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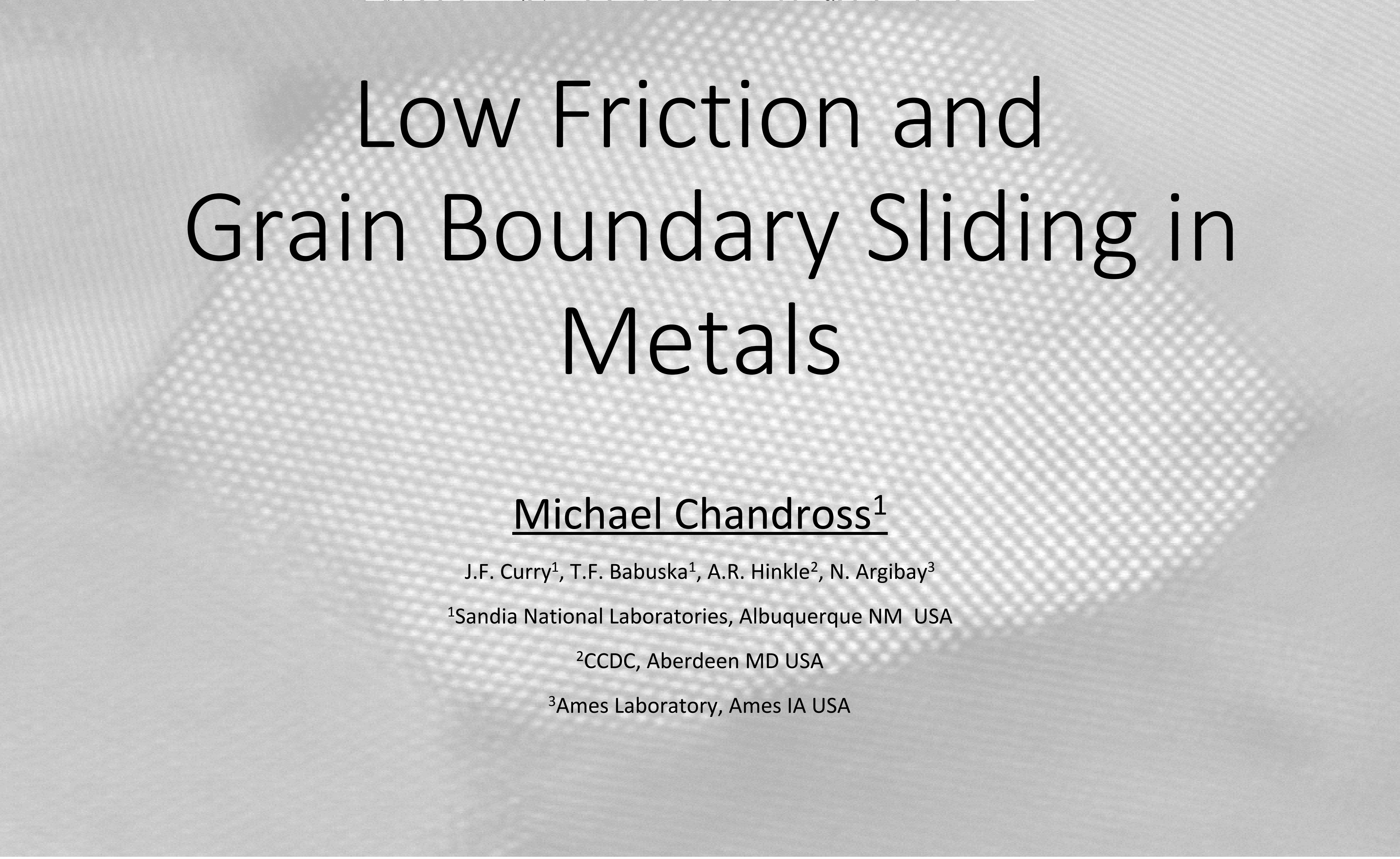

Low Friction and Grain Boundary Sliding in Metals

Michael Chandross[1]

