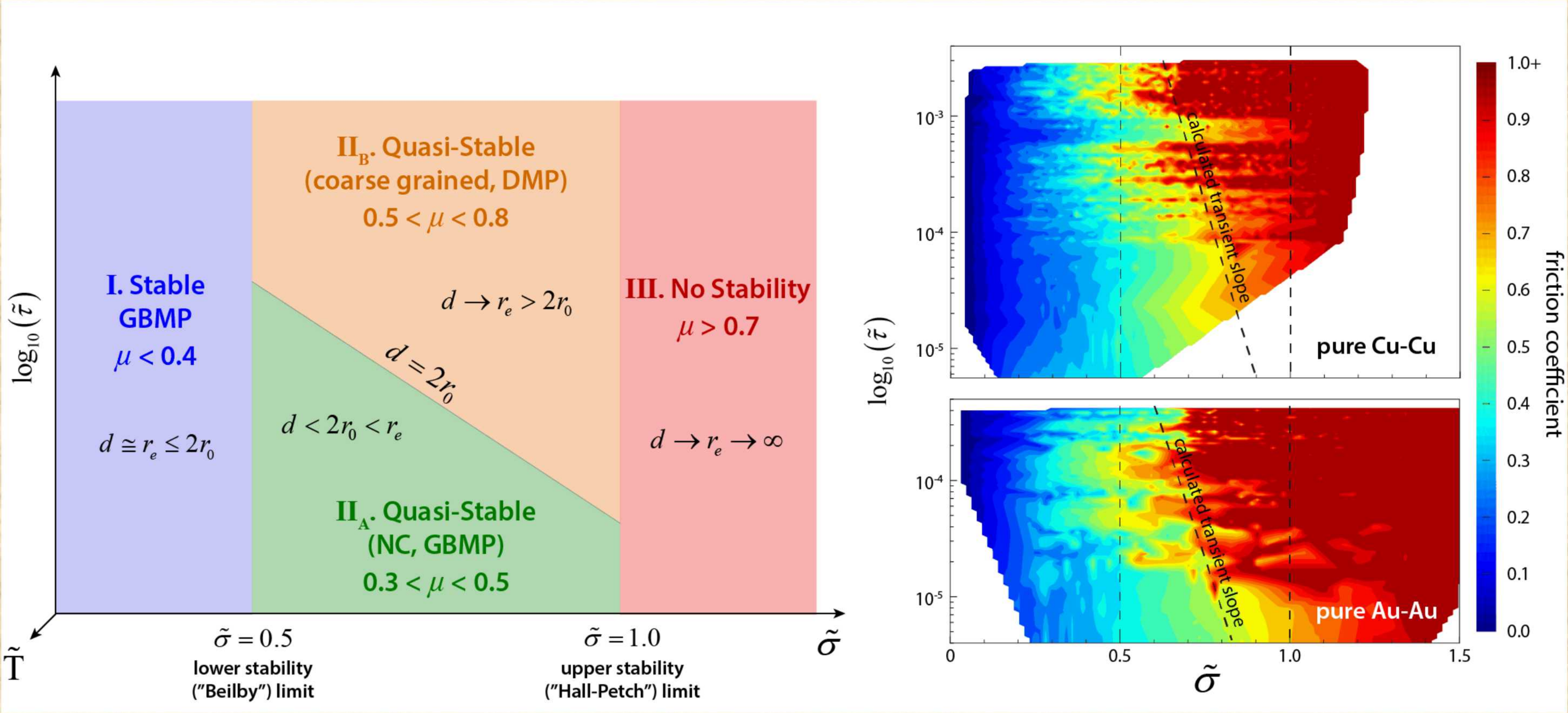
- Self-mated pure copper @ 20^{o}C
- Convert force to surface stress via μ

Plug In Values

property	material system				
	Au	*Cu*	*Al*	*Ni*	*units*
shear modulus, G	27	48	27	76	GPa
Poisson ratio, v	0.44	0.36	0.35	0.31	-
lattice constant, a	4.08	3.61	4.05	3.52	A
Burgers vector, b	2.88	2.55	2.86	2.49	A
SFE, γ_{sf}	45	78	166	128	mJ/m^2
GBE, γ_{gb}	378	625	324		mJ/m^2
HAGB mobility, M_0	3.84×10^{-6}	30	2×10^{-2}		m/s-Pa
HAGB activation energy, Q	1.33	2.01	1.05		$x10^{-19}$ J
calculated parameters					
equilibrium splitting distance, r_0	8.7	5.9	2.0	2.8	nm
σ_∞	312	611	1,117	1,808	MPa
$\sigma(r=2r_0)$	156	306	580	904	MPa

σ_∞ and $2r_o$ are the important derived parameters

Compare the Predictions



- Excellent agreement for multiple different systems
- All predictions purely from materials parameters; no fudging!

