SAND2013-3490C

Atomic Origins of Friction Reduction in Nanocrystalline Metal Alloys and Composites

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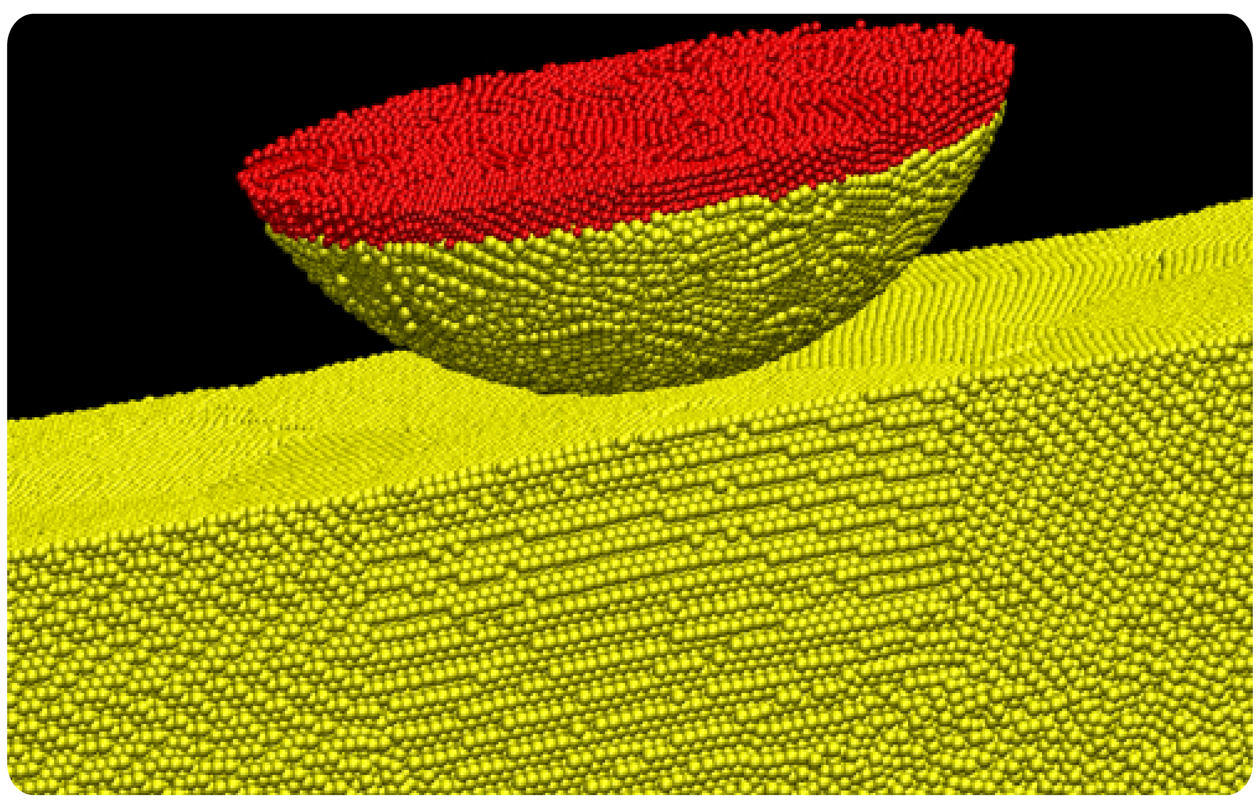

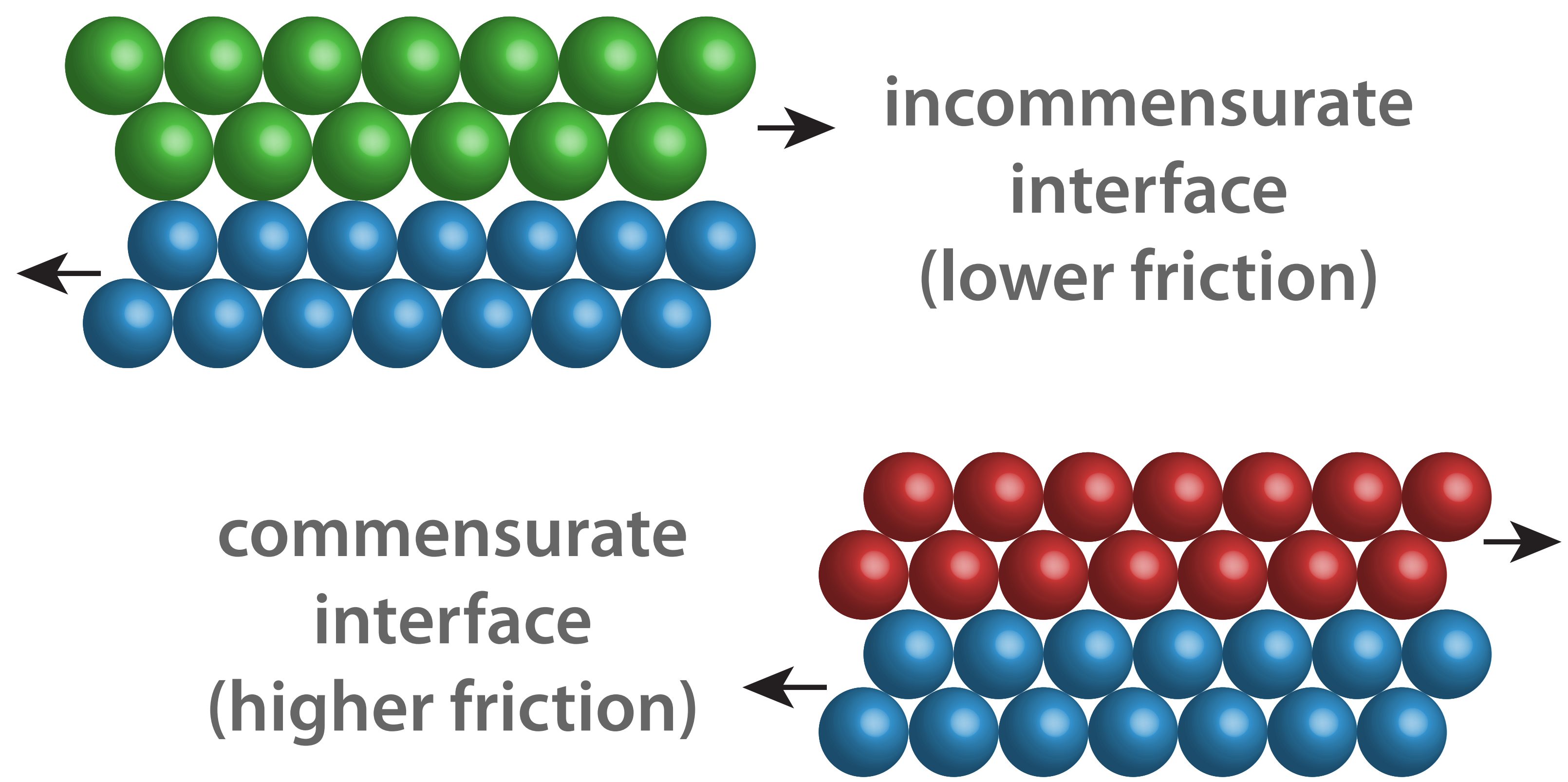

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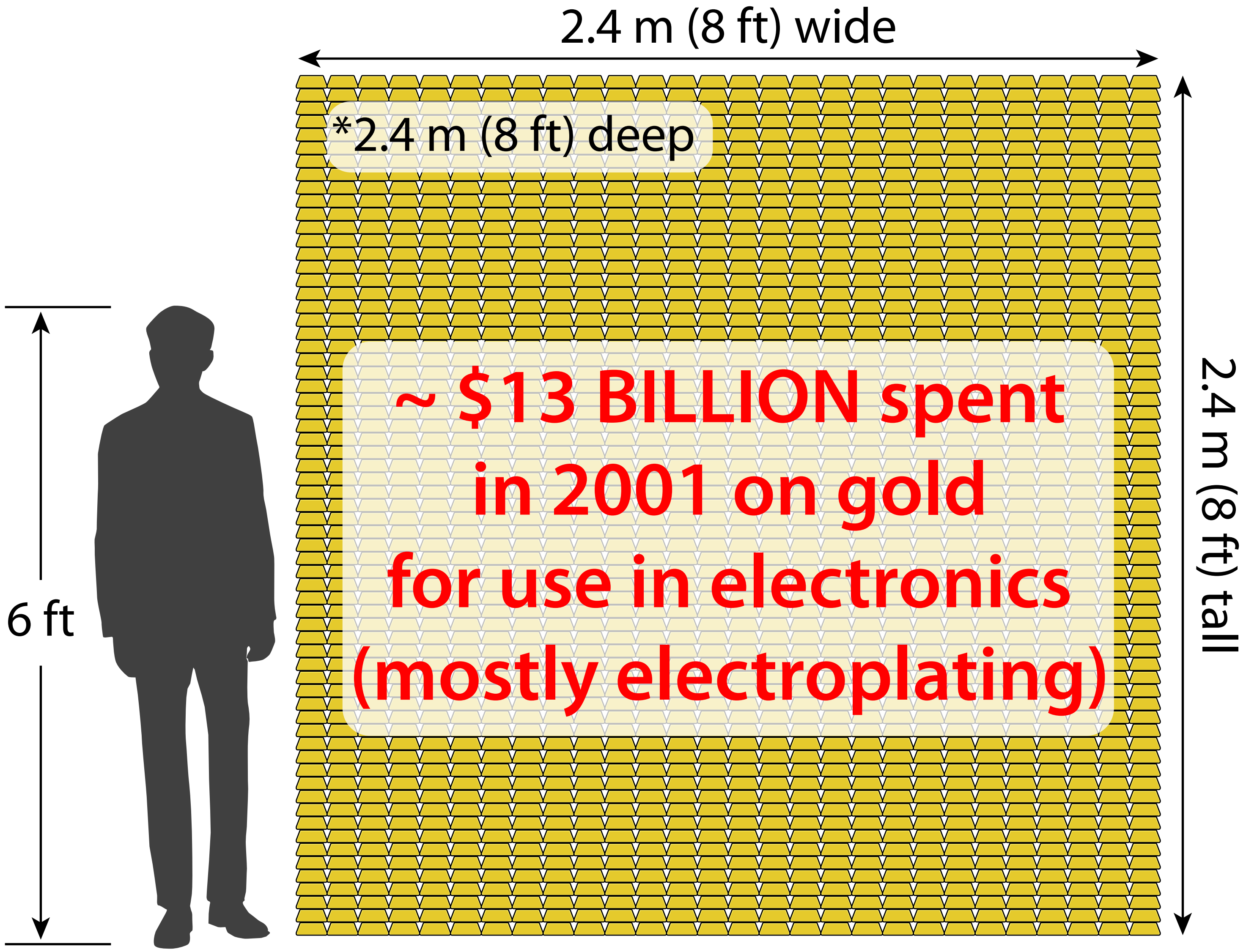
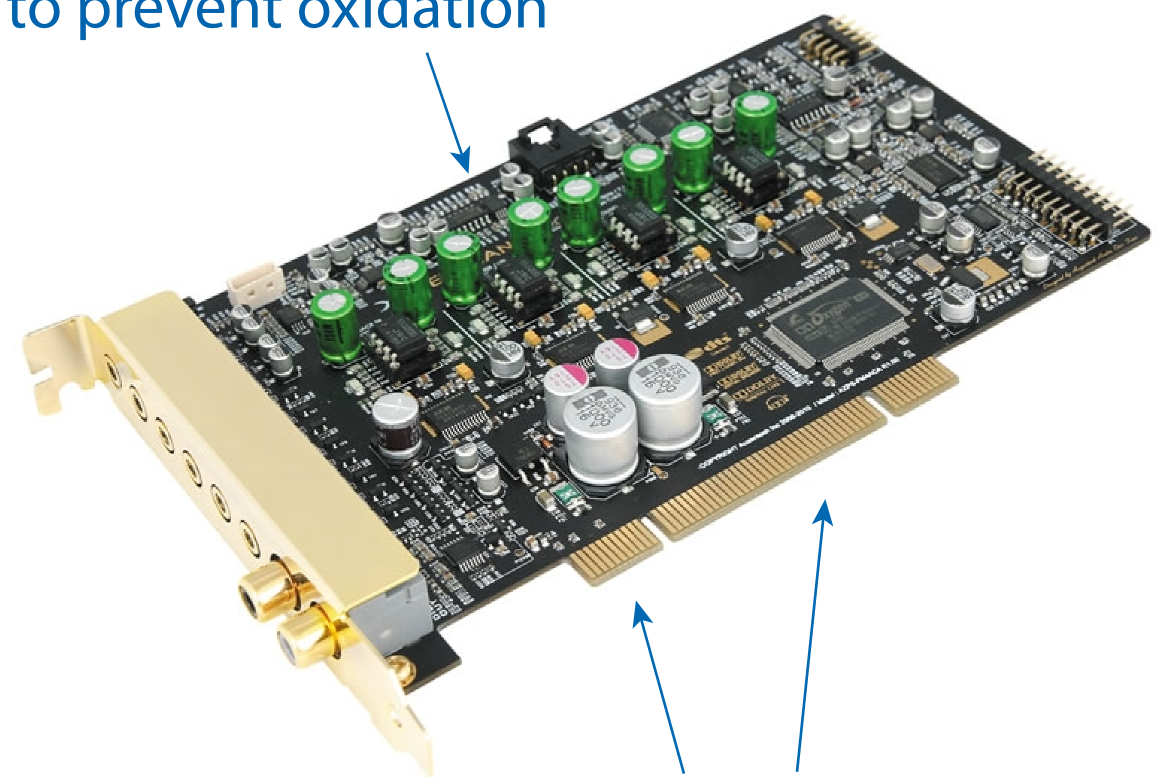
280 METRIC TONS of gold used in 2001 on electronics related applications, most of it in electroplated connectors and contacts (0.15% of world supply per year)

equivalent to a cube comprised of ~23,333 standard gold bars (12 kg/26.4 lb each):



Ni or Co hardened Au films (electroplated and electroless) protect copper connectors in many printed circuit boards (PCBs)

200 - 500 nm thick electroless plating on soldered connections to prevent oxidation

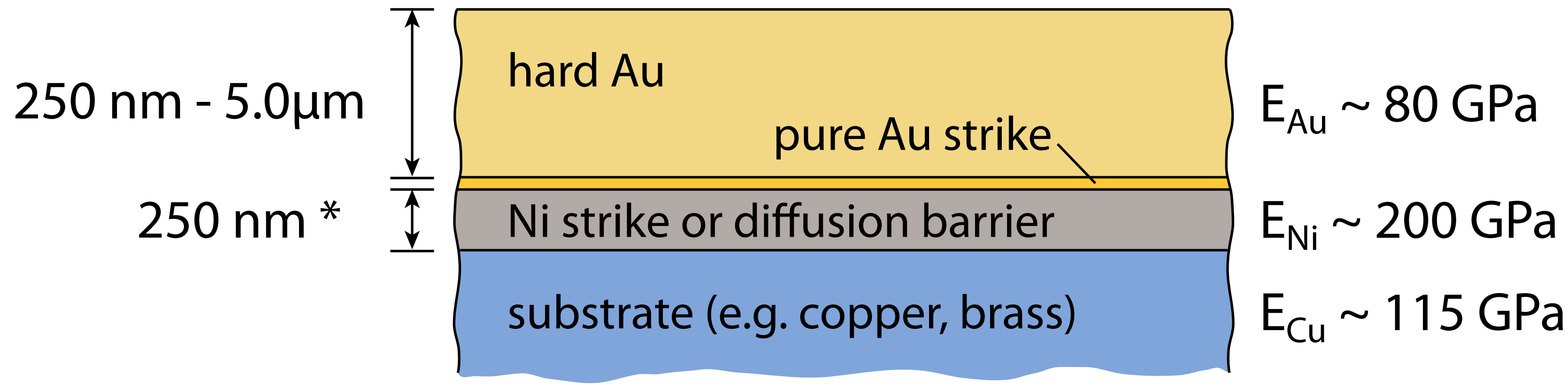


1 - 3 μm thick electroplate used on edge connections that are susceptible to wear

Reference: Gold Survey, Gold Fields Mineral Services Ltd., 2001

hard gold films are defined by the following specifications:

type (purity) / code or grade (hardness) / class (minimum thickness)



* if operating at high temperature and on a Cu substrate then > 1.2 µm is recommended

	type	suggested applications (ASTM)
> 99.7% Au	I	general-purpose, high-reliability electrical contacts
(hardest) > 99.0% Au	II	general-purpose, wear resistance; low temperature only
(softest) > 99.9% Au	III	soldering; limits impact of oxidation of codeposited material
(softest) > 99.9% Au	IIIA	semiconductor components, nuclear eng., high temperature

more Ni/Co/Fe content (in the 0 to 2 vol. %) → ***increased hardness*** → ***reduced wear and increased electrical contact resistance***

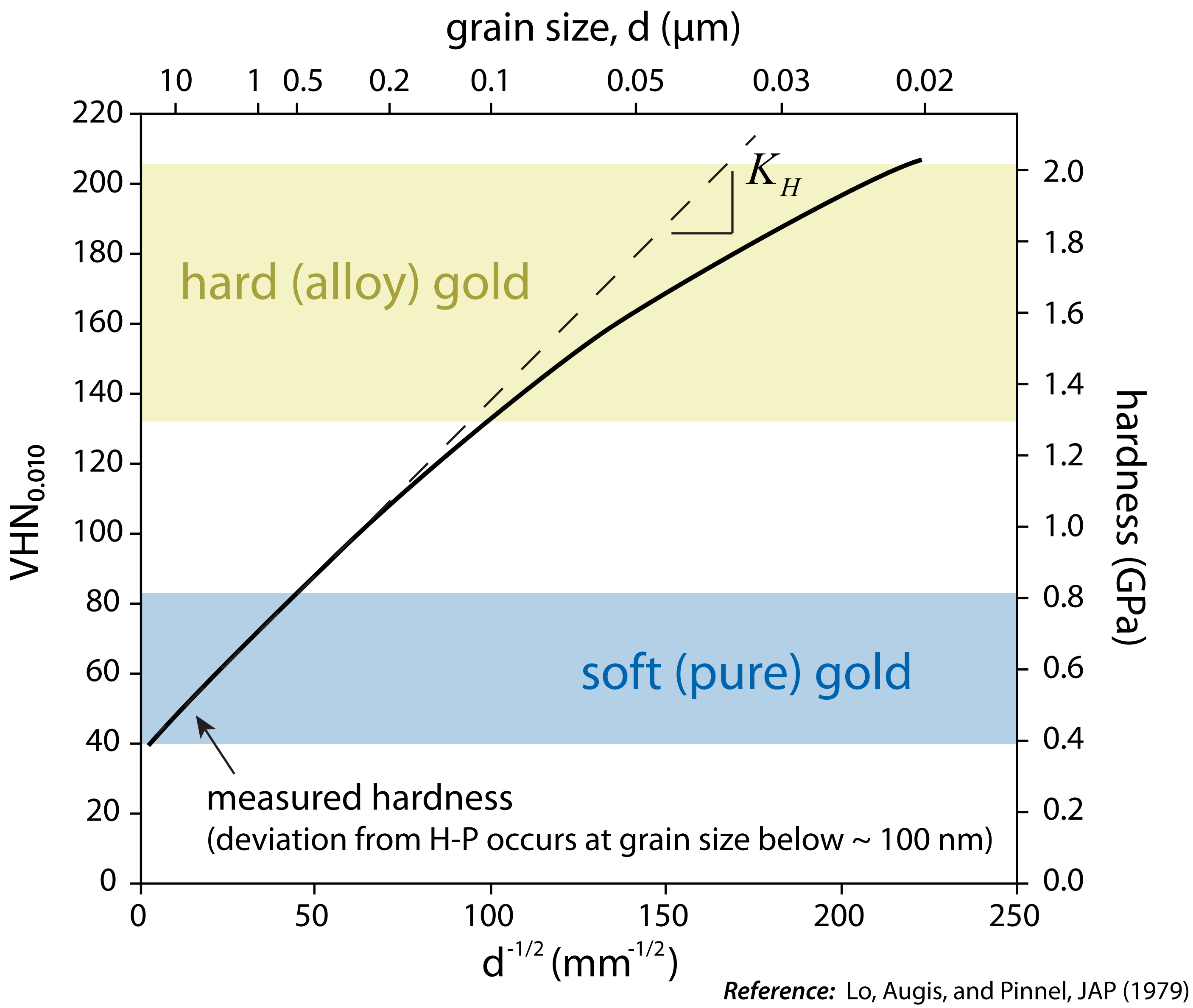
For metal contacts the real area is a function of hardness and contact force (Bowden & Tabor, 1939):

$$A_r \cong \frac{F_n}{H}$$

... adhesion related to real area.