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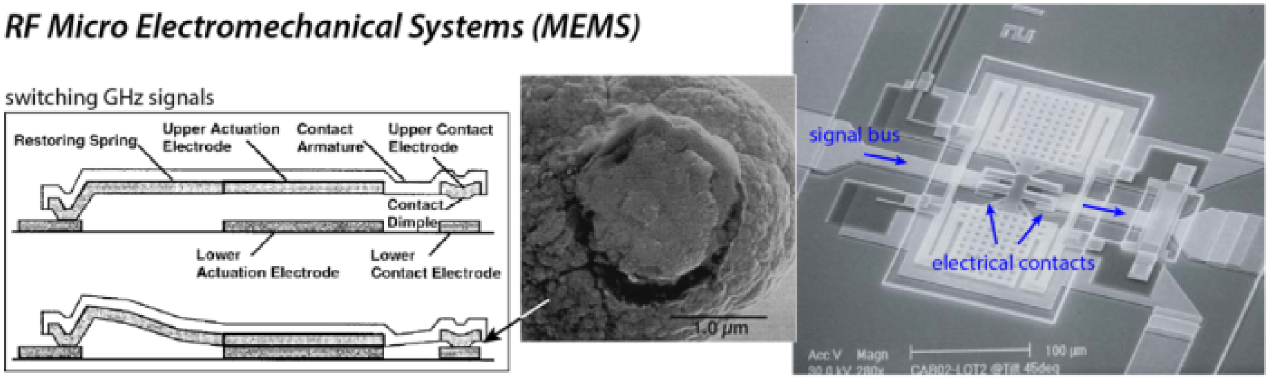
Electrical Contacts use Bare Metal

Phone Interconnects

RF Micro Electromechanical Systems (MEMS)

switching GHz signals



Source: D. Hyman and M. Mehregany, IEEE Trans. & Pack. Tech. 22-3, 1999

Source: Rockwell Scientific metal-metal switch

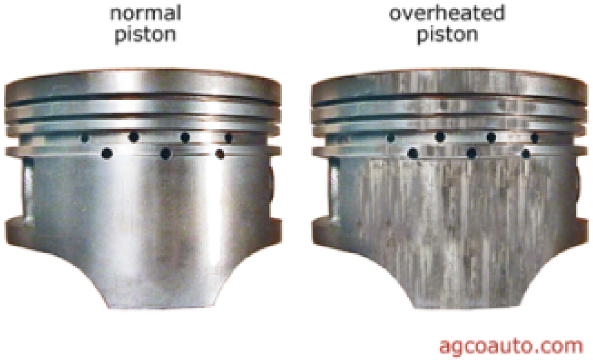
Electronics (e.g. PCB blade connectors):

200 - 500 nm thick electroless hard gold

Aerospace and Energy

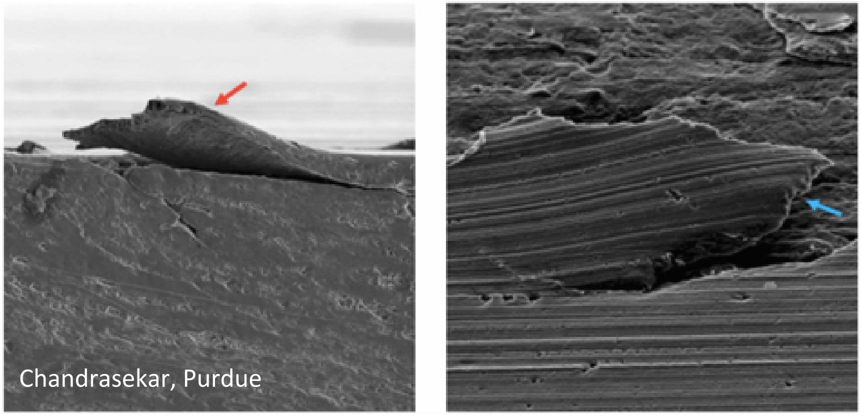
Source: Honeybee Robotics (http://www.honeybeerobotics.com/portfolio/rolling-contact-connector/)

Metals are Ductile and Sticky

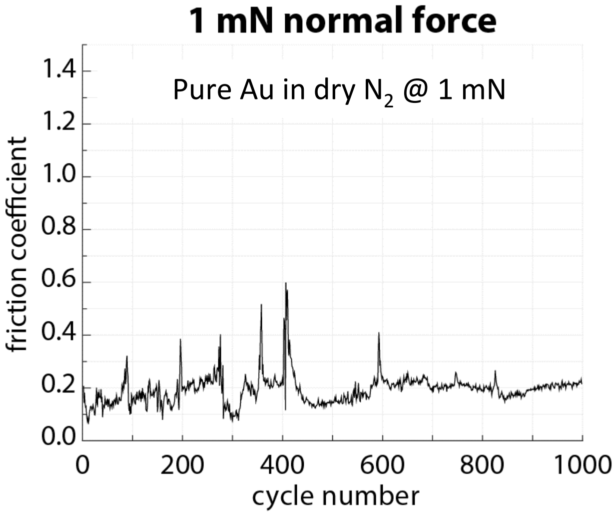


Materials	μ
Aluminum/Aluminum	1.2
Copper/Copper	1.0
Nickel/Nickel	0.9
Rubber/Asphalt	0.9
Waxed Ski/Snow (0^o C)	0.05