Conclusions

- Model accurately predicts stress and time regimes
  - Low stress = UNC with persistent low friction
  - High stress = coarse grained and high friction
  - Intermediate = transient regime with evolving grains and friction
- Feedback loop determines properties
  - μ determines σ, σ determines r and r determines μ
- Connects friction and hardness though atomistic mechanisms
  - Equilibrium dislocation splitting distance
  - Transition between GBMP and DMP

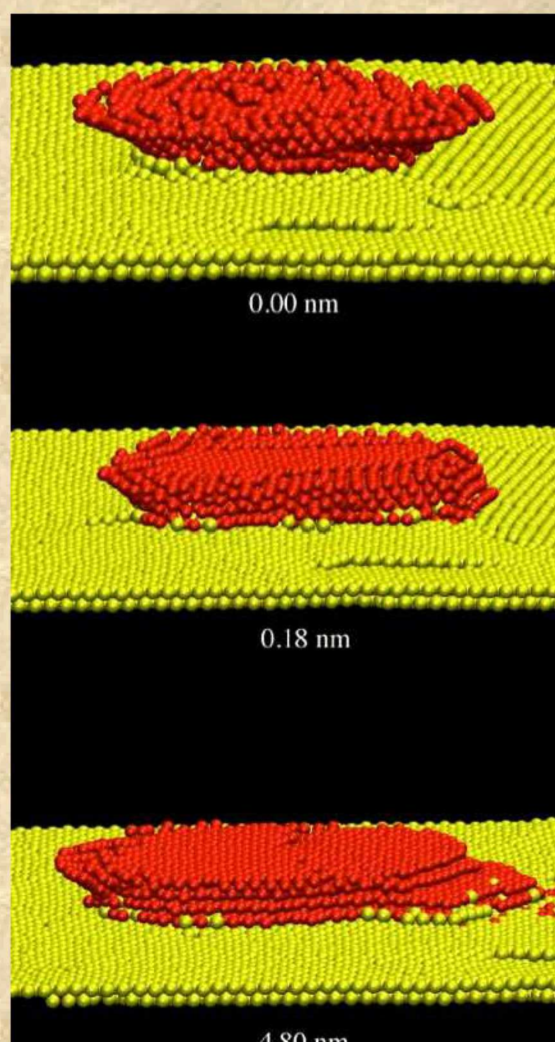
Outlook

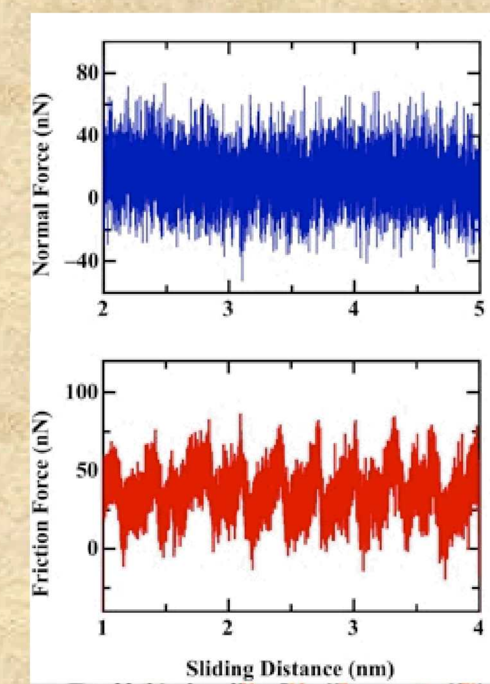
- A lot of places to go from here!
- Define temperature axis (recover Lim & Ashby)
- Provide explanations for current problems (i.e.hip implants)
- Use model to back out mobilities and stacking fault energies
  - Understand effects of alloying
  - Design new alloys
  - Intrinsic stability?

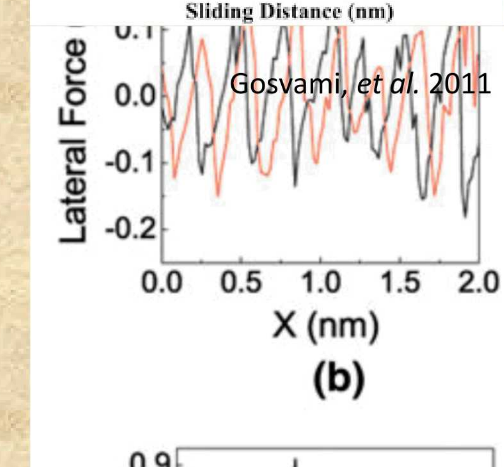
Backup Modeling Slides

Pure Ag Shows Stick/Slip

- Stick-slip in friction signal
- Layering / ordering of tip atoms
- Shear induces commensurate contact
- Commensurability => high friction
- Does alloying suppress this?