Hardness of hard gold is primarily the result of Hall-Petch strengthening (Lo, Augis, Pinnel, JAP 1979):

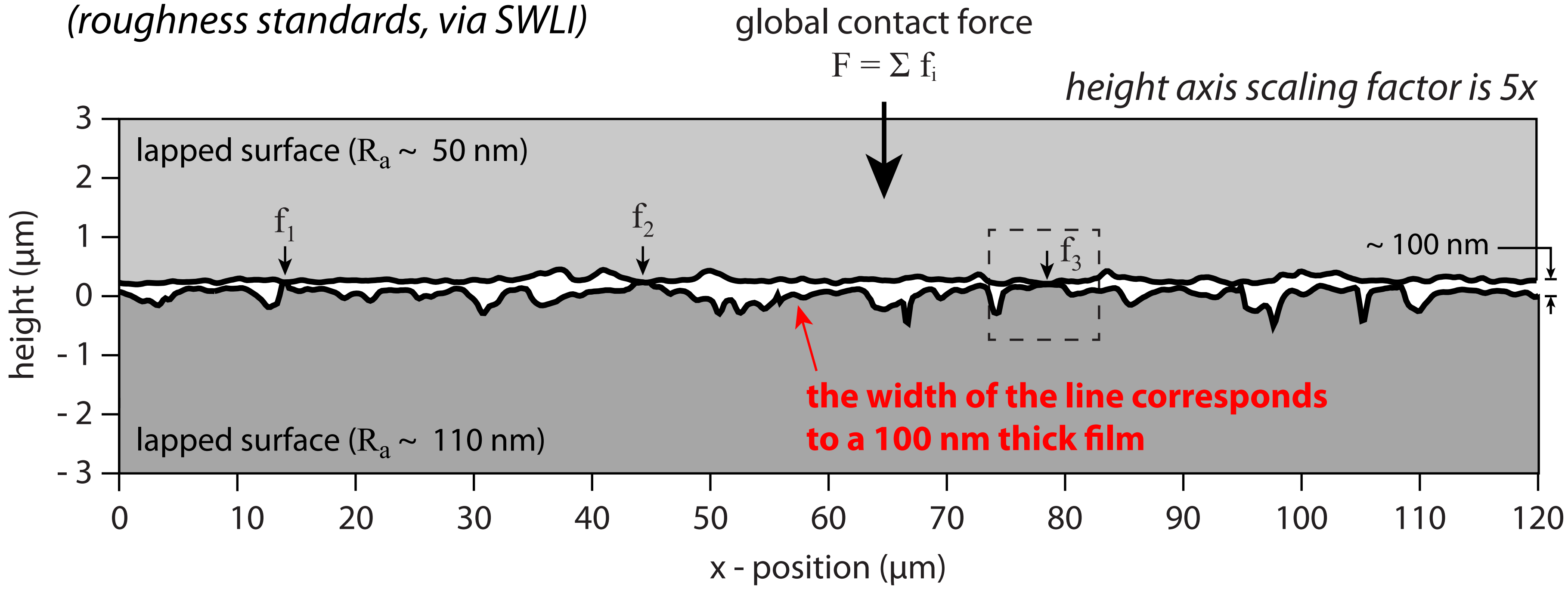
$$H = H_0 + K_H d^{-1/2}$$

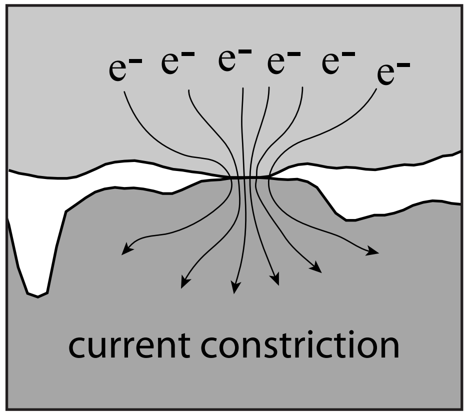


Reference: Lo, Augis, and Pinnel, JAP (1979)

Example of actual surface roughness:

(roughness standards, via SWLI)





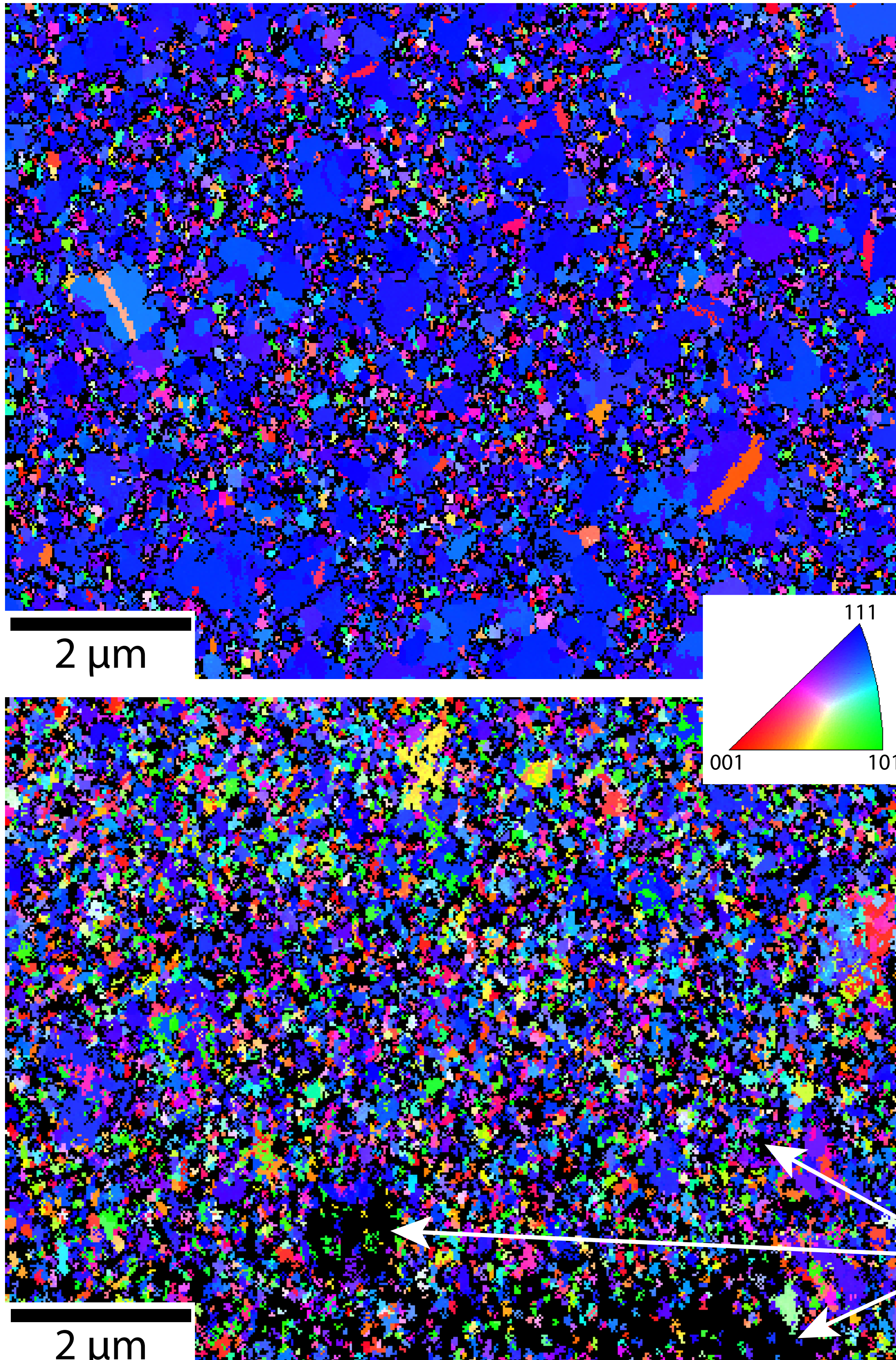
constriction of electrical current leads to **large** local current density (~ 1-100 MA/cm^2 is typical!)

Film surface EBSD maps of pure and 0.1% alloy gold reveals 5x grain size reduction

(EBSD = electron backscatter diffraction)

pure gold film
(highly textured)

pure gold grain size was bimodal and textured in the surface normal direction, with
average grain size > 500 nm



surface normal orientation

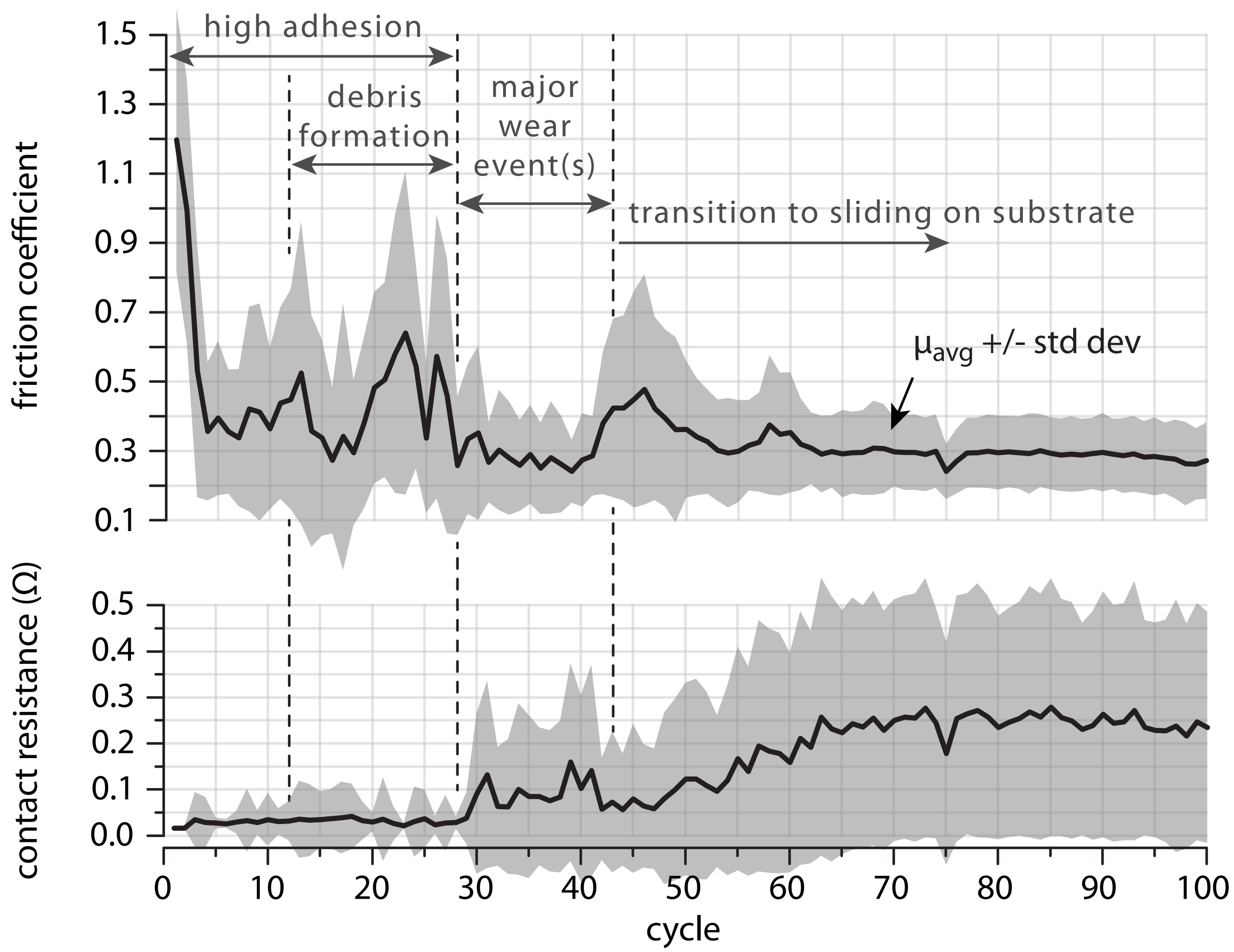
0.1 vol. % alloy
(random texture)

gold nanocomposite grain size was significantly smaller and not preferentially oriented, with an
average grain size ~ 100 nm

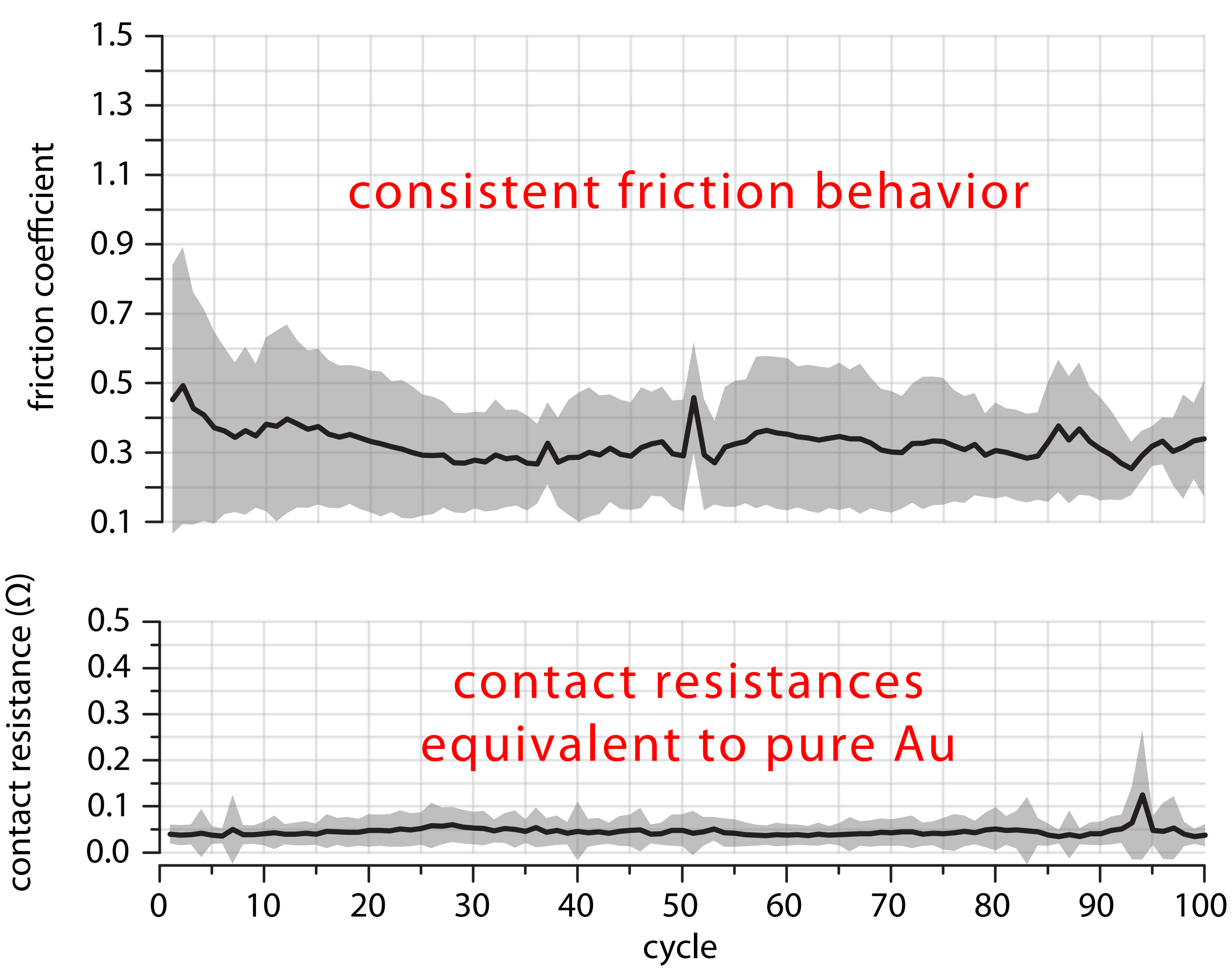
black pixels imply regions with grain sizes < 50 nm