- High adhesion (cold welding)
- High friction
- High Wear (galling)
- Plasticity


Chandrasekar, Purdue

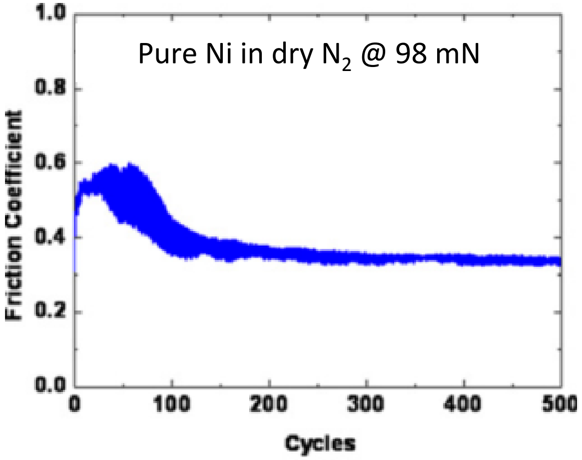
Low Friction starting from Bare, Soft, Pure Metals

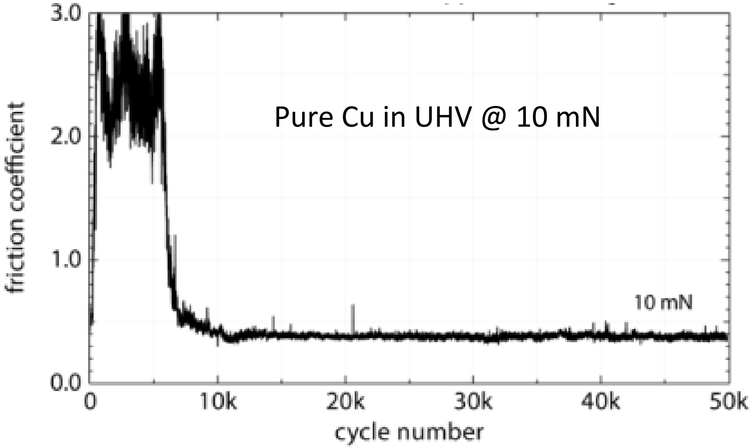


> “When surfaces are cleaned in a good vacuum, the sliding friction… becomes vanishingly small.”
> - Bowden & Hughes, *Nature* 1938.

> “It was found quite unexpectedly that with some metals, very low friction less than 0.10 was observed.”
> - Tamai, *J. Appl. Phys*. 1961

Prasad, *Scripta Mat.* 2011

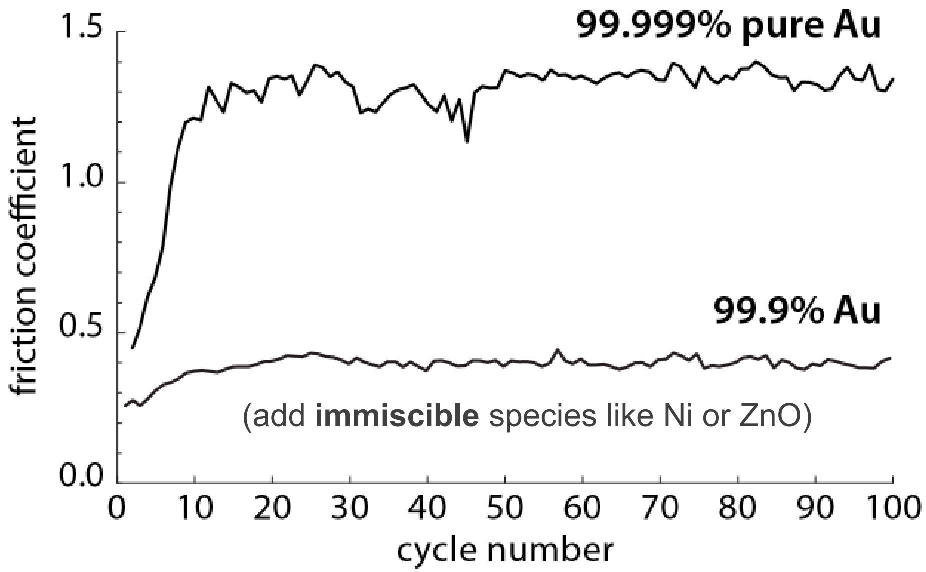




Low friction with pure metals is achievable.