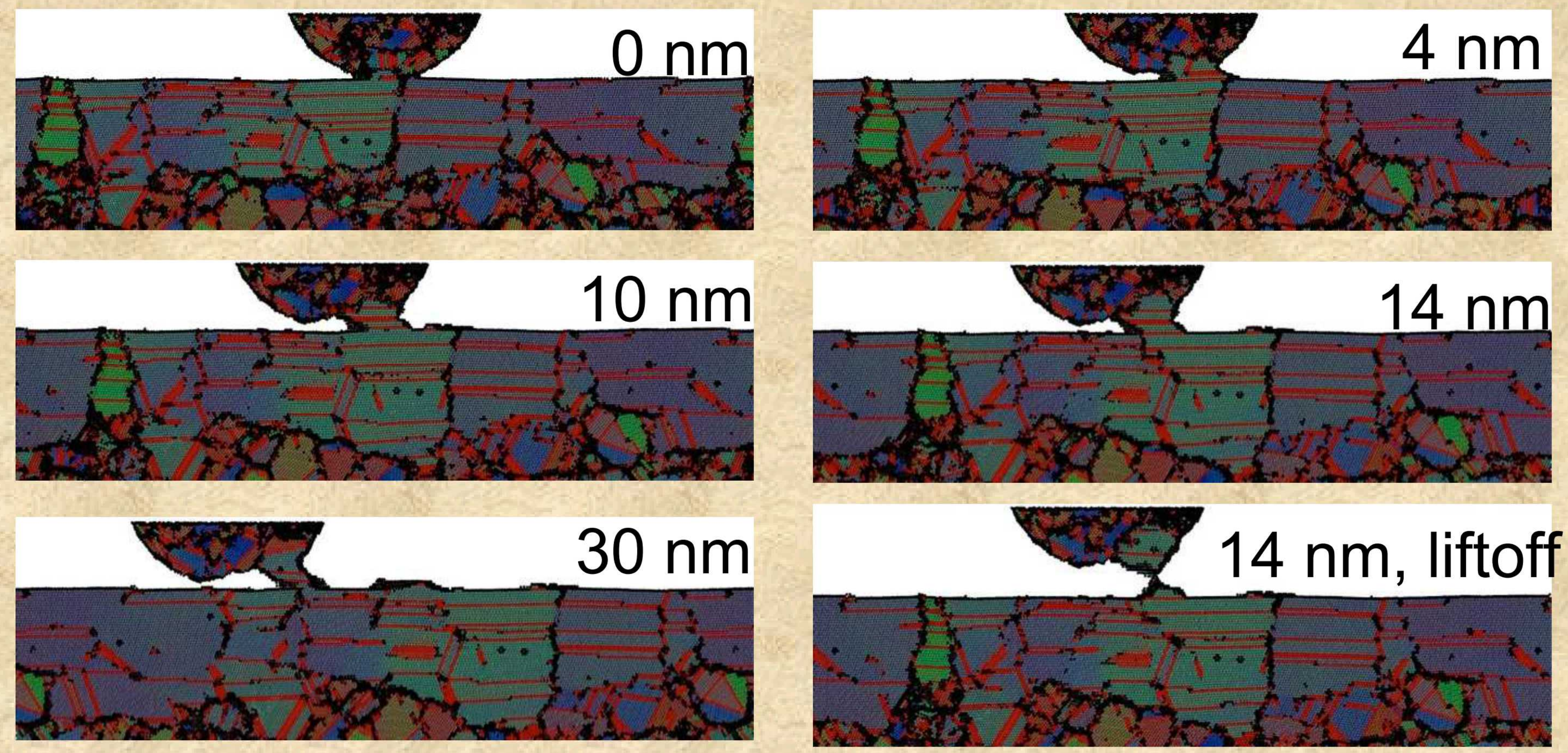






Gosvami, *et al.* 2011

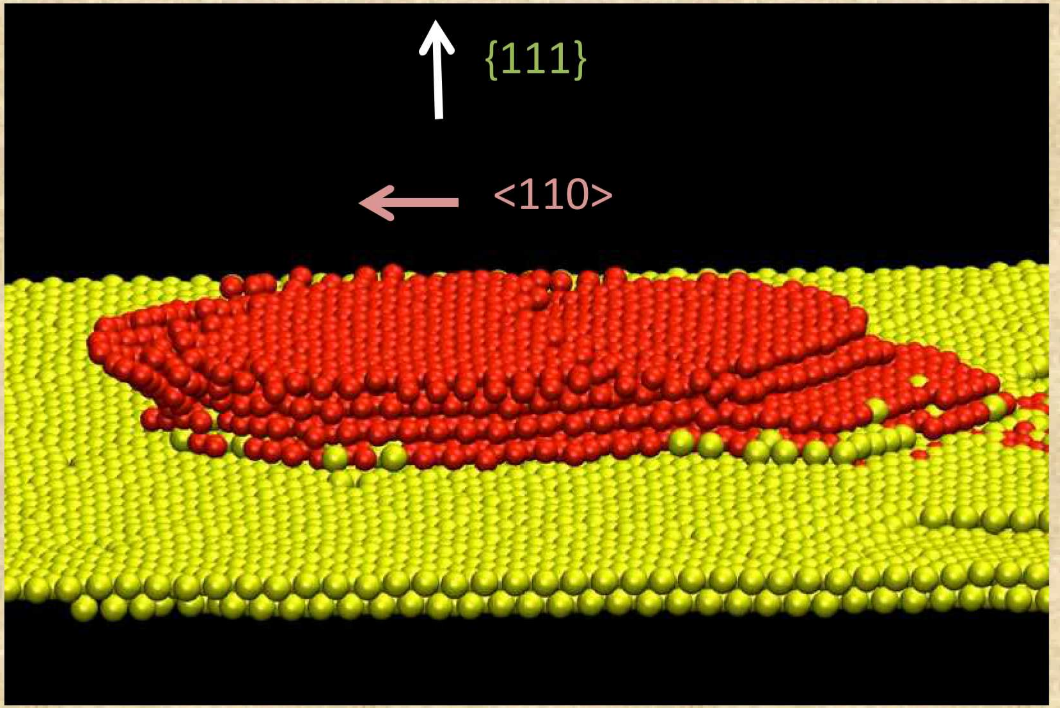
Grain Level Snapshots



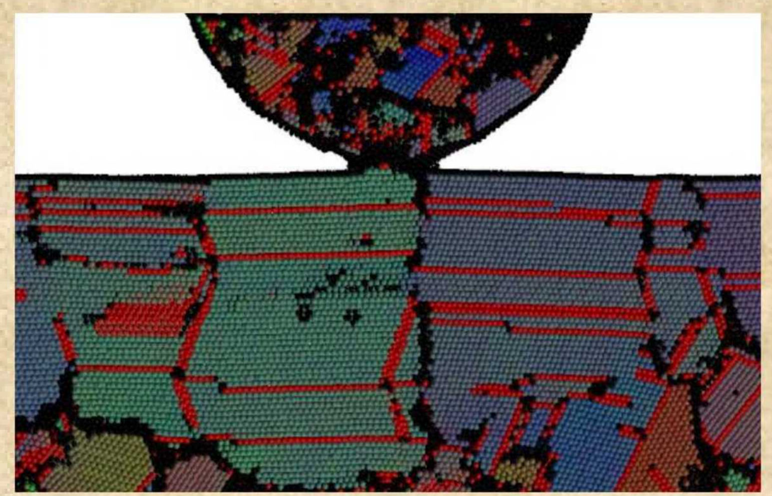
- Initially distinct grains
- After shear (adhesive load), coalescence – now a mode II crack
- Single grain forms across interface – stress induced grain growth

Shear Accommodation through FCC Slip Systems

- Mechanism is due to grain growth
- Slip along {111} plane in <110> direction
- Ductility, plastic deformation
- *Dislocation mediated plasticity (DMP)*