Alloying produces more consistently "low" friction & contact resistance

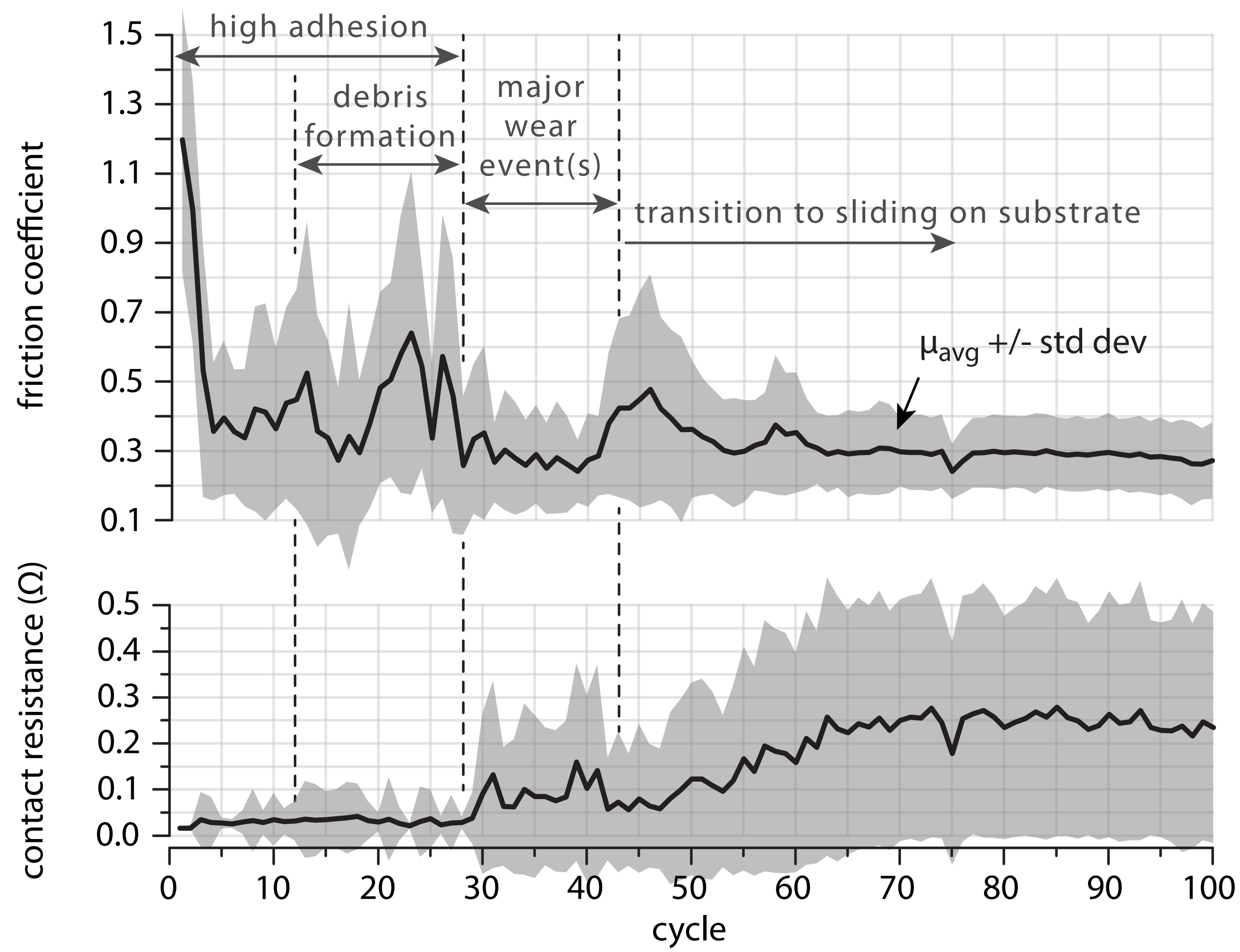
Neyoro G rider sliding against a pure Au film



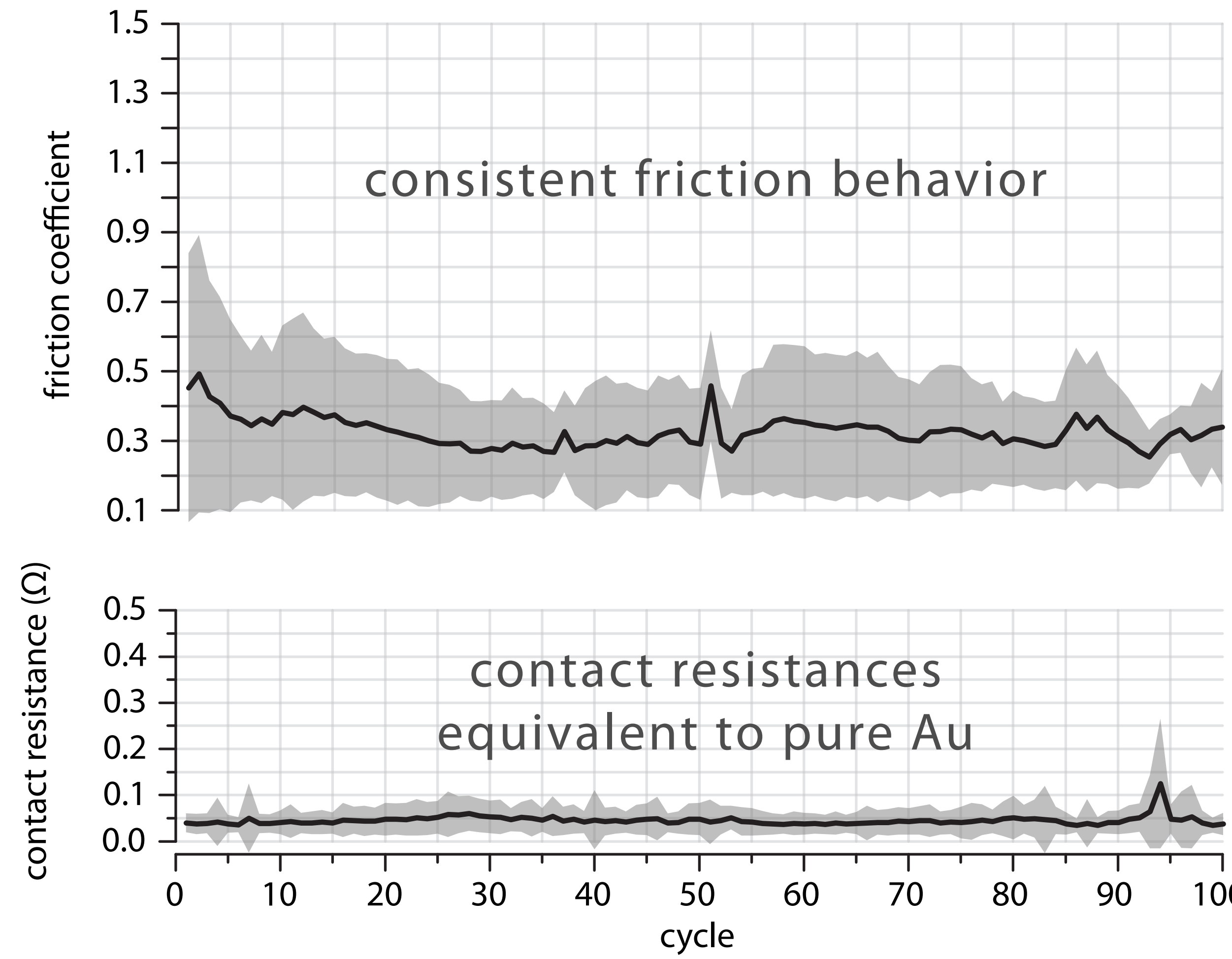
Neyoro G rider sliding against a "hard" (alloyed) 98% Au film



Neyoro G rider sliding against a pure Au film

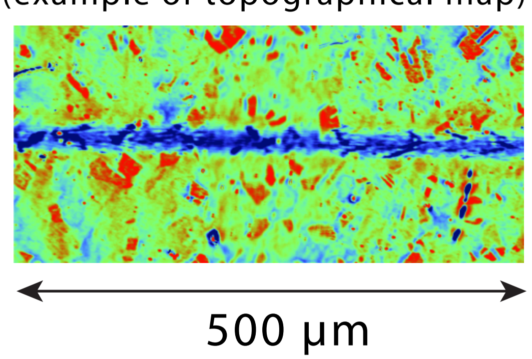


Neyoro G rider sliding against a 98% "hard" (alloyed) Au film

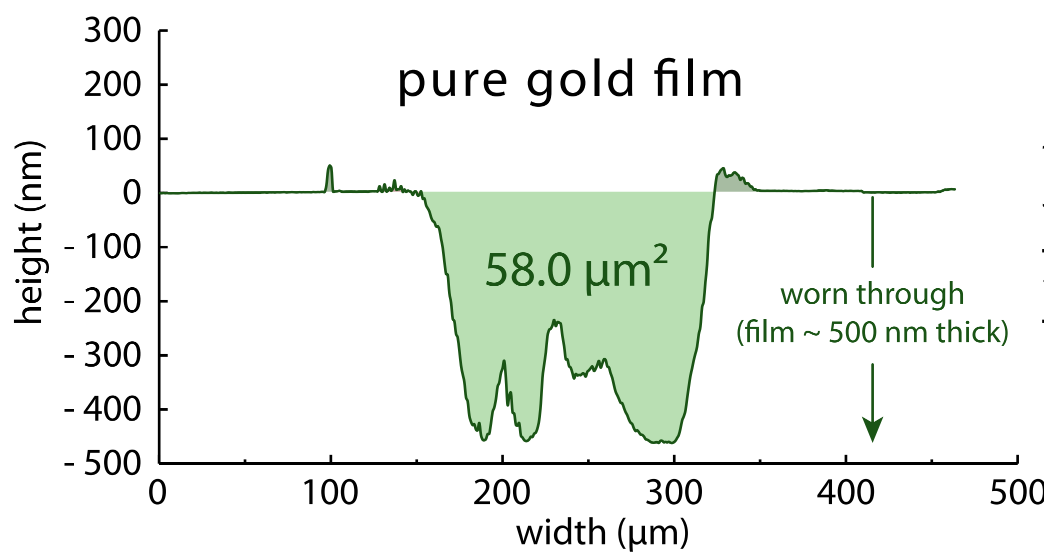


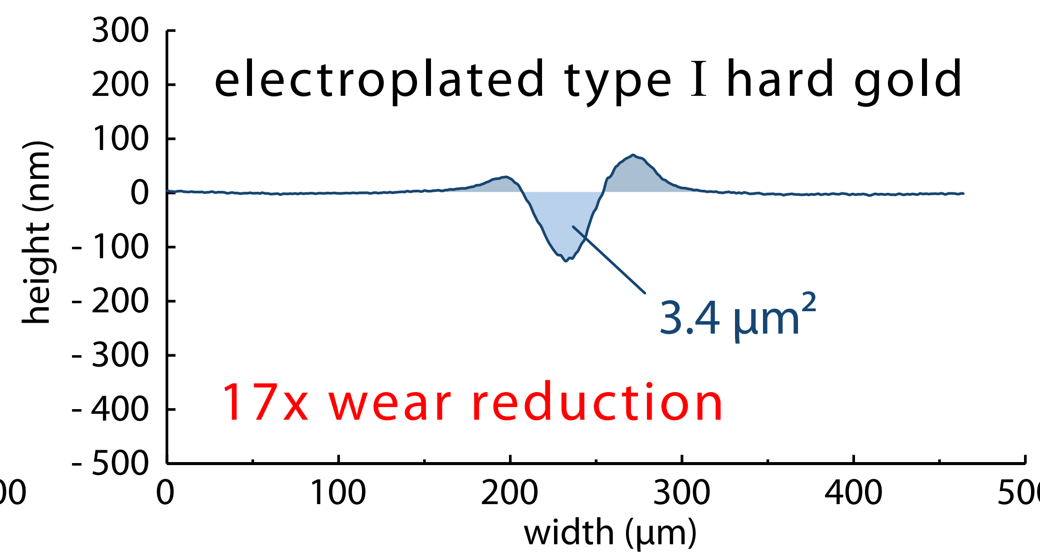
average wear track cross-section in same sliding conditions against Neyoro G rider:

(example of topographical map)



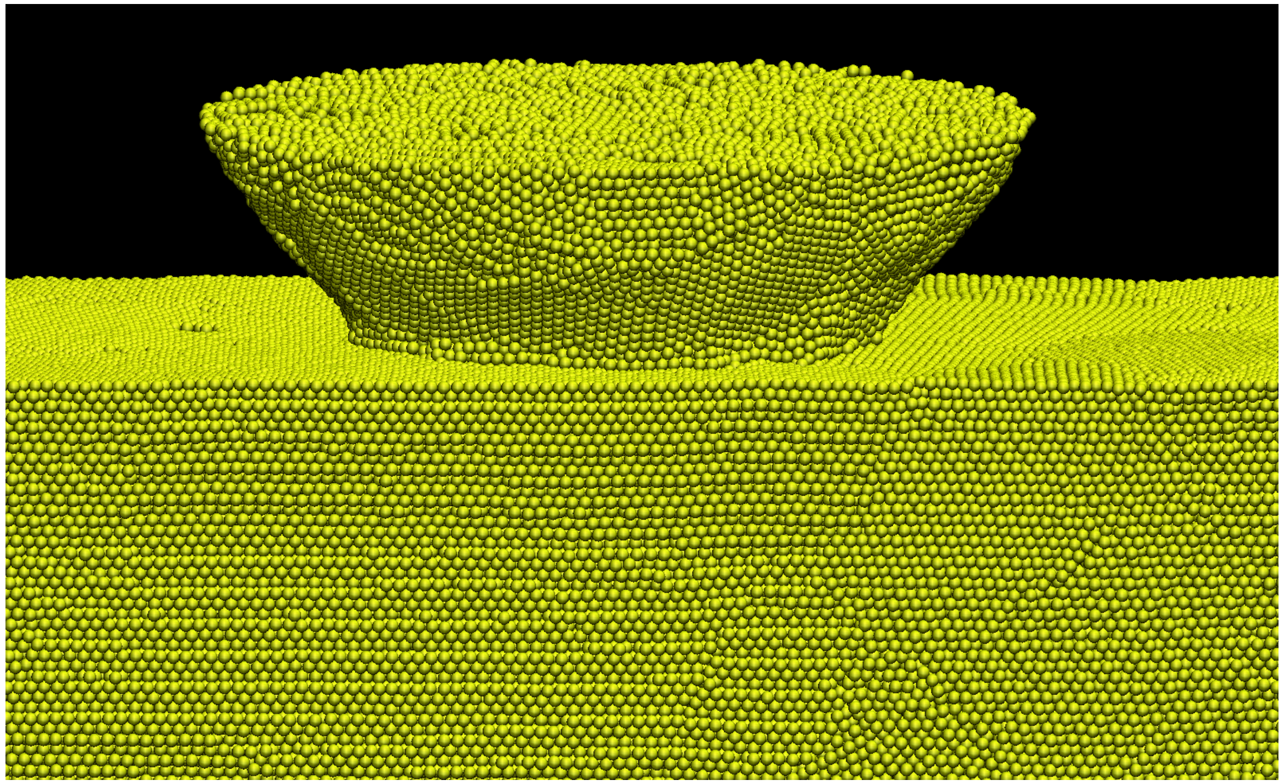
average linescans over 50% of wear track length

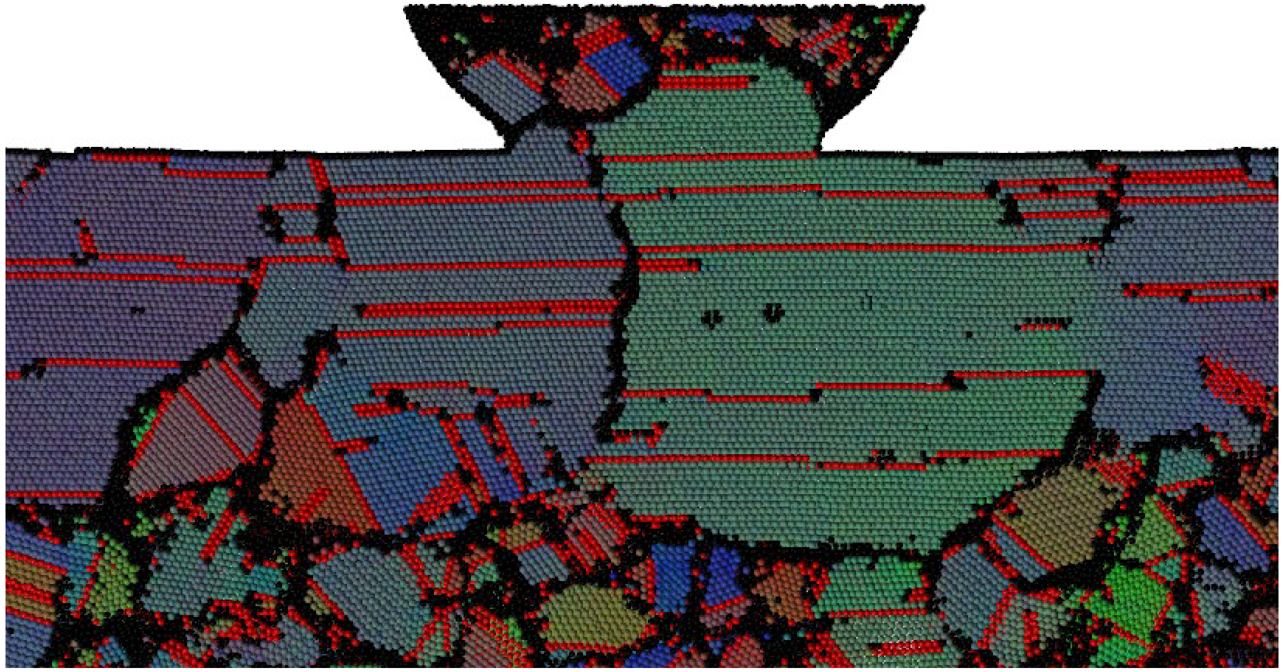




Question

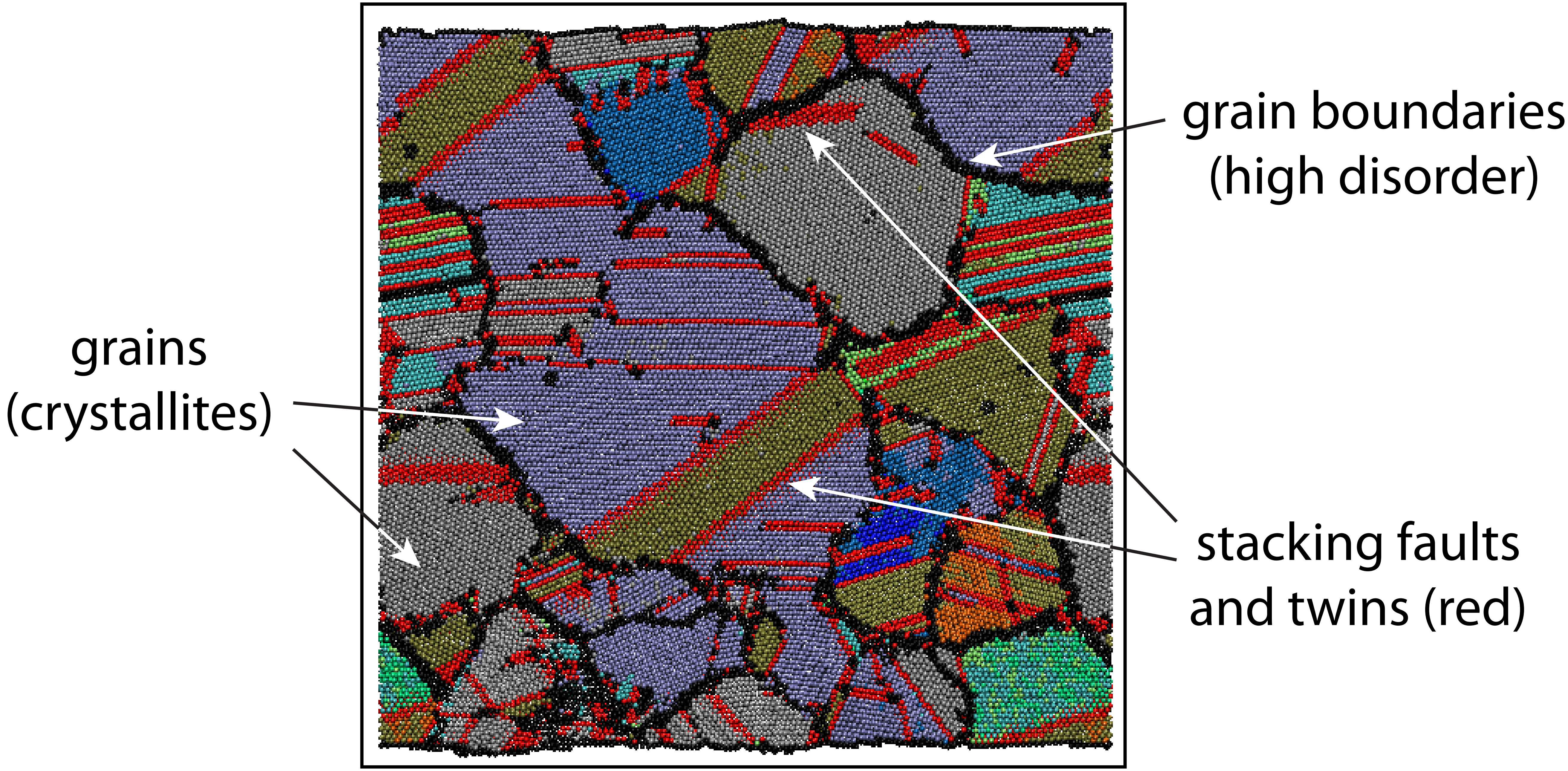
What is the atomic origin of reduced friction/wear?