Reduced Friction and Wear of Nanocrystalline Metals

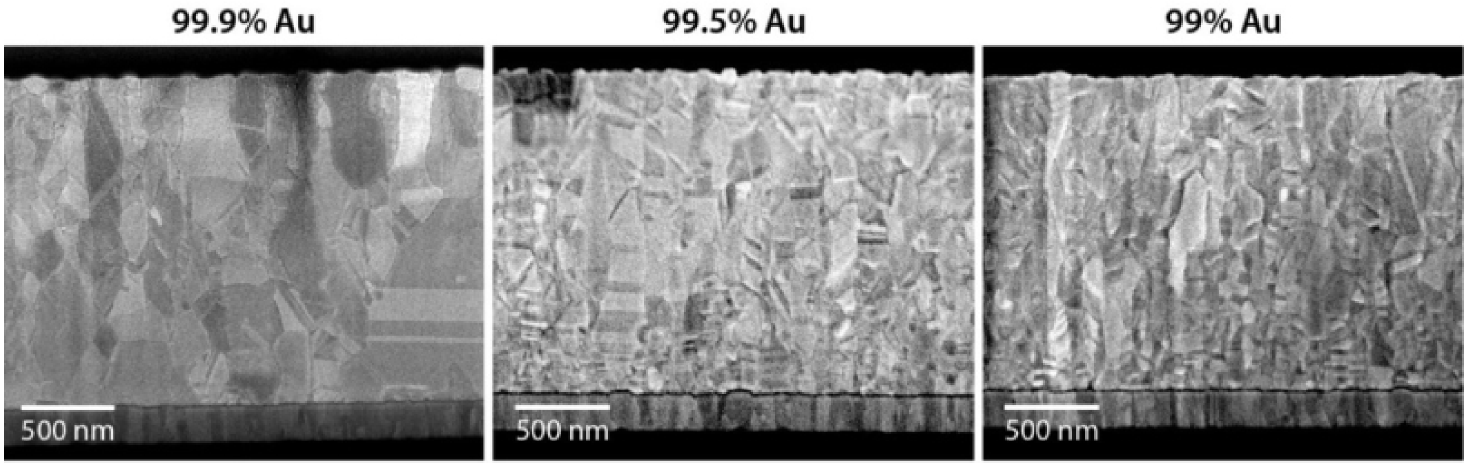
Alloying reduces friction coefficient:



(add **immiscible** species like Ni or ZnO)

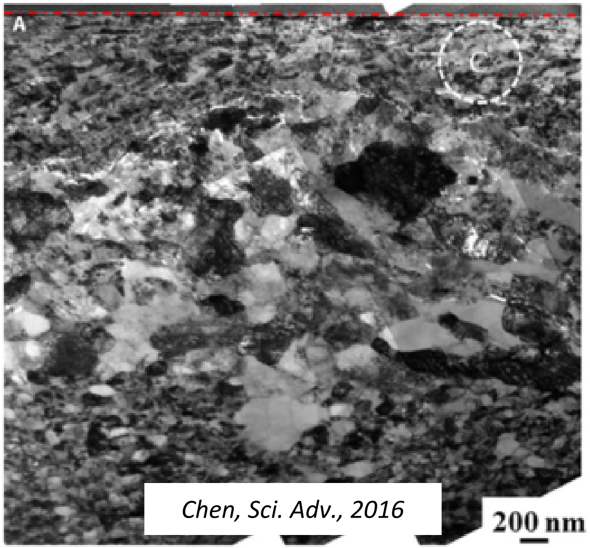
Alloying improves
friction & wear performance by reducing
and stabilizing grain size

…by reducing grain size:



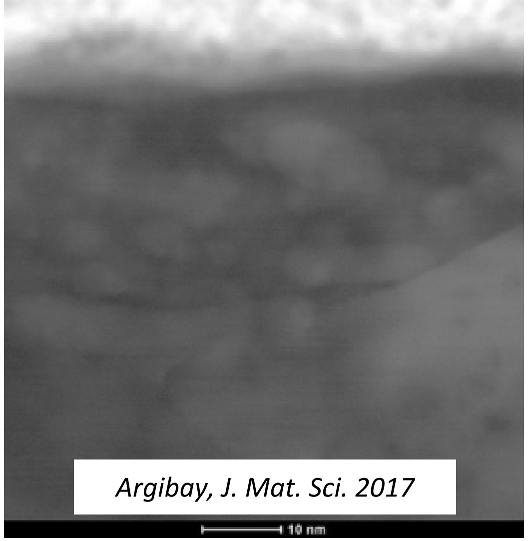
Friction depends on grain size

Pure Cu in air @ 50 N, μ ~ 0.37



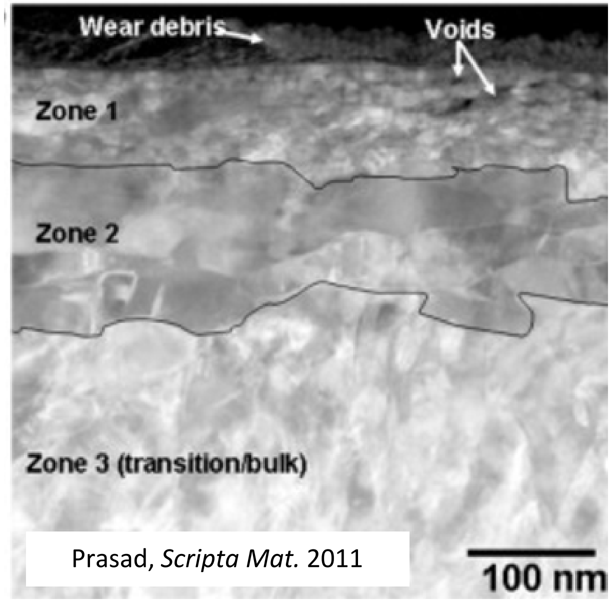
Chen, Sci. Adv., 2016

Pure Au in dry N_2 @ 1 mN, μ ~ 0.2



Argibay, J. Mat. Sci. 2017

Pure Ni in dry N_2 @ 98 mN, μ ~ 0.2



Prasad, *Scripta Mat.* 2011

Low friction is associated with the formation of a highly surface localized UNC layer.