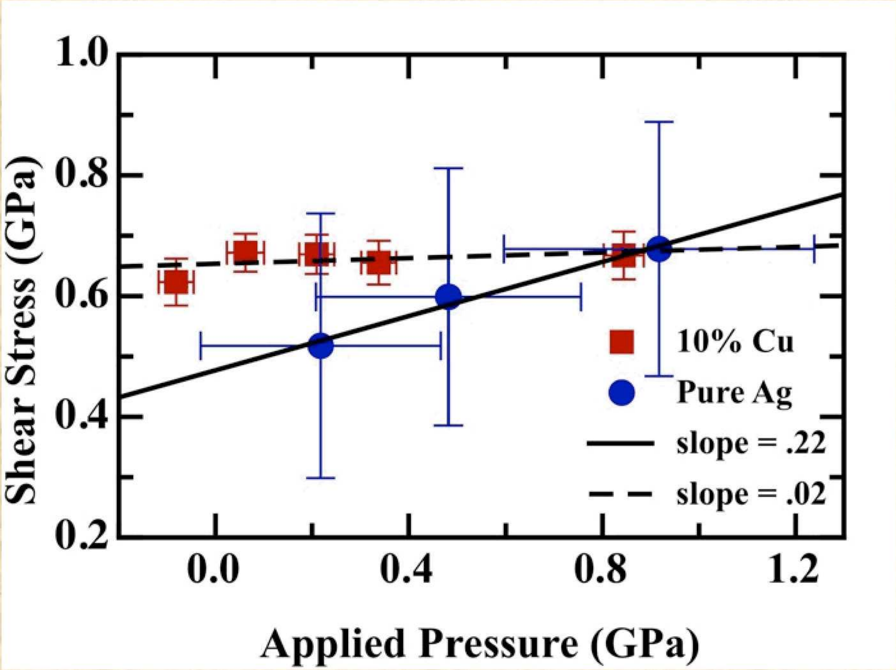


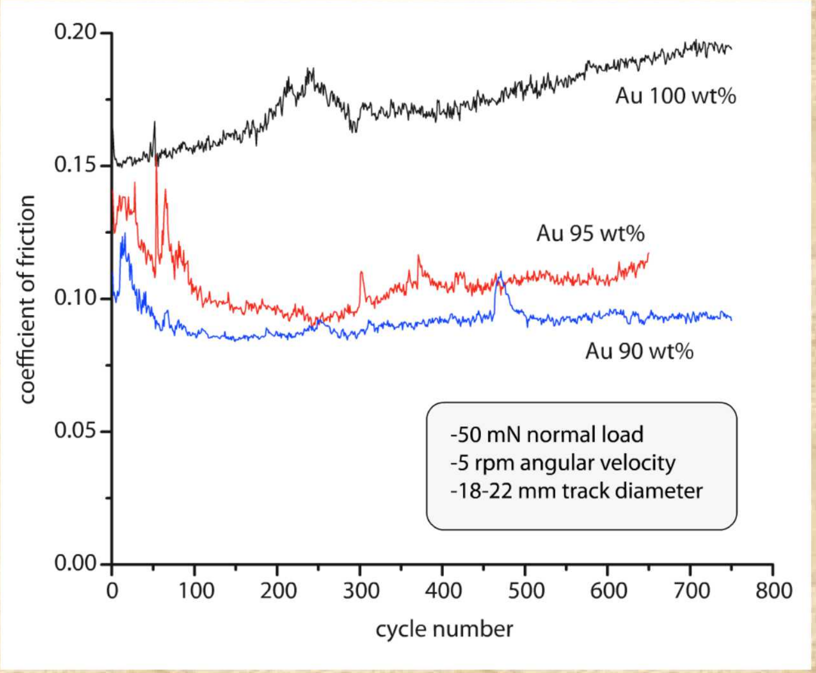
Alloying Suppresses Grain Growth



- Experiments
  - Alloy element collects at grain boundaries
  - Stabilization of grain boundaries through solute drag
  - Prevents growth
- Simulations
  - Grain growth is prevented due to solute drag, enforced by lattice mismatch
  - Sliding interface is now a stabilized grain boundary (GBS)
  - Non-commensurate interface = lower friction
  - Grain growth results shown later

Comparison of Friction





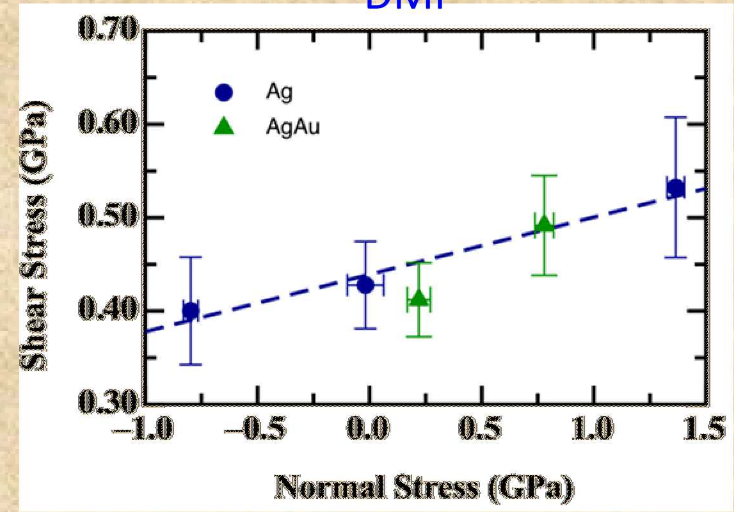
Courtesy: WG Sawyer, U. Florida

- Alloy has lower friction
- Qualitative agreement with experiment
- Pseudo-quantitative: Factor of 3-4 between slab & tip results for pure Ag
  - Also seen in our previous work, & Harrison's work on different systems
  - "Tip" friction: $\mu(Ag) \cong 0.22$ $\mu(AgCu) \cong 0.08$

Different sliding mechanisms lead to different friction coefficients
DMP = higher friction **GBS = lower friction**