Approach

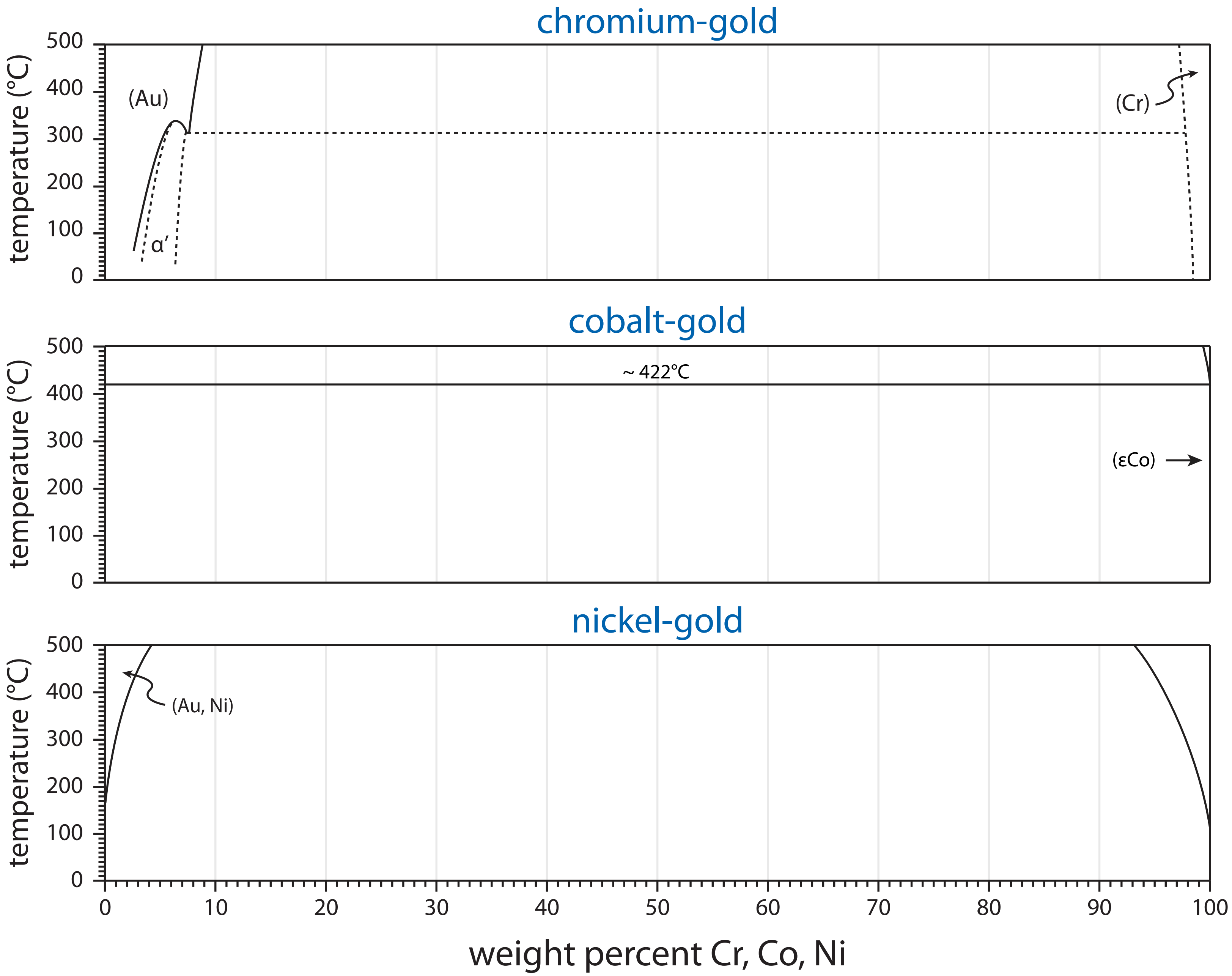
Large scale MD simulations
utilizing embedded atom method
(particularly suited to metals)

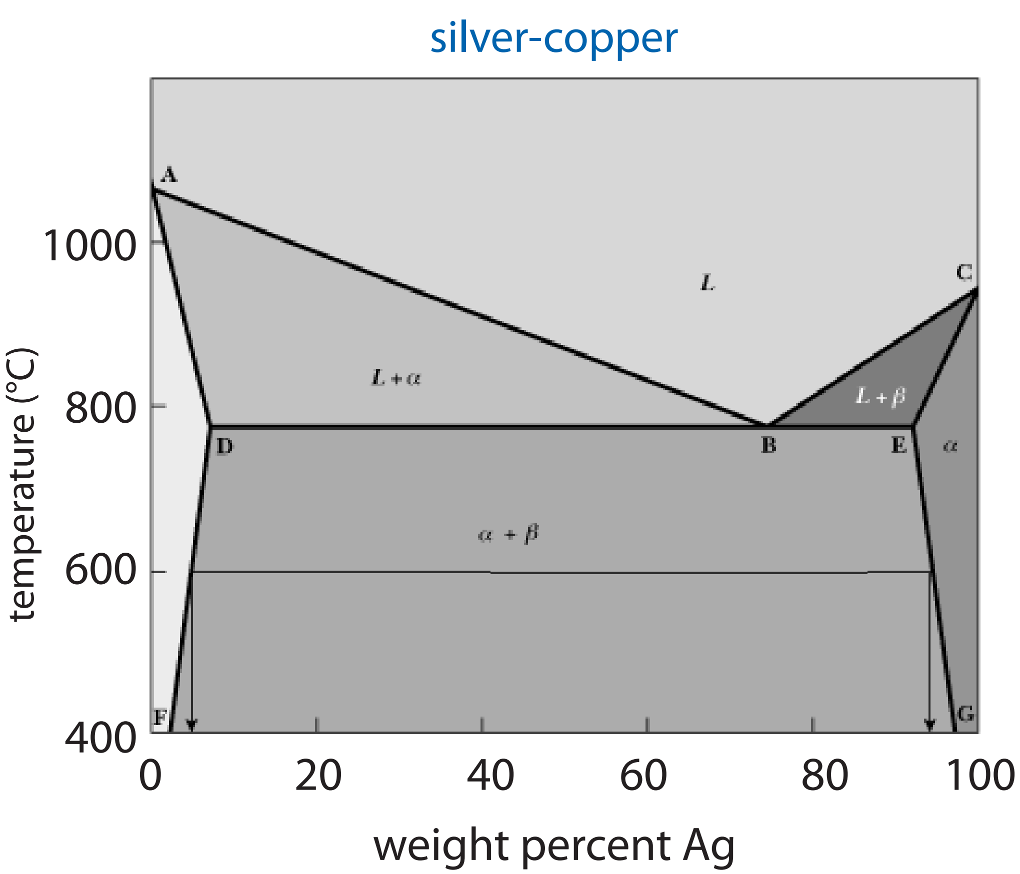


- locally FCC atoms colored according to Euler angle
- locally HCP atoms colored red (twins & stacking faults)
- grain boundaries colored black

MD simulations done with silver and copper, not gold (comparable systems)

- Few potentials for Au and Ag alloys available, but Ag/Cu works
- Cu/Ag are similarly insoluble (at deposition temperatures, T < 300°C) as Au/Ni, Au/Co, etc. (hard gold)
- Sterling silver (7.5 wt. % Cu) was used as a substitute





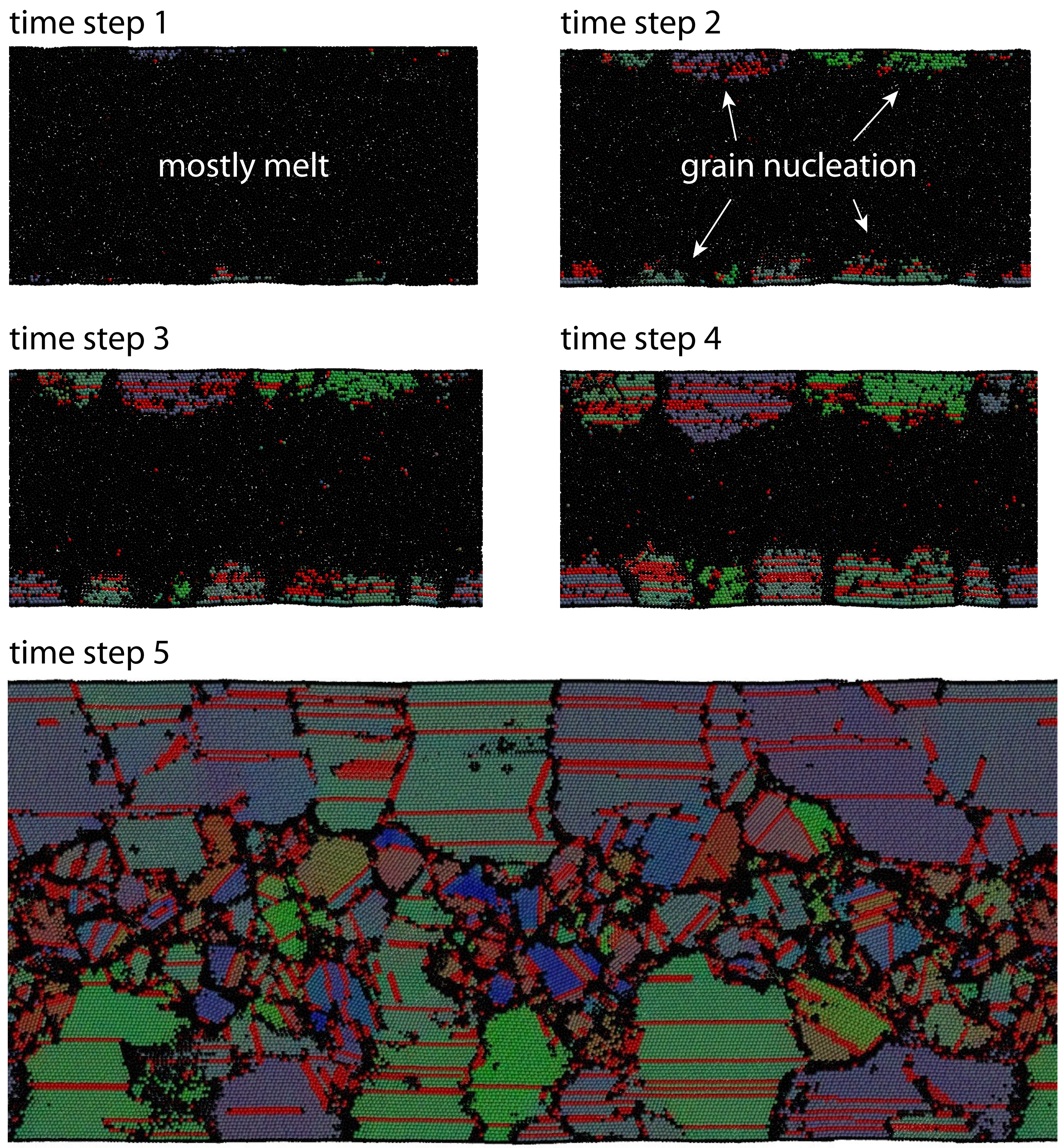
Melt and quench

- start with bulk FCC
- melt at 1800K (20 ps)
- rapid quench (100 ps)
- grains ~ 5 nm
- can then grow grains easily

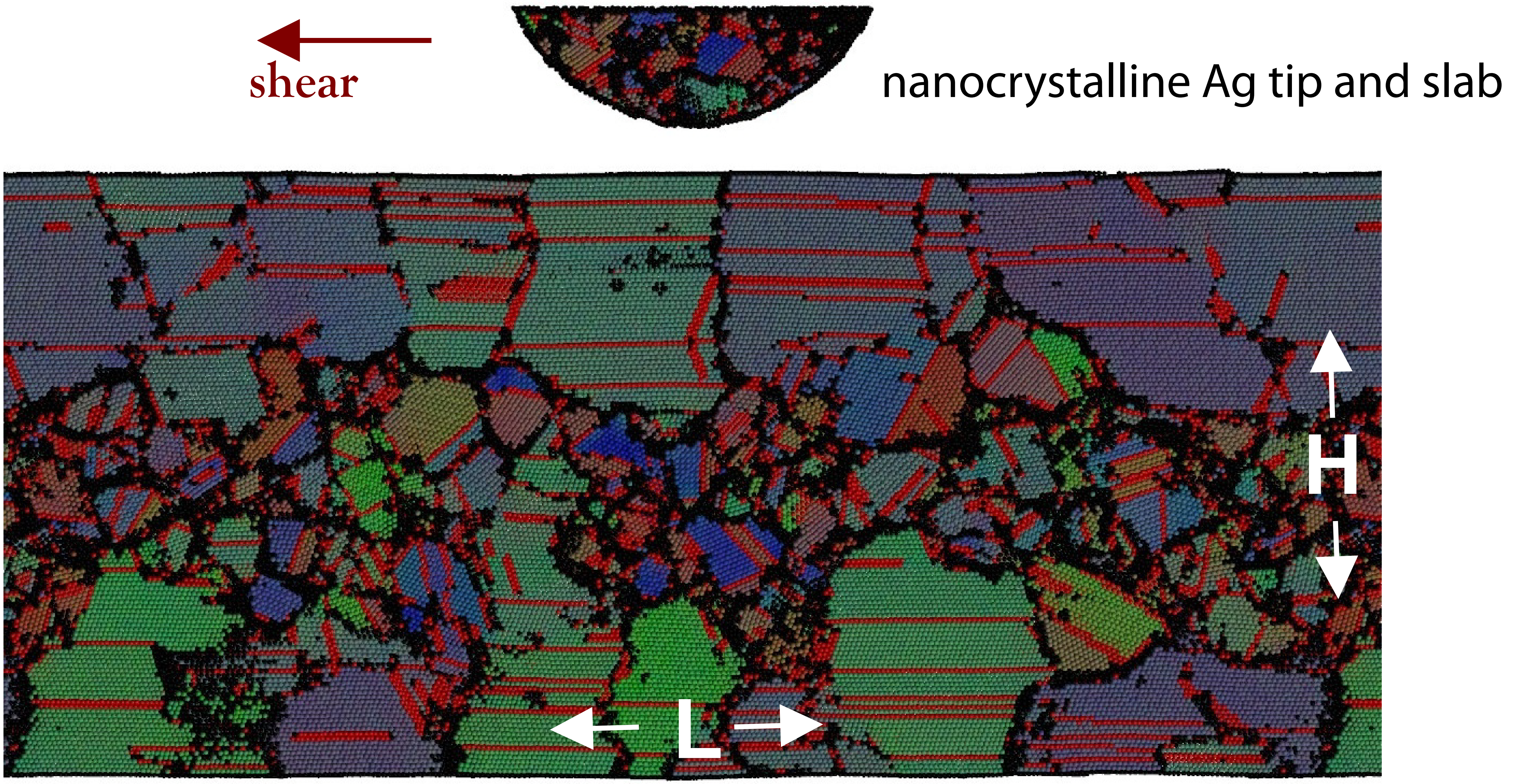
Note on metallurgy...