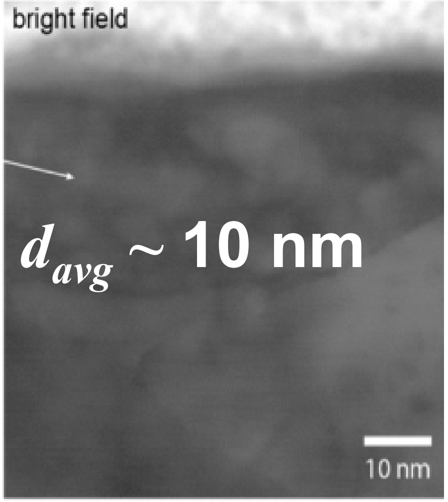
There is a crossover around 10 nm

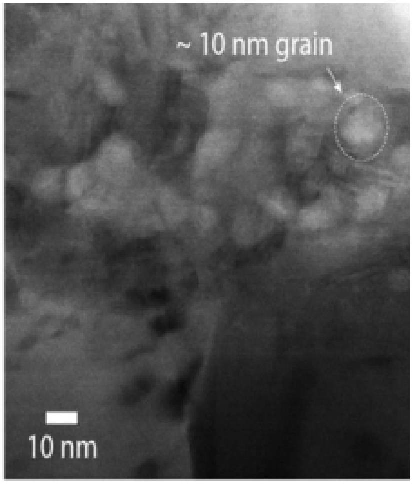
low friction

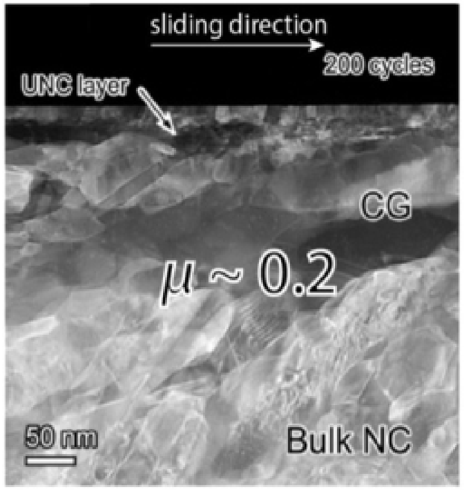
gold on gold

copper on copper

sapphire on nickel





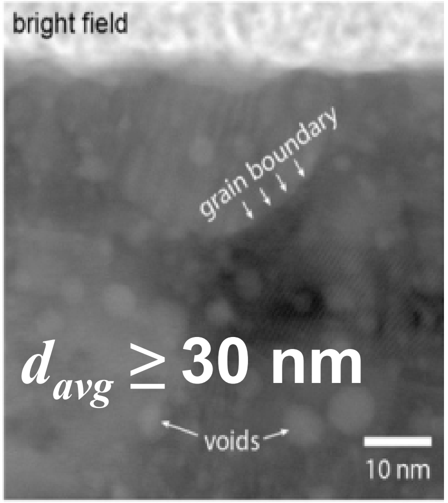


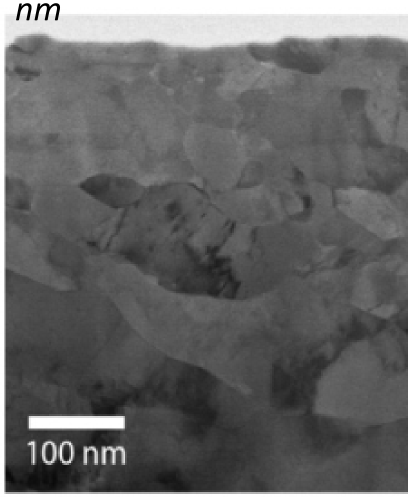
critical grain size = *17.4 nm*

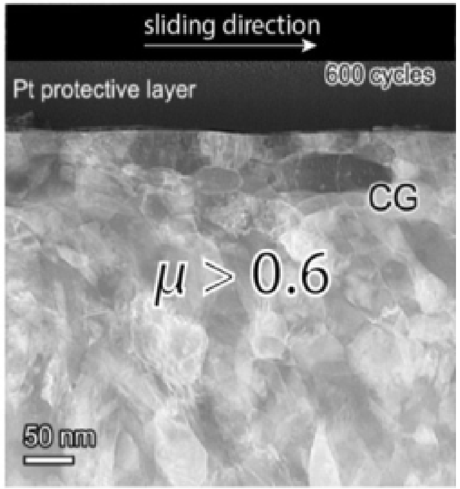
critical grain size = *11.8 nm*

critical grain size = *9.8 nm*

high friction





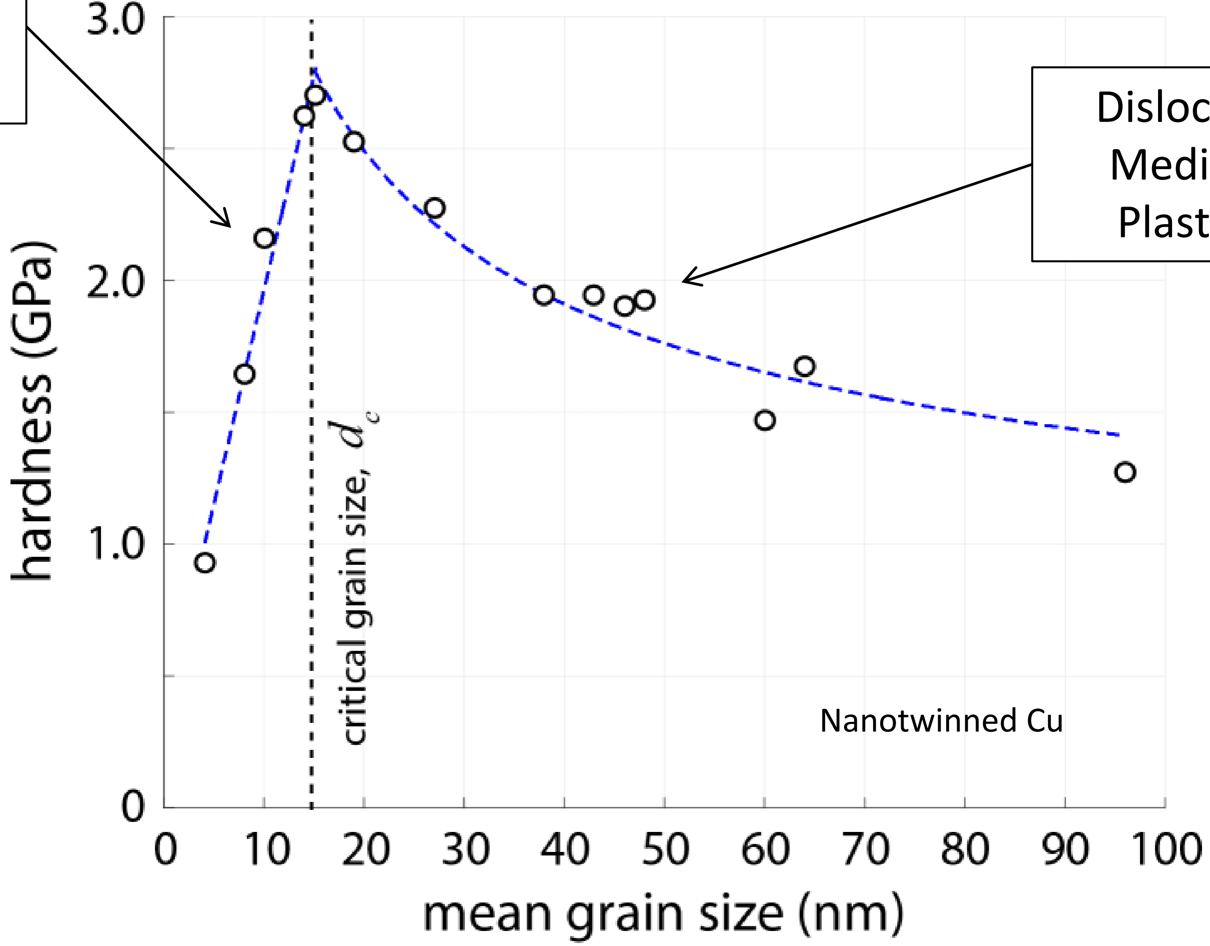


Prasad et al., Scripta Mat. 2011

Grain size and Materials Properties

Grain Boundary Sliding

MD
low friction