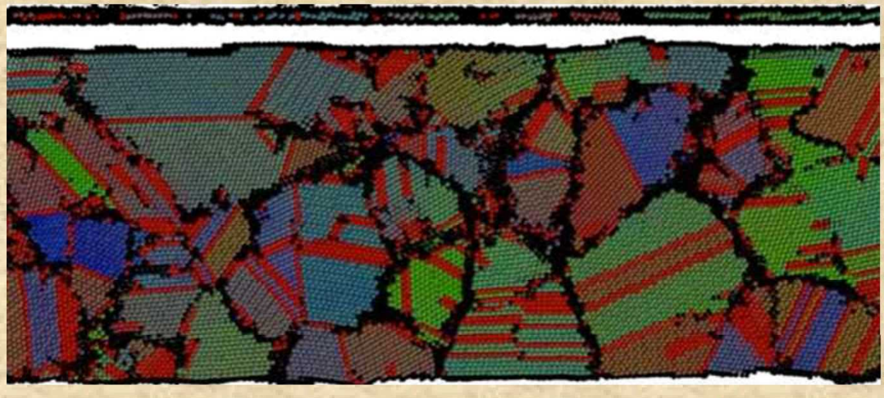
Enforcing the Different Mechanisms

DMP



GBS

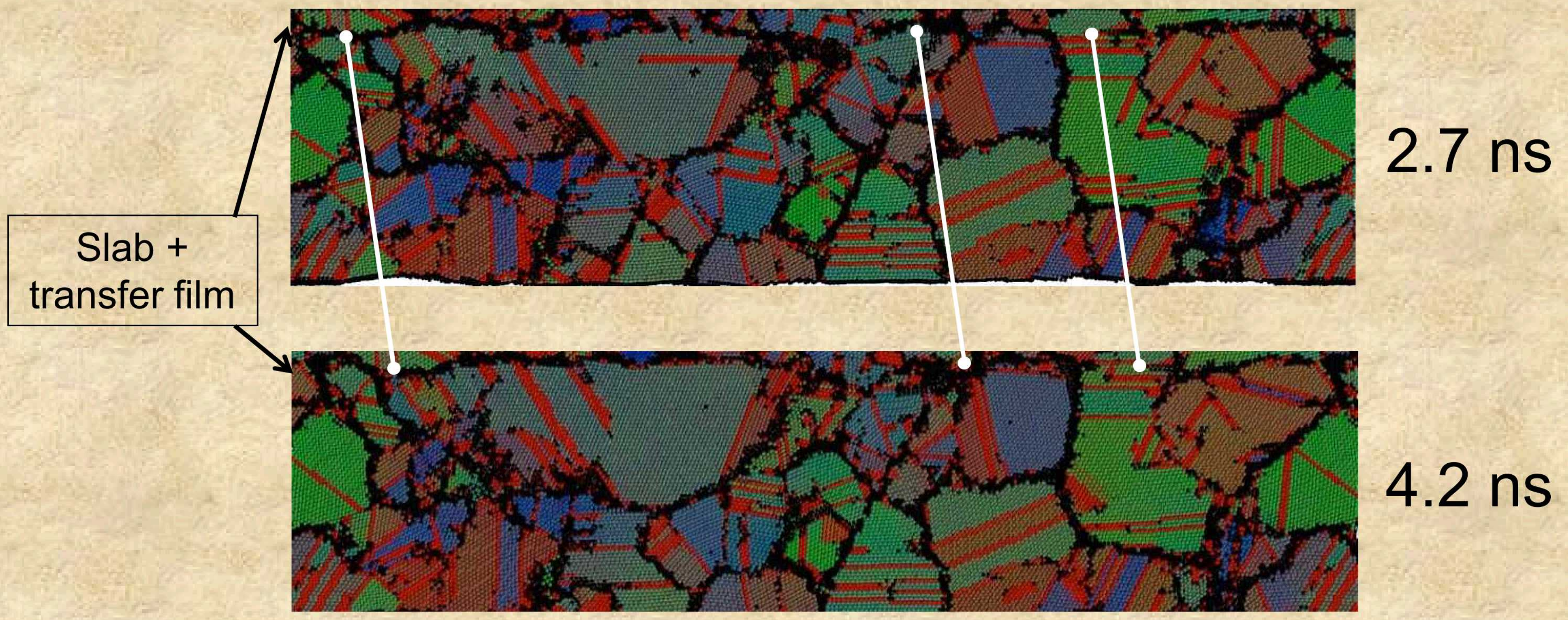
rigid



dynamic

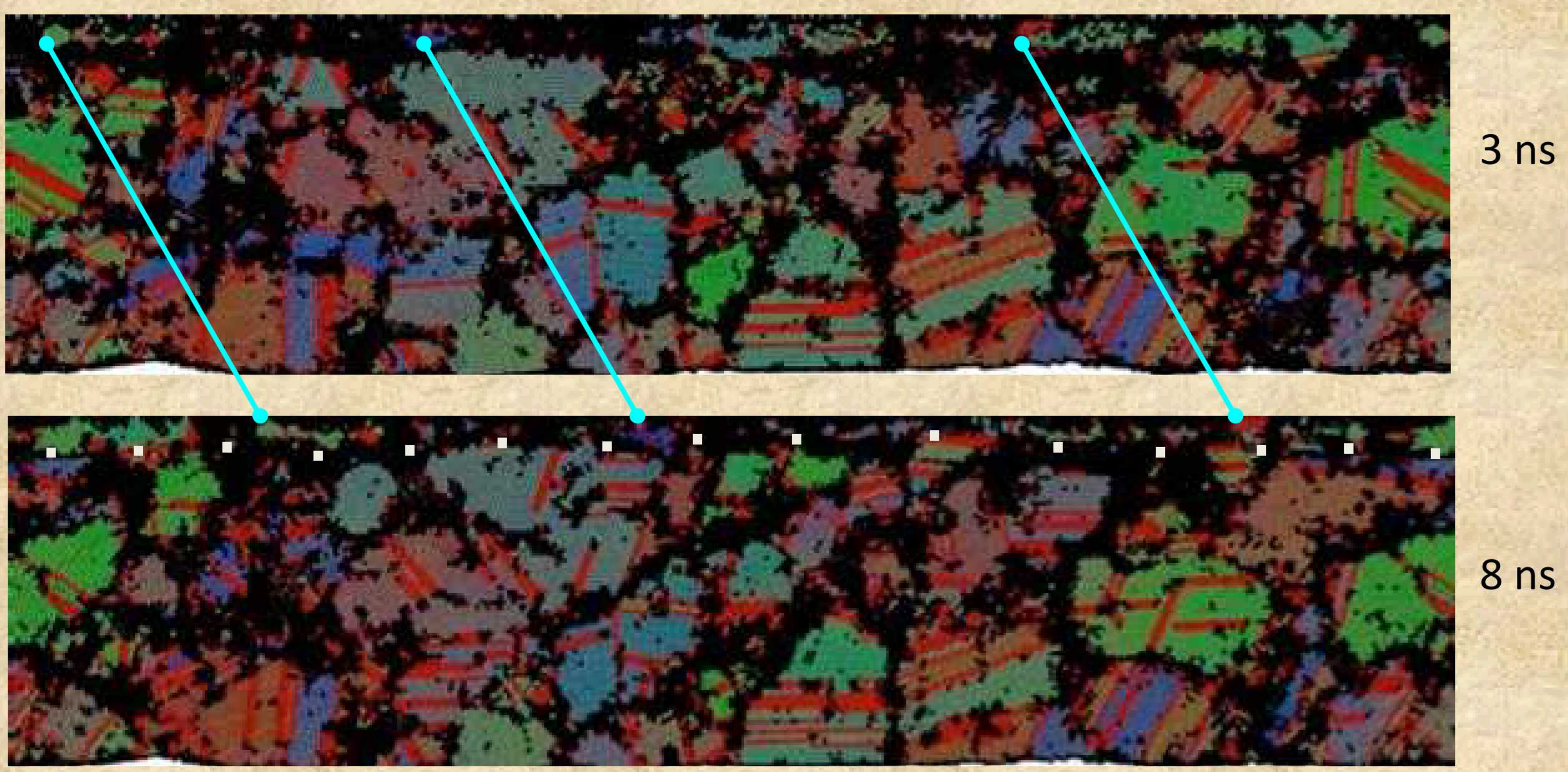
- Demonstrate that same mechanism = same friction
  - Force alloy to use DMP
    - AuAg alloy
    - Pure Ag (a=4.09) and alloy with Au (a=4.08) show indistinguishable friction
  - Force pure metal to use GBS – rigid, infinite, nanocrystalline slabs
- Rigid slabs suppress grain growth
- No plowing is possible, unlike with rigid tips