- twins indicate {111} surface
- growth nucleates at surface

greater disorder/finer grain size where the grain nucleation fronts meet



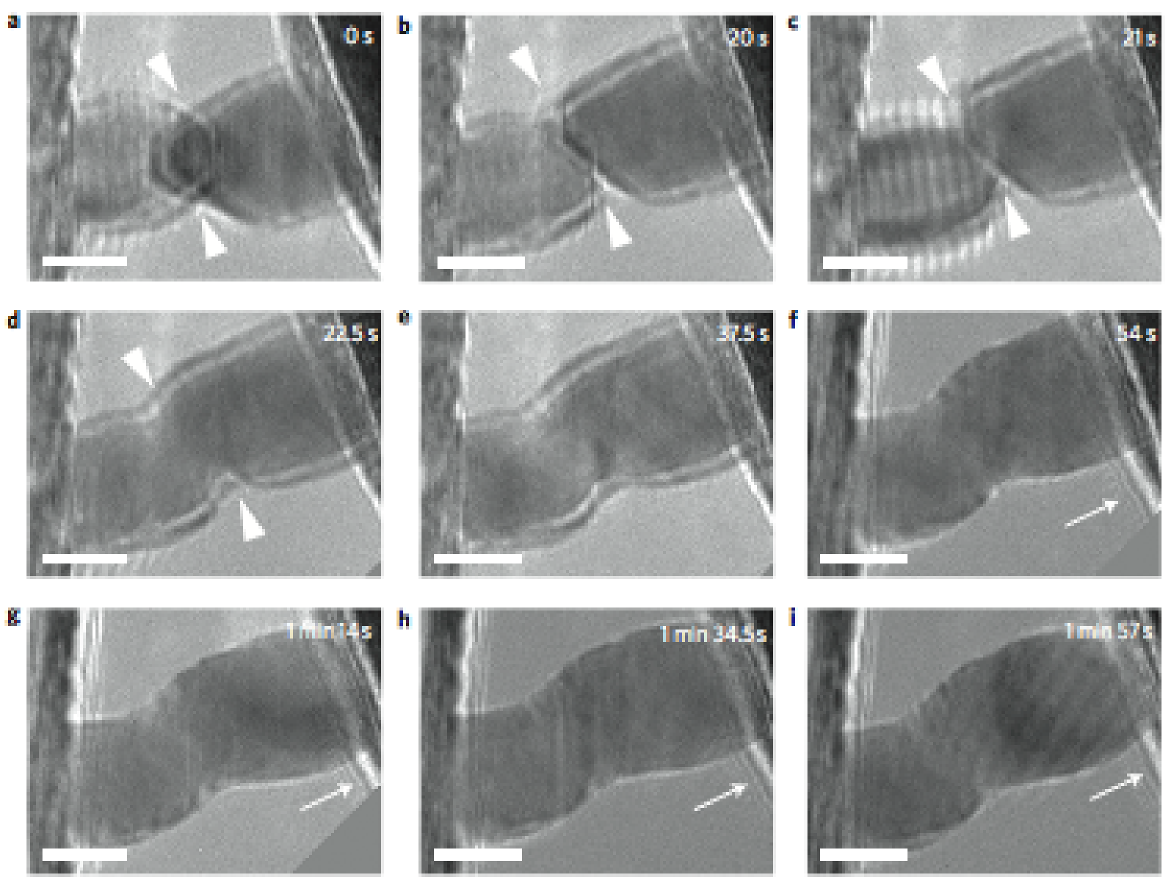
Nanocrystalline tip on slab shear simulation of pure Ag



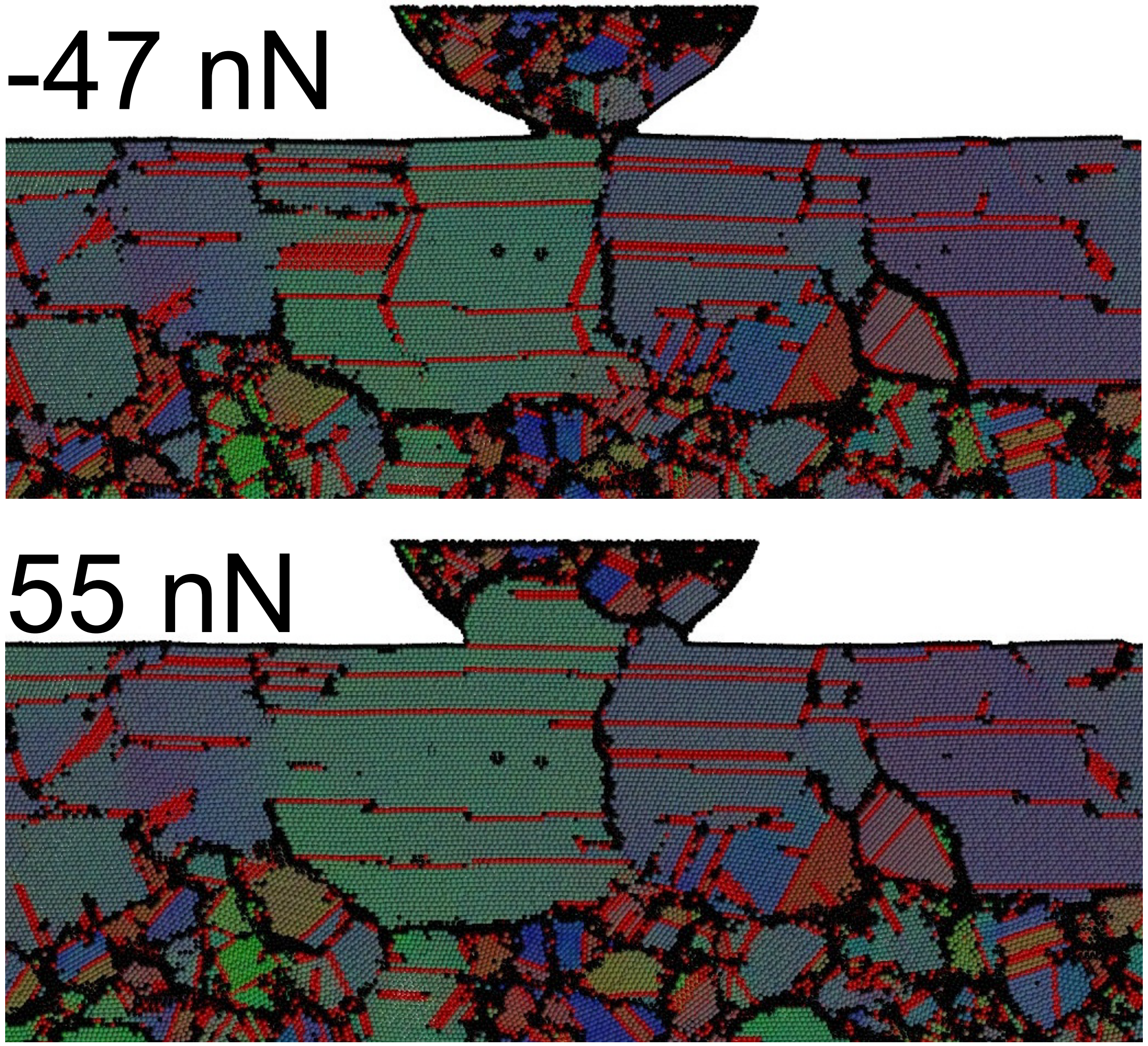
- slab dimensions:
  - width = 17 nm
  - height = 34 nm
  - length = 67 nm
- tip radius = 10 nm
- shear velocity was 2 m/s (constant)
- constant separation *or* force

Cold welding verified in single asperity experiments

Lu, *Nature Nanotech*, 2010

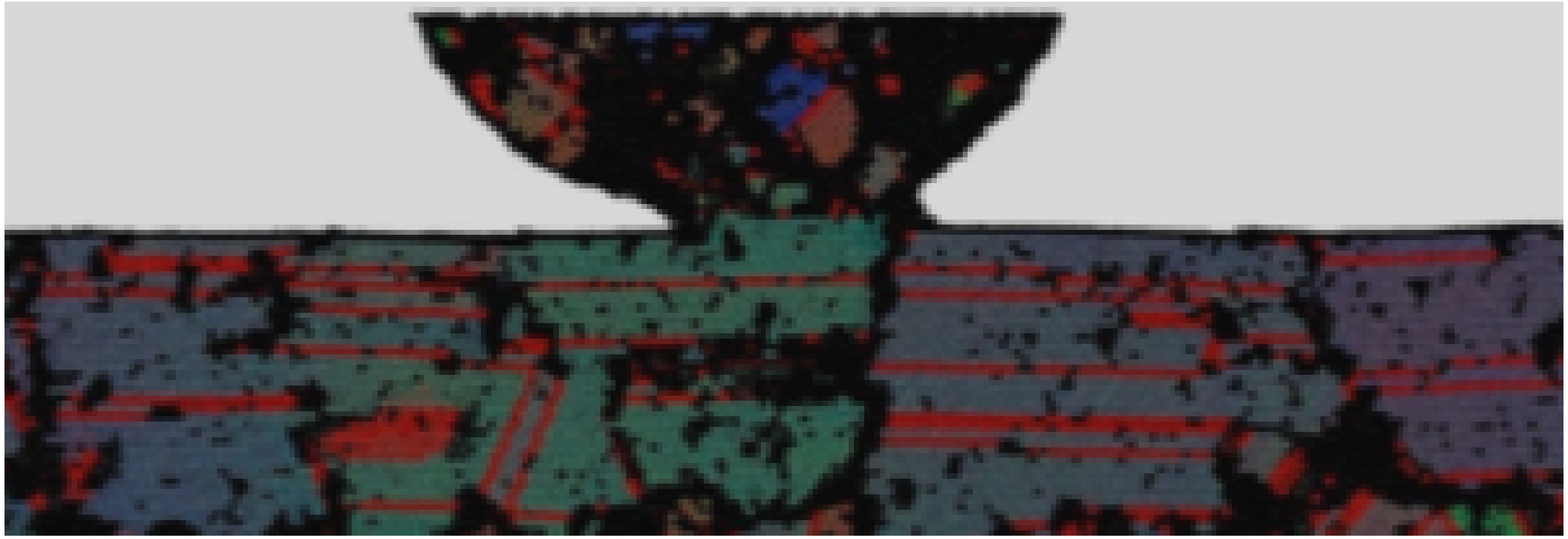


cold welding of gold nanowires
occured with little external force
during 1.5 seconds
(single crystals)

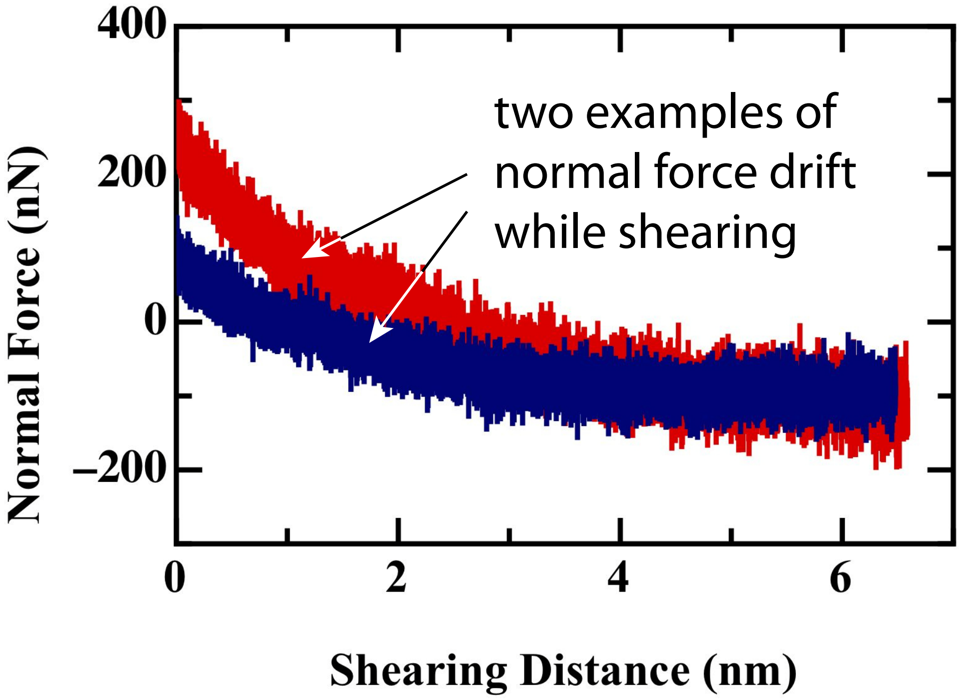


simulation shows coalescence
and grain growth after 2 ps
of contact under compression
(without sliding)

Can't measure alloy friction with tip/slab geometry… switch to slab/slab

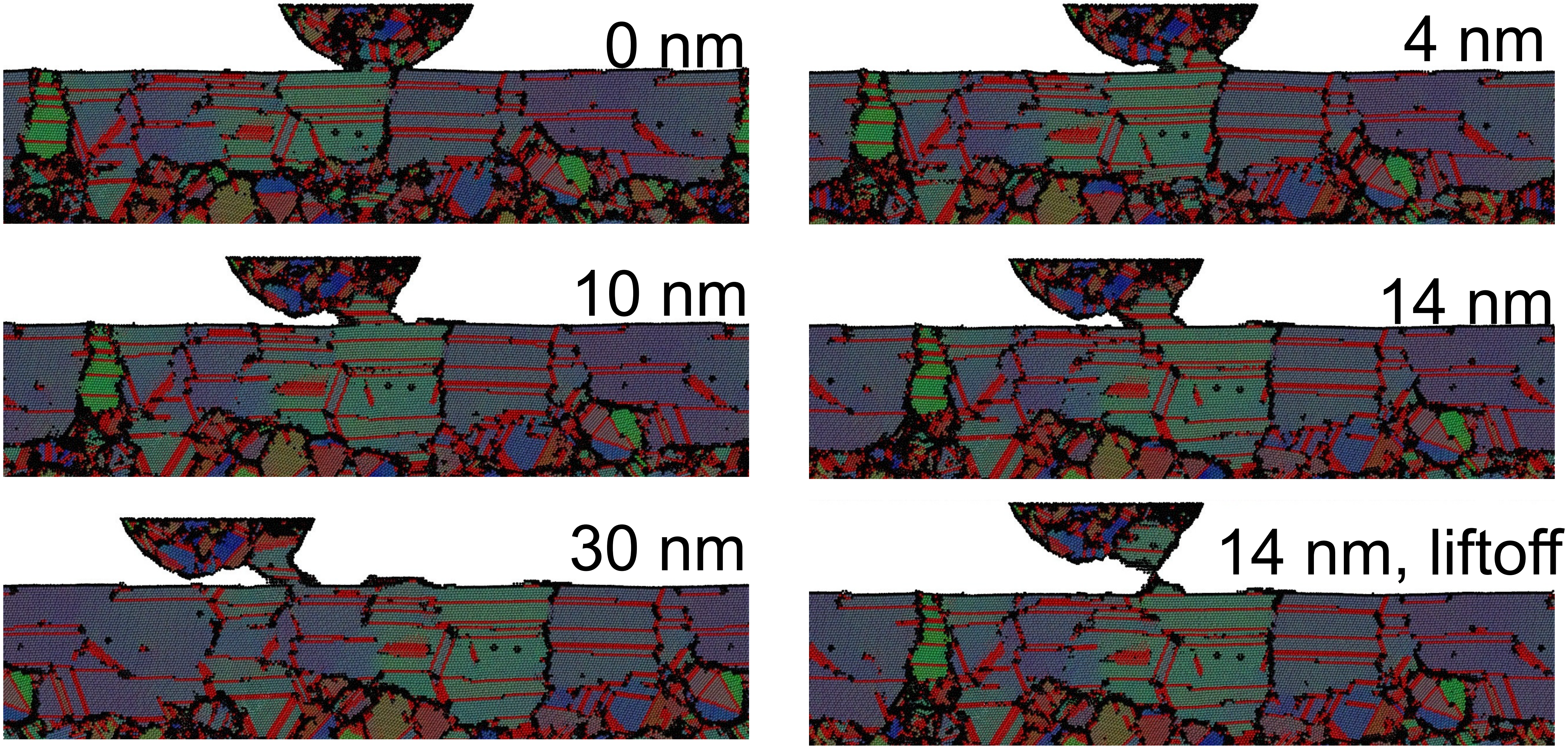


Alloying suppressed coalescence (commensurate contact) due to shear



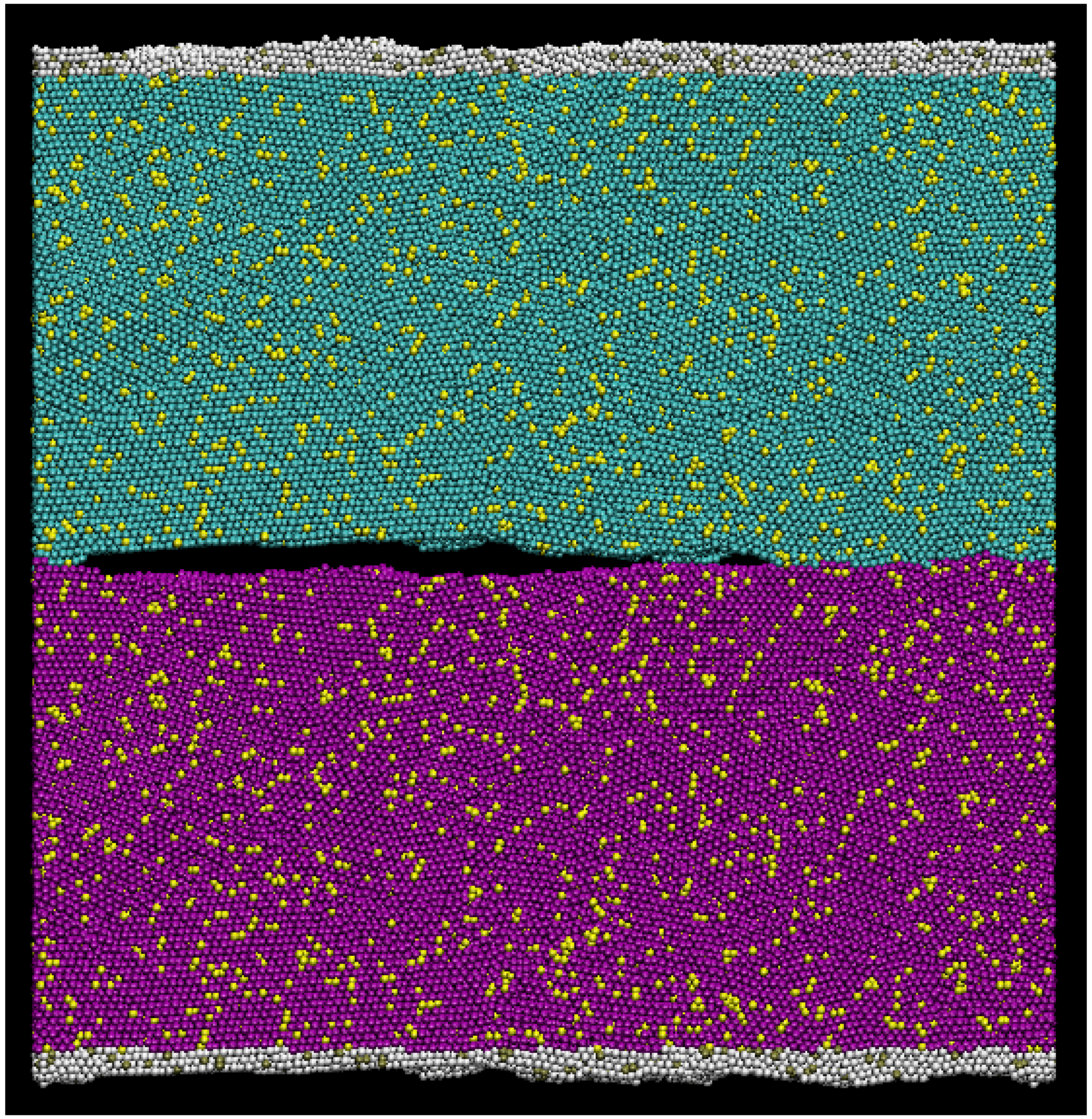
Cannot measure friction with tip/slab due to significant normal load drift, perhaps related to work of adhesion (Ag/Cu alloy exhibits 2x that of Ag/Ag)

Nanocrystalline pure metal surfaces coalesce and weld (high friction)