from Lu et al., Science, 2009

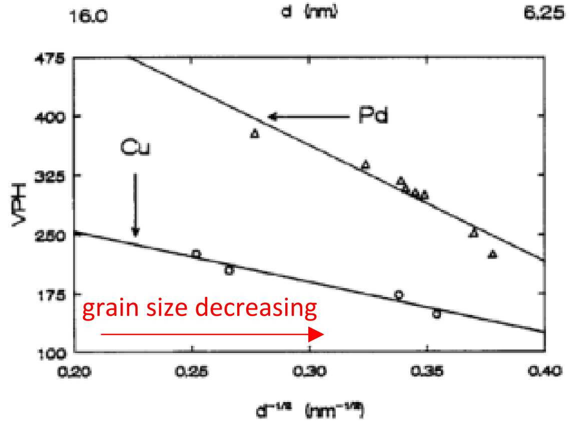
Dislocation Mediated Plasticity

MD
high friction

Hall-Petch Breakdown Occurs around 10 nm

FCC Cu and Pd experiments

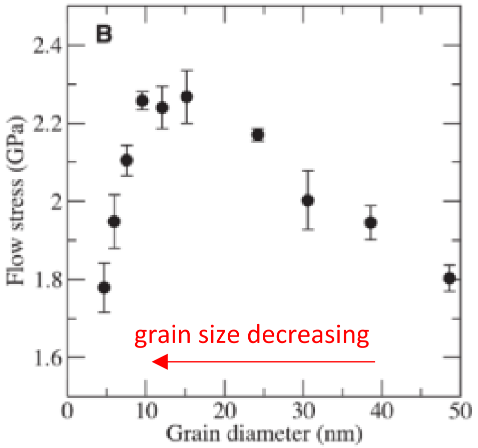
Chokshi, et al., Scripta Mat., 1989



grain size decreasing

FCC Cu simulations

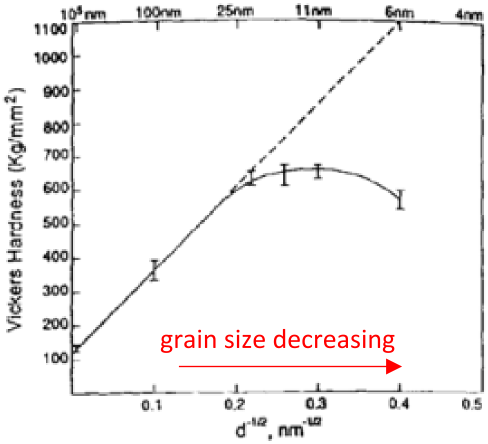
Schiötz and Jacobsen, Science, 2003



grain size decreasing

FCC Ni experiments

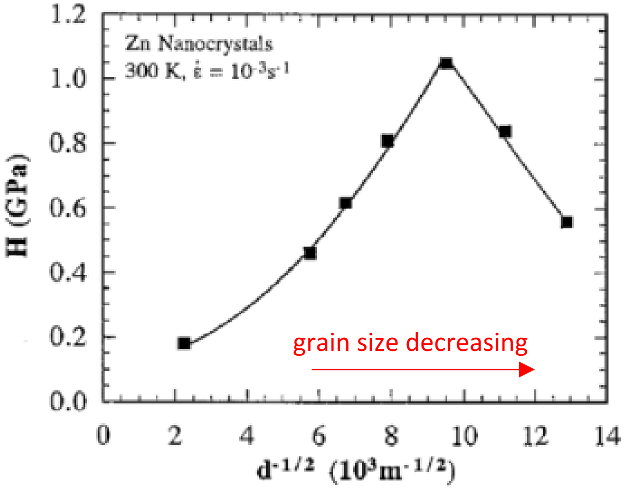
Erb, Nanostructured Matls., 1995



grain size decreasing

HCP Zn experiments

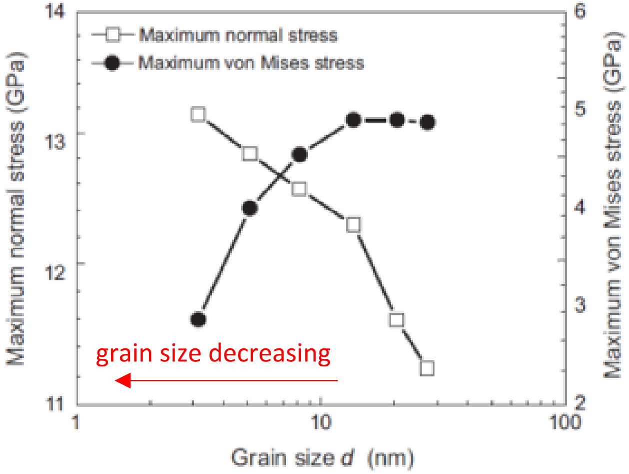
Conrad and Narayan, App. Phys. Lett., 2002