Rigid Slab – Pure Ag



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

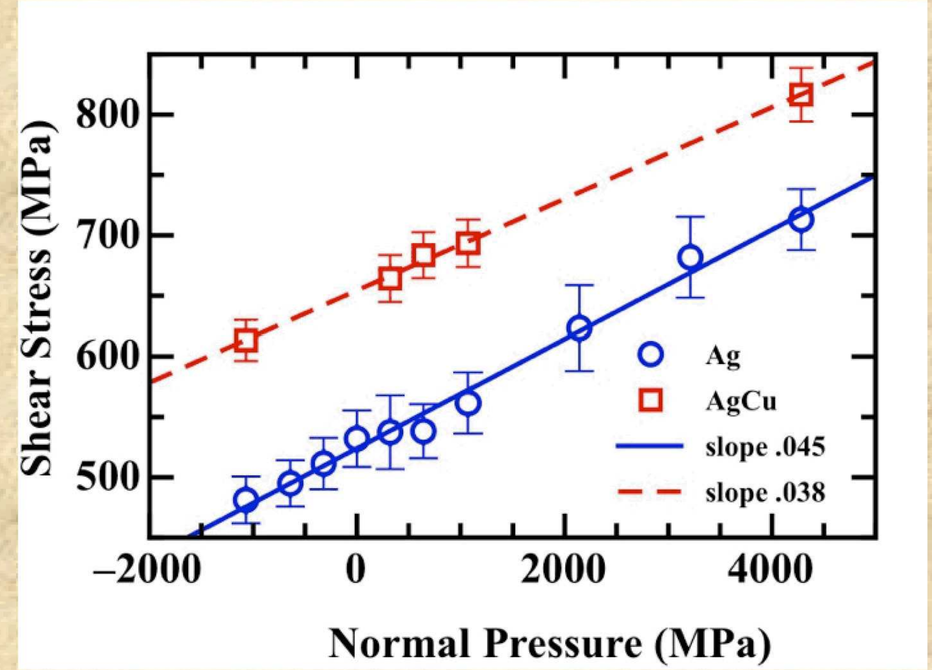
Rigid Slab – Alloy



- Alloy slides at boundary, but also throughout substrate

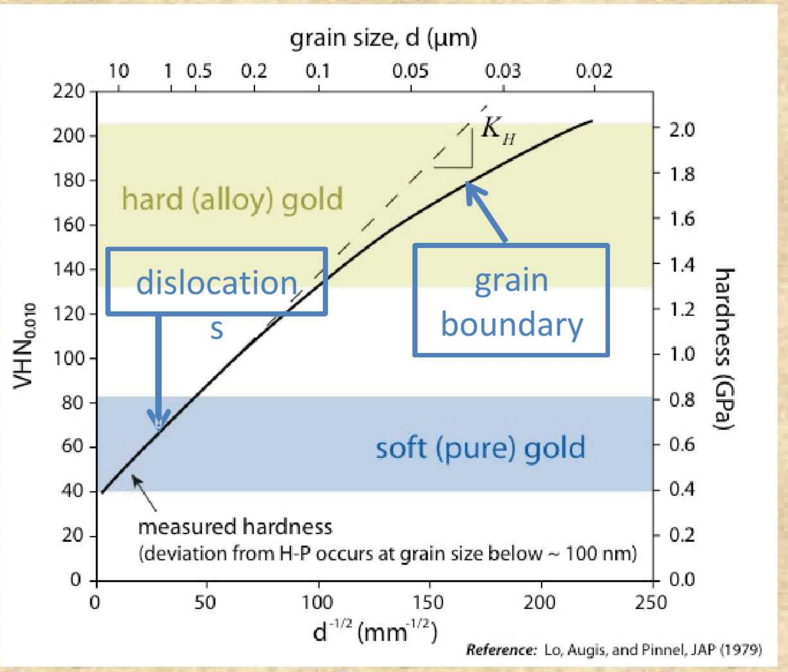
Rigid Slab Friction

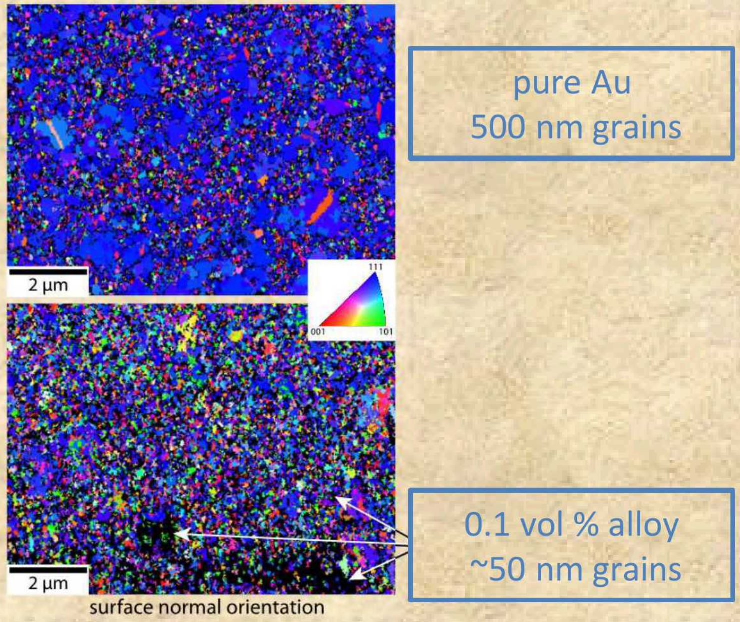
- μ essentially identical ($\cong$ 0.04)
  - Ag, AgCu with rigid slabs
  - AgCu with dynamic slab
  - Grain boundary sliding leads to lower friction



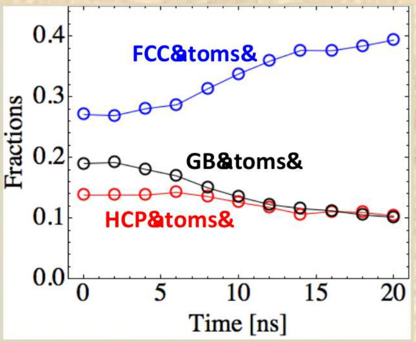
- Suppression of grain growth changes the sliding mechanism
  - Allowing GG = DMP
  - Disallowing GG = GBS

Grain Growth Suppression

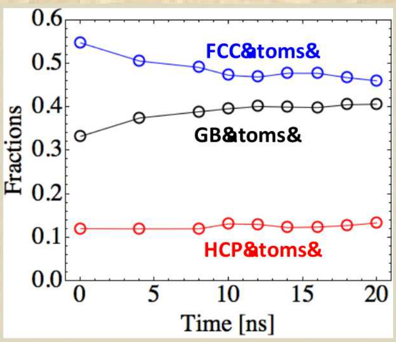




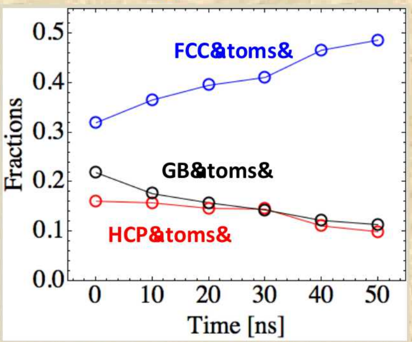
pure Ag



AgCu alloy



AgAu alloy



- Experiments: alloys stabilize grain boundaries, prevent grain growth
- Simulations: alloys prevent grain growth through lattice mismatch
- Both: Lack of grain growth avoids formation of commensurate interface, lowering friction