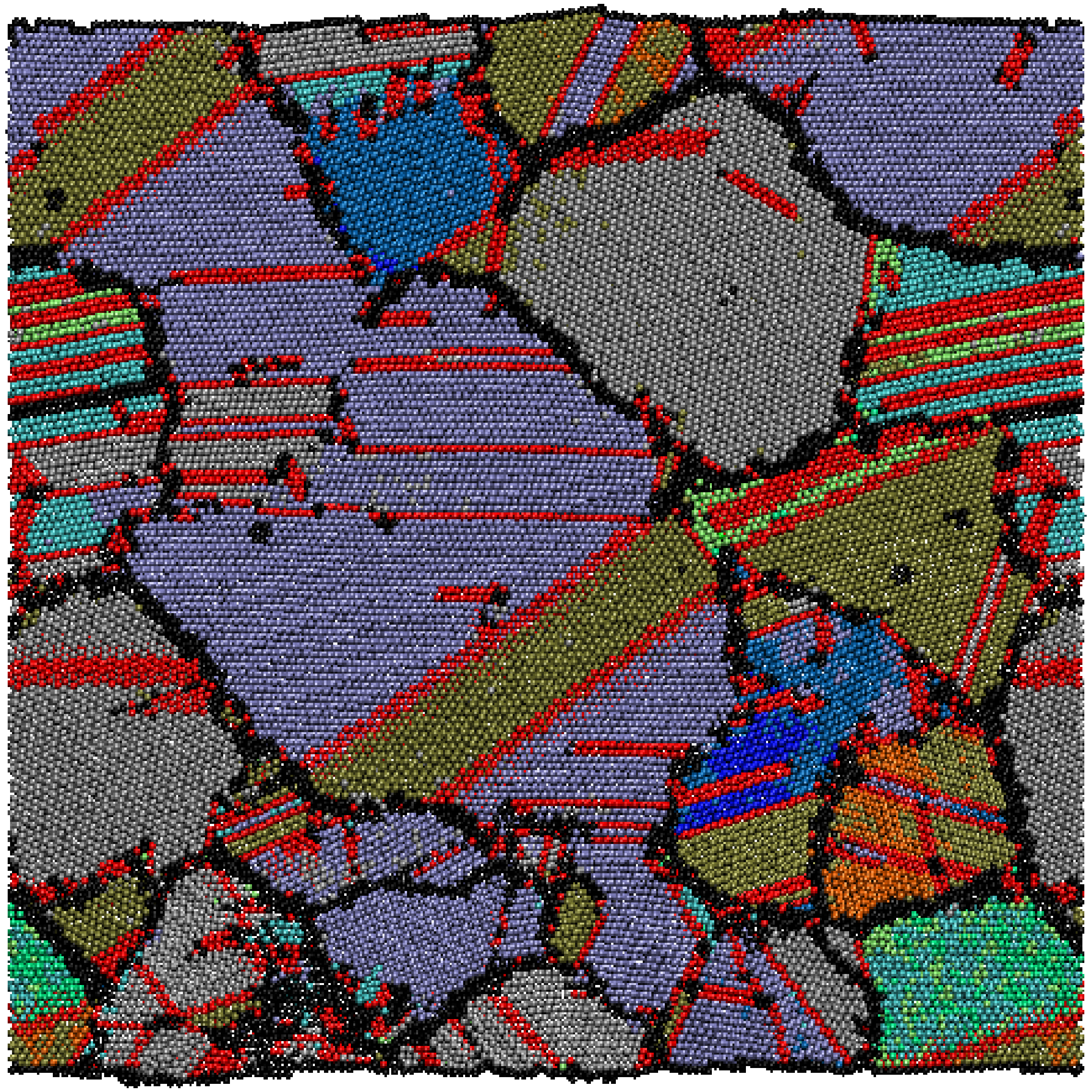


- initially distinct grains
- after shear (adhesive load), coalescence occurs -- now a mode II crack
- single grain forms across interface -- stress induced grain growth

Instead, used Ag slab/slab geometry, made by duplicating and rotating a slab (now using a compressive normal load, about 50 nN)



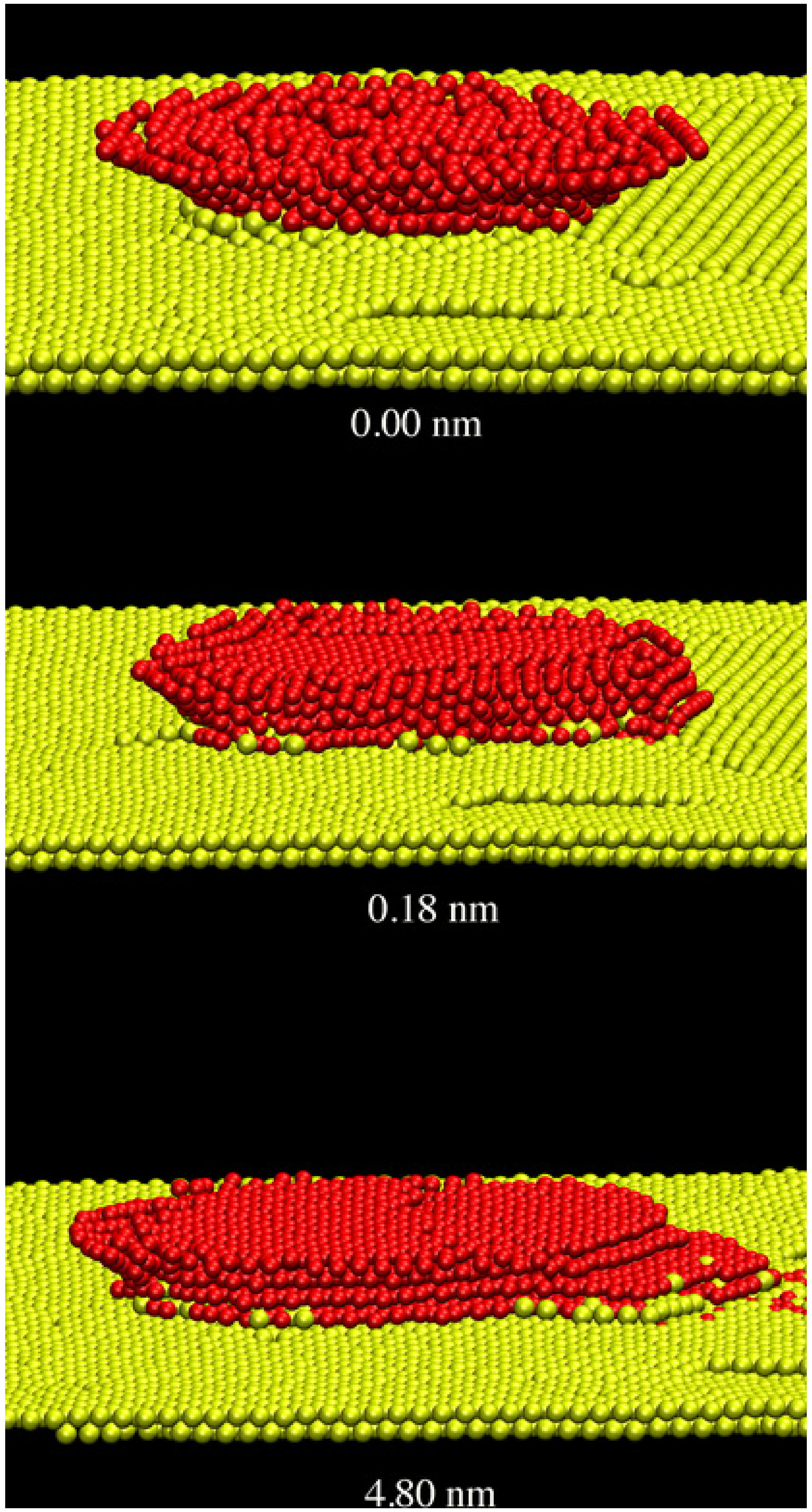
example of alloy slabs with initial roughness (yellow = Cu)



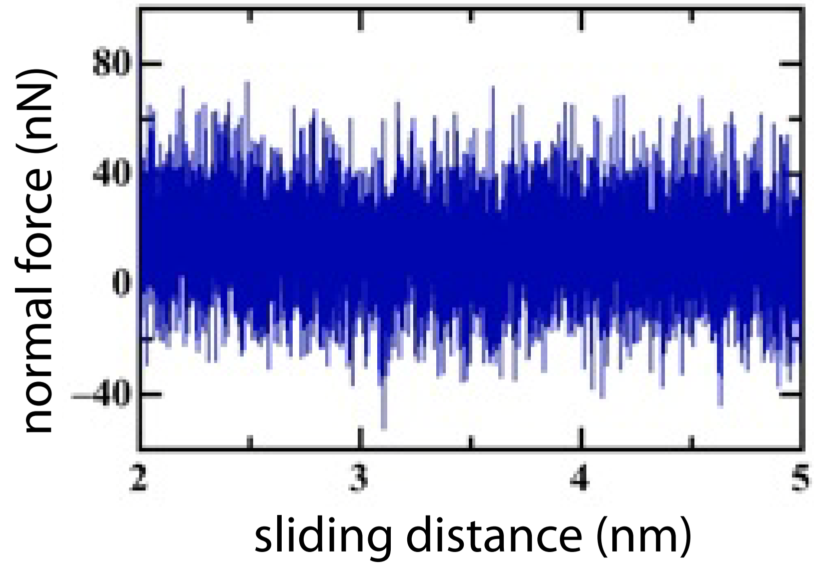
pure Ag slabs after shearing (completely welded)

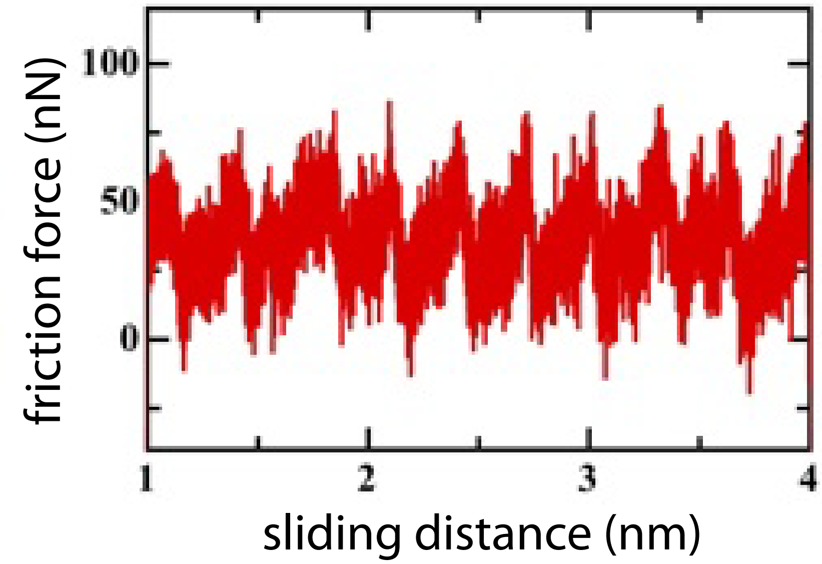
- observed stress induced grain growth, as with tip/slab
- shear occurred at stacking faults, not the junction -- slabs coalesced

Shear induces commensurate contact for Ag/Ag contact (high friction, μ >1)



friction coefficient, μ > 1

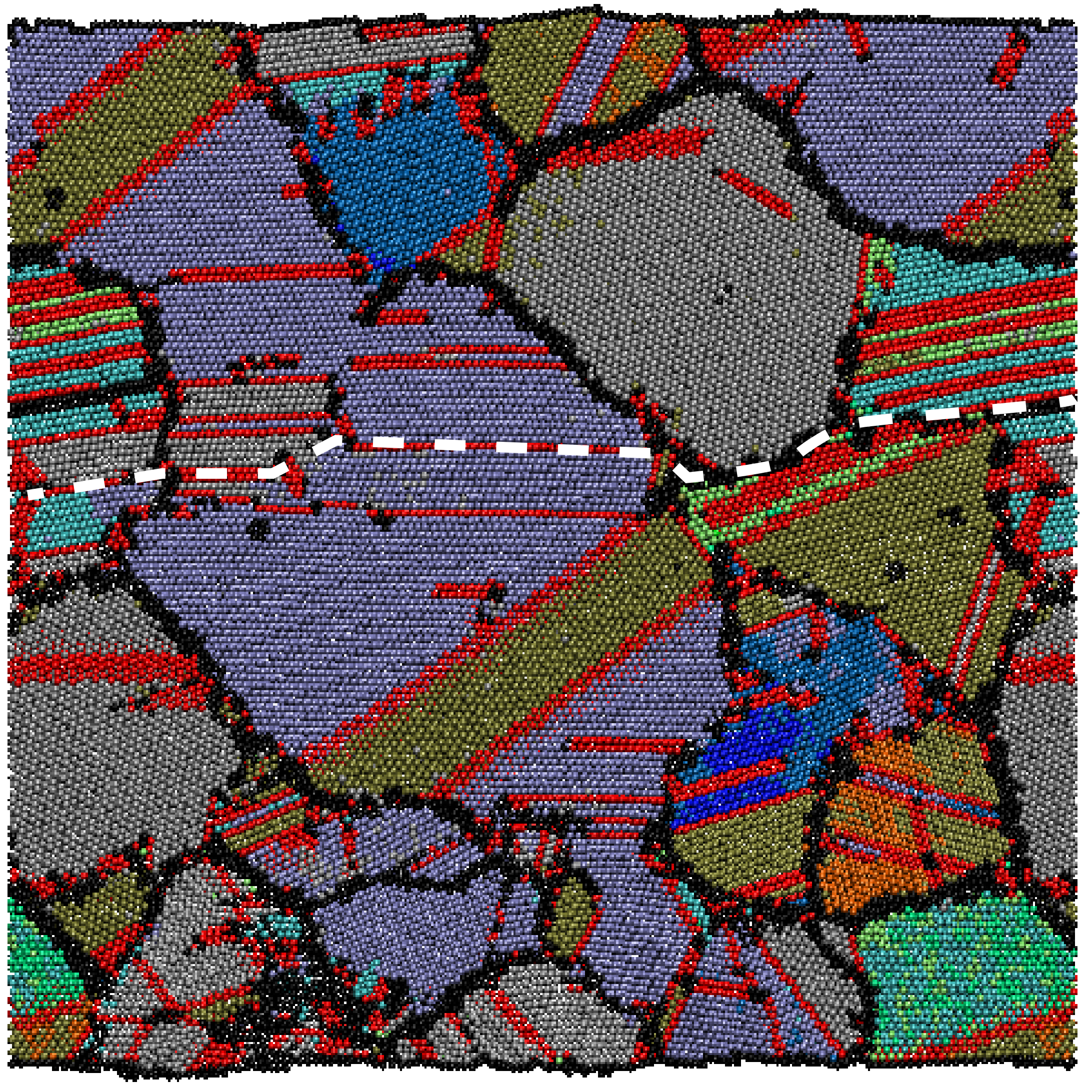




- layering of tip atoms
- stick-slip behavior
- shear induced commensurate contact
- commensurability leads to high friction

... do composites/alloys supress this behavior?

Ag slabs

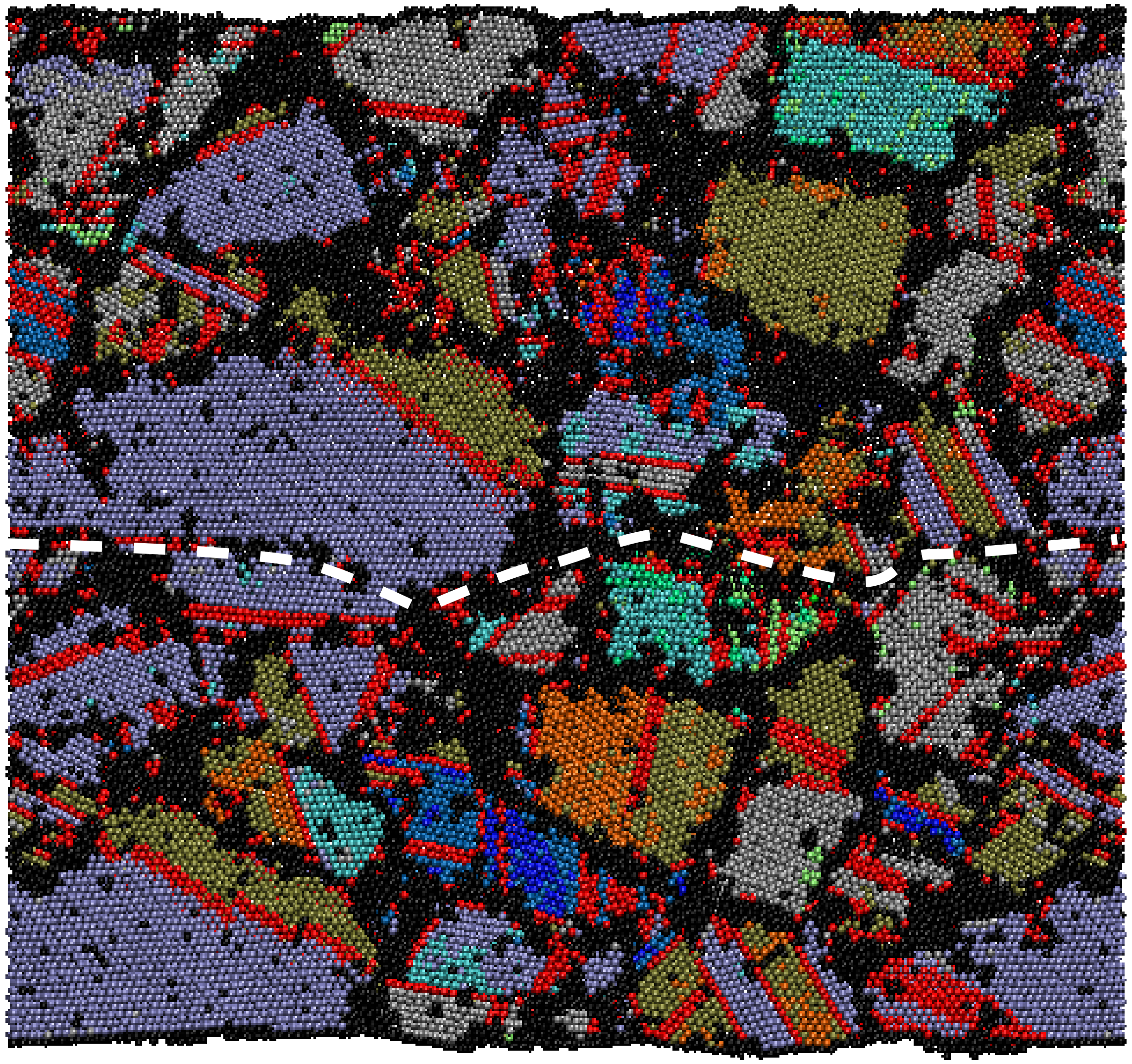


friction coefficient, μ ~ 0.22

- shear occurred primarily at stacking faultsin the bulk

- grains coalesced and grew across junction

Ag/Cu slabs



friction coefficient, μ ~ 0.02

- higher disorder

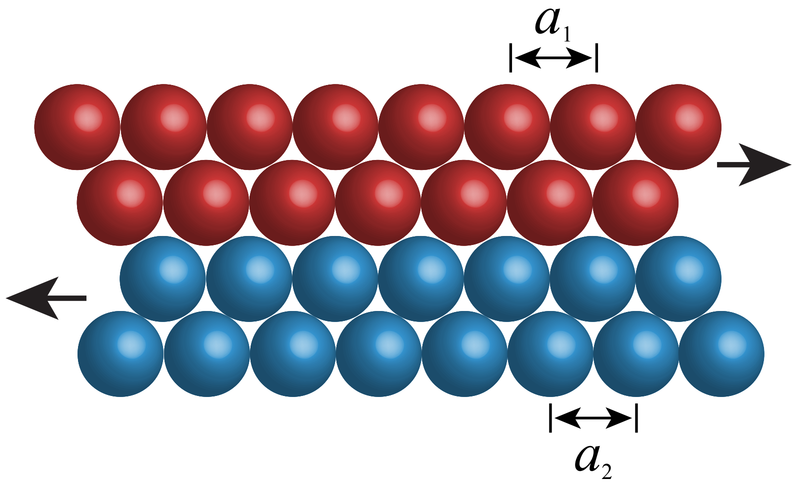
- shear occurred primarily at the *junction*

- coalescence was suppressed

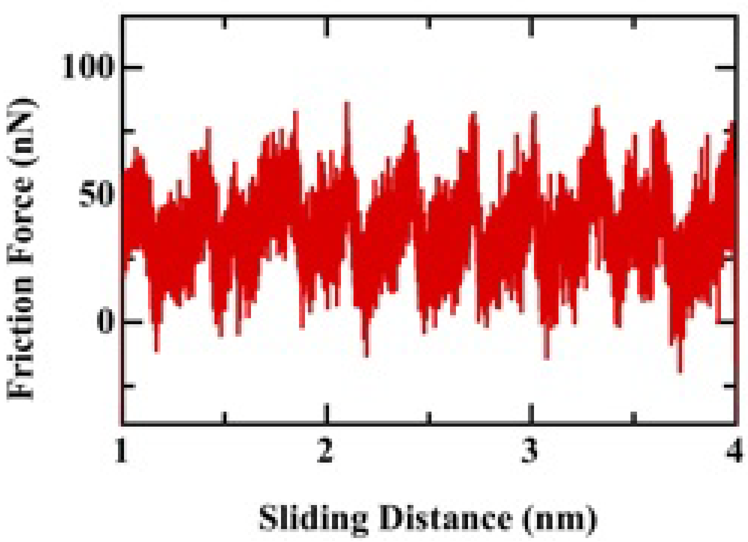
At the nanoscale, commensurate means high friction

commensurate interface
(stick-slip)

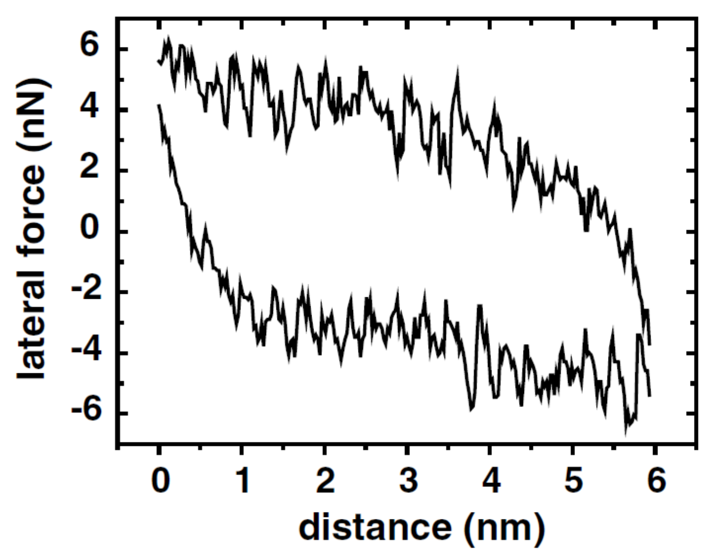
$$a_1 \cong a_2$$



MD simulation



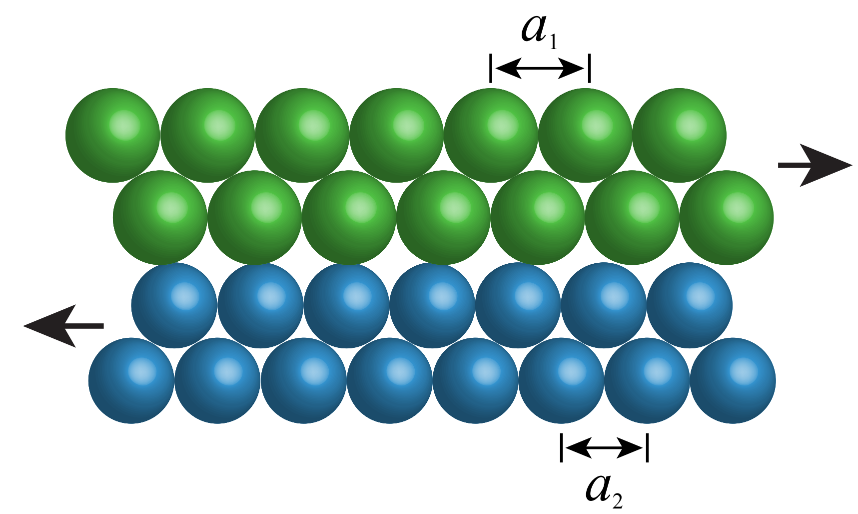
experimental (AFM) data



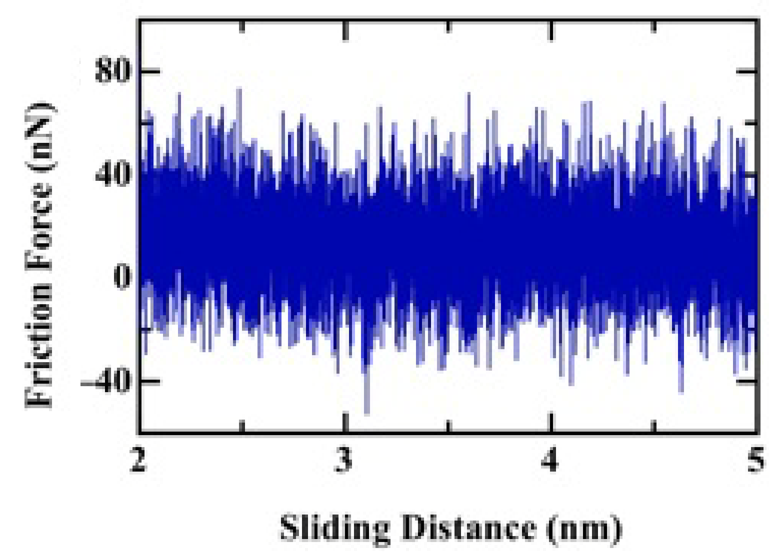
Ref: Gosvami et al, Phys. Rev. Lett. 2011

incommensurate interface
(smooth sliding)

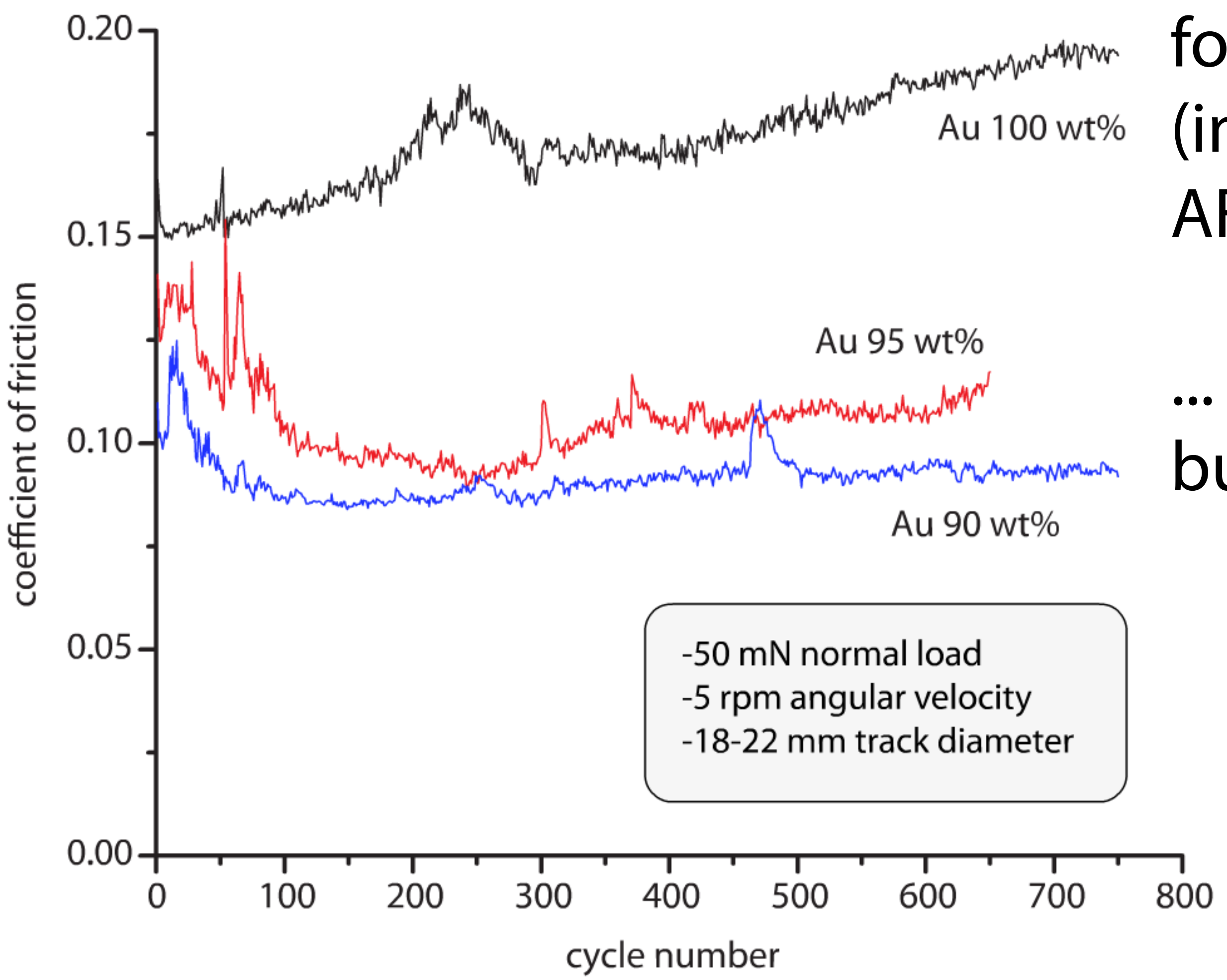
$$a_1 \neq a_2$$



MD simulation



Qualitative agreement with low contact stress experiments

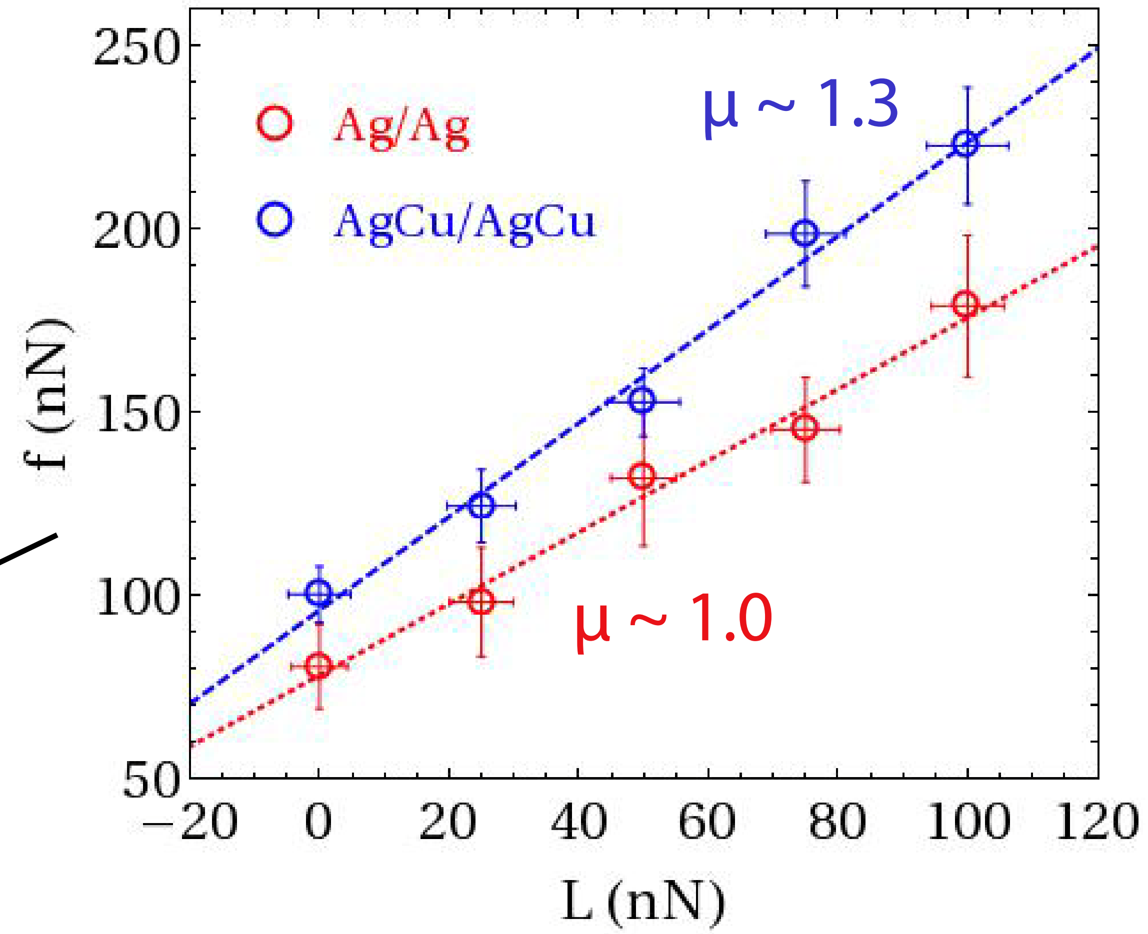


Courtesy: WG Sawyer, U. Florida

for pure Au contact μ ~ 0.2
(in agreement with simulation AND with AFM experiments; soft tip = no ploughing!)

... reduction with alloying,
but not to μ ~ 0.02

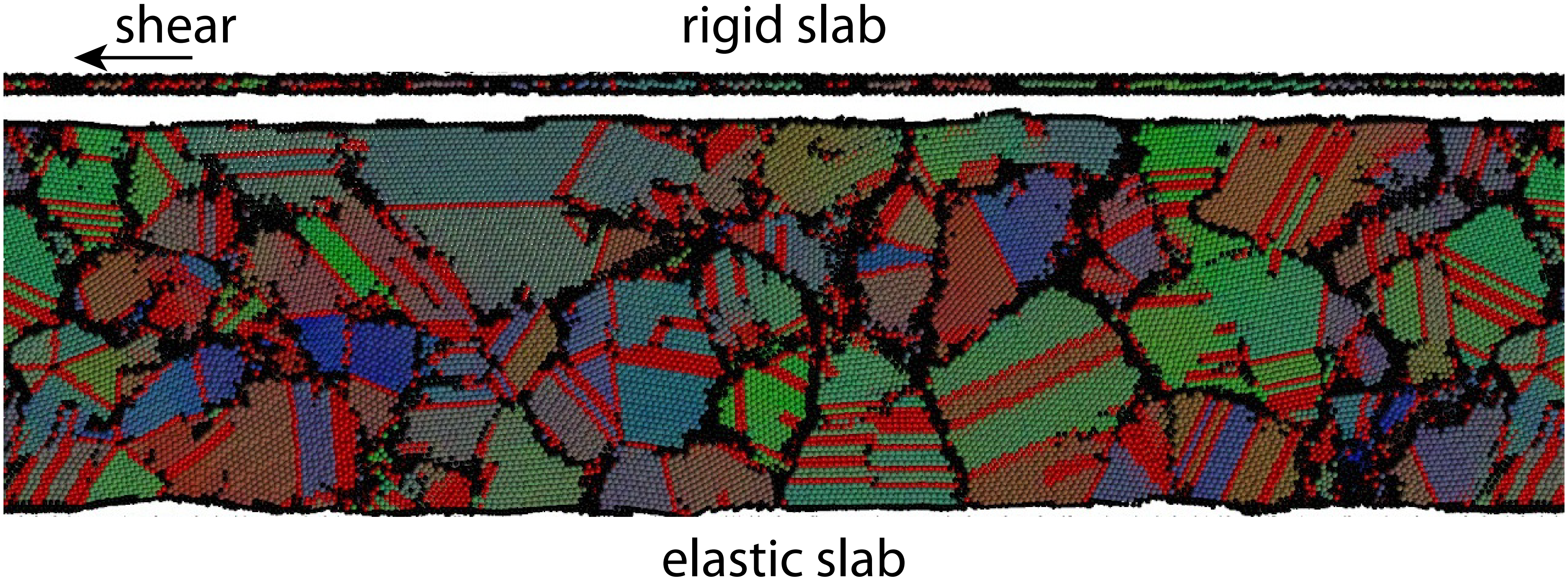
Using rigid tip in tip/slab contact can artifically supress grain growth:



material independent friction behavior was observed
(all friction was ploughing)

alloy μ was ***higher***

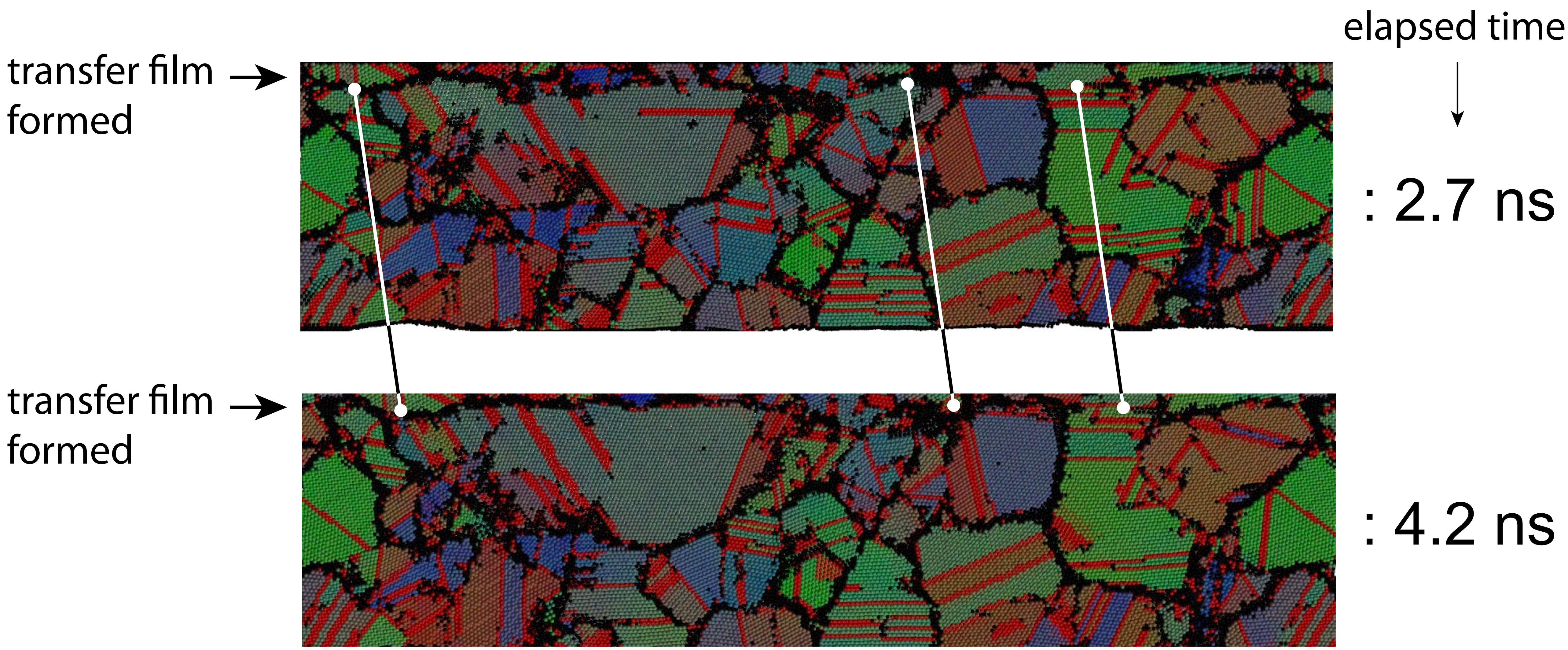
Rigid slab sliding on slab supresses grain growth and ploughing...



By using a slabs -> suppress ploughing

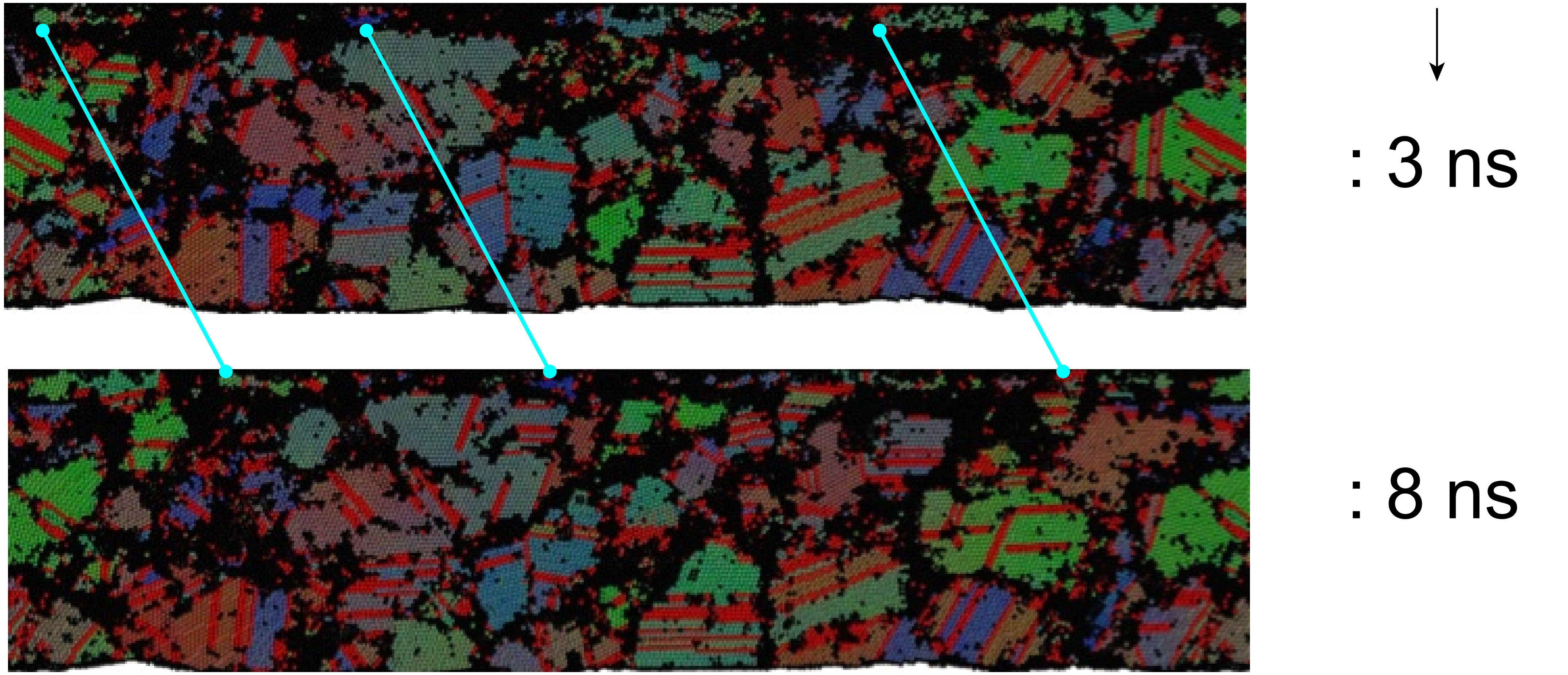
By rigidizing top slab -> suppress grain growth

Pure Ag slabs (one rigit/one elastic) formed transfer film, sheared at junction



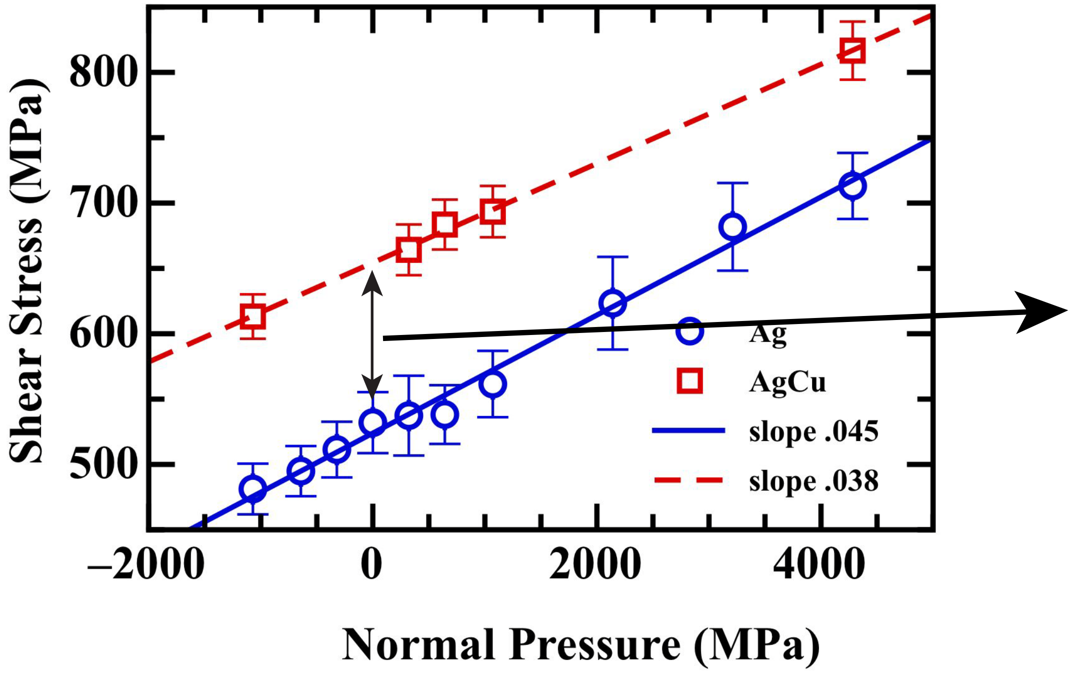
- transfer film formed between rigid/elastic slabs
- sliding occurred along grain boundary of transfer film, or stacking fault, depending on local availability
- grain growth mostly suppressed

Alloy slabs sheared at boundary *and* throughout substrate; friction was reduced



Alloy slabs slide at boundary and also throughout the substrate

Friction behavior was materials dependent



Alloy shear stress 23% higher than pure metal (650 MPa vs 530 MPa)

Macro-scale experiments with hard gold (”engineering”)

1. Reductions in friction and wear are attributed to grain refinement and grain boundary segregation of alloy species (typically an insoluble material) in the 1-2 wt. %
2. Friction reduces from $\mu > 1$ to $\mu \sim 0.3$ to 0.5 with order 1 wt. % alloying of various species -- wear reduces 17x over pure gold for a “gold/gold” contact (Neyoro G vs Au film) -- grain size reduced from > 500 nm to ~ 100 nm with 0.1 vol. % alloying

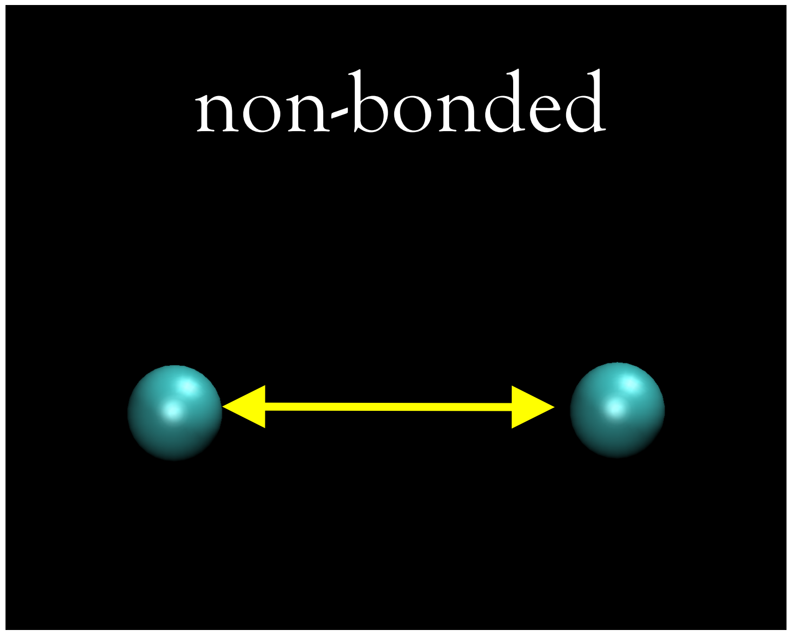
MD simulations with hard gold-like materials (”fundamental science”)

1. Pure metal contacts (without protective oxide films) will cold weld and undergo grain reorientation -- shear will occur along slip planes (dislocation mediated plasticity) -- and commensurate interfaces (self-mated materials) will exhibit the highest friction ($\mu > 1$)
2. Alloys such as hard gold will still cold weld, but grain reorientation is suppressed -- shear occured along transfer film boundary -- grain boundary mediated shear

Acknowledgments

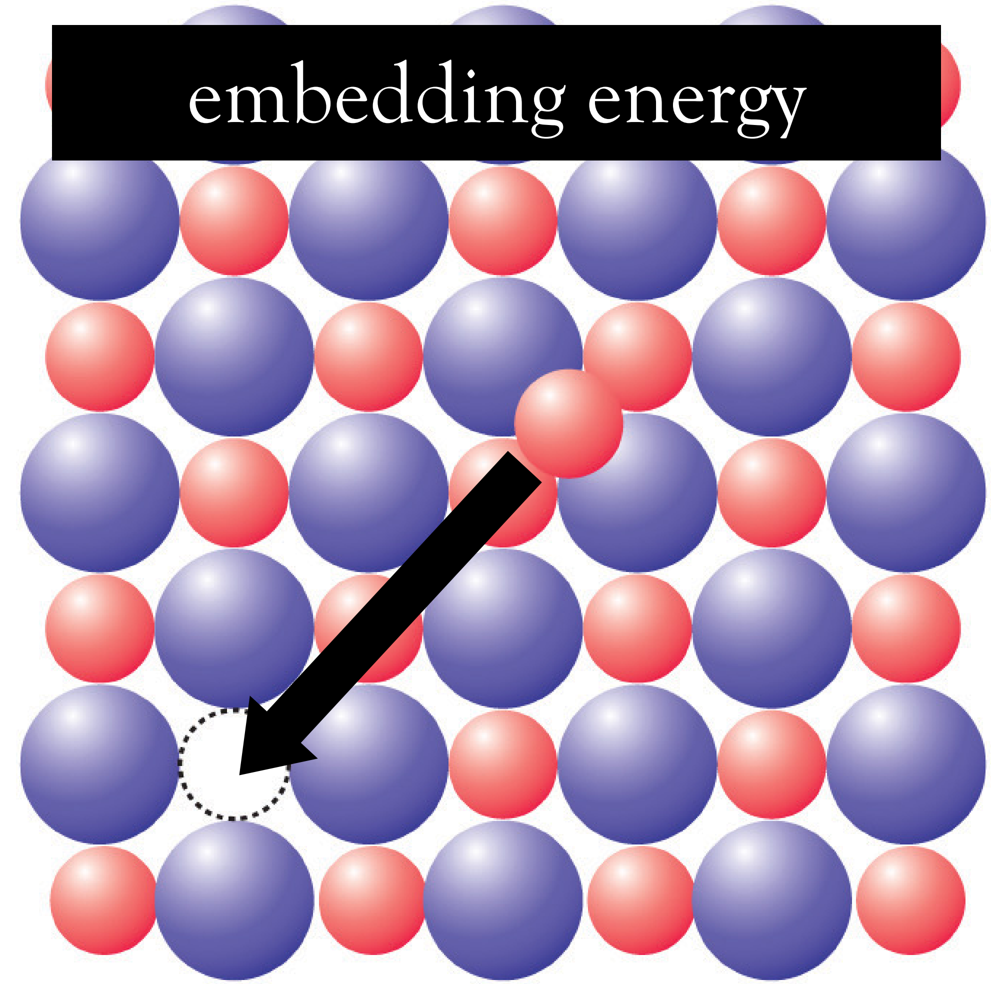
- Somuri Prasad and Michael Dugger for fruitful discussions and support
- Joeseph Michael and Bonnie McKenzie for SEM/EBSD microscopy
- Rand Garfield for tribotesting specimen preparation

Embedded Atom Method



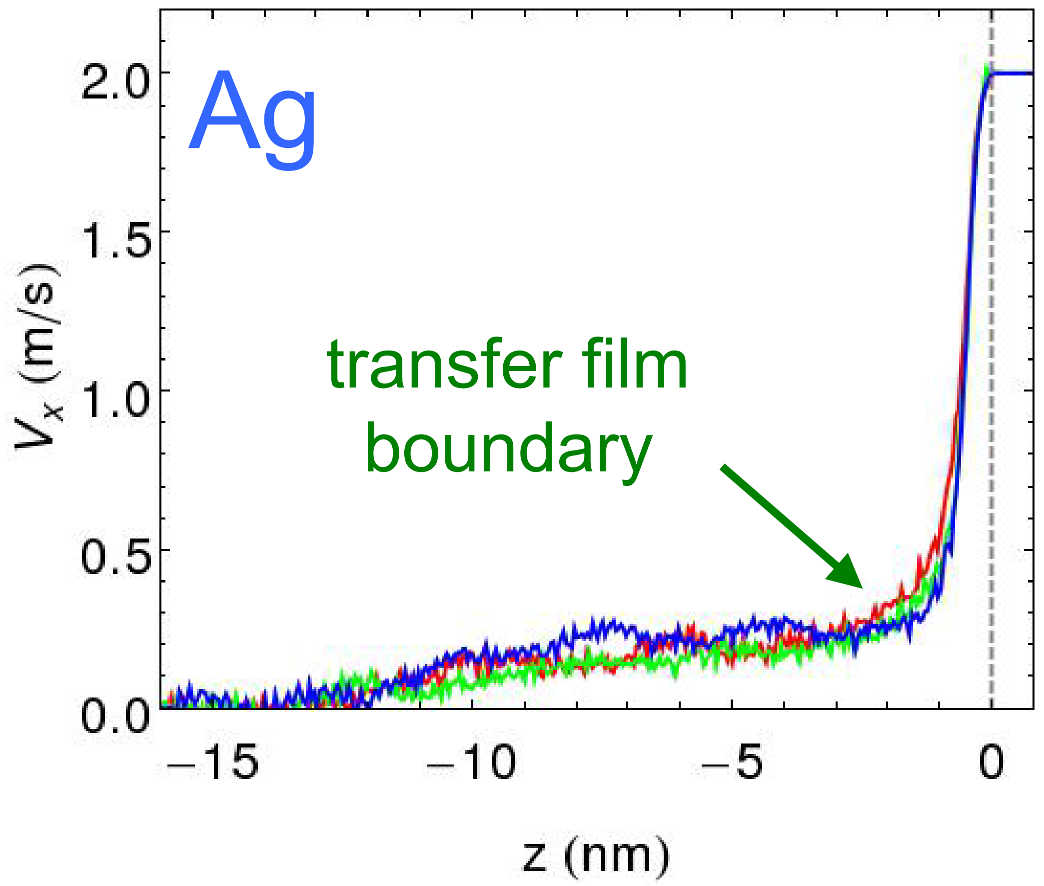
$$4\varepsilon \left[(\sigma/r)^{12} - (\sigma/r)^{6} \right] \quad r < r_c$$

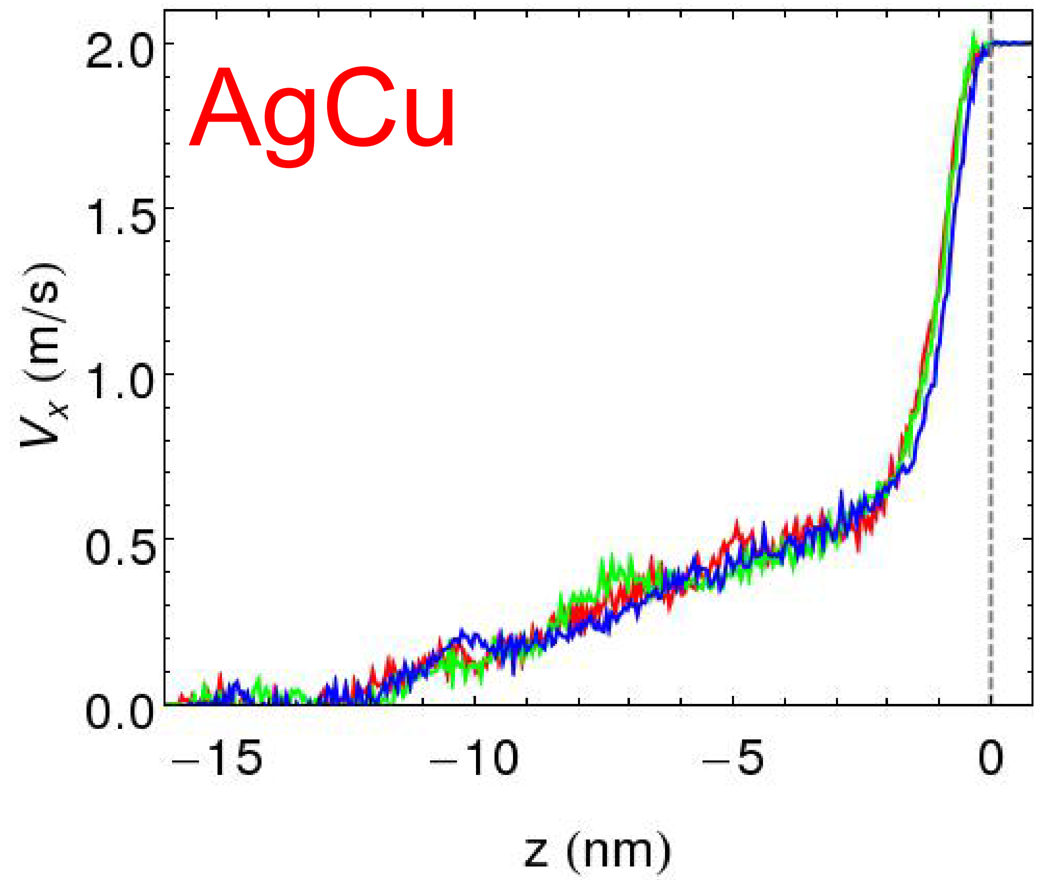
+



$$F_\alpha\left(\Sigma_{i \neq j}\rho_\beta(r_{ij})\right)$$

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