grain size decreasing

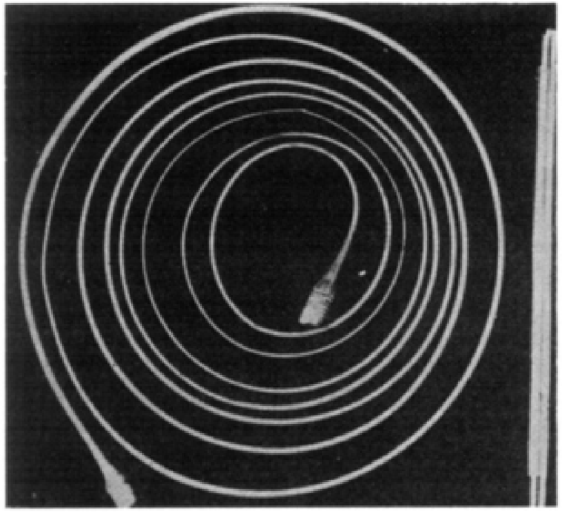
BCC Ta simulations

Tang, et al., Mat. Sci. & Eng. A, 2013



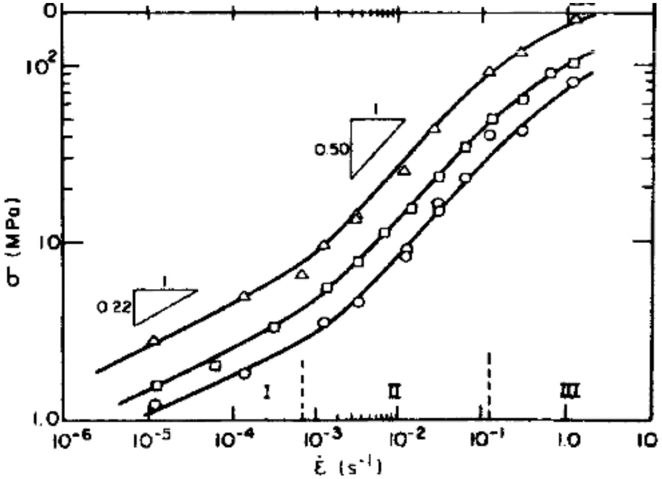
grain size decreasing

Link Between GBS and Superplasticity

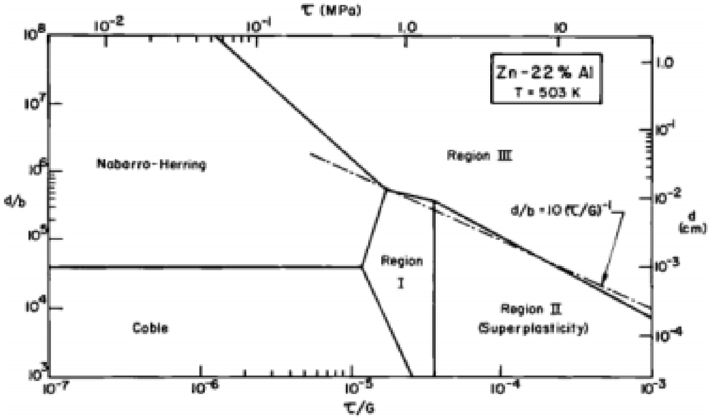


Edington, J.W., K.N. Melton, and C.P. Cutler. "Superplasticity." Progress in Materials Science, 1976

Edington, J.W., K.N. Melton, and C.P. Cutler. "Superplasticity." Progress in Materials Science, 1976



- General equation: $\dot{\varepsilon}^m = K(\sigma_f - \sigma_0)$
- When m=1, pure GBS
  - $\dot{\varepsilon} = \dfrac{\sigma_f - \sigma_0}{\eta}$
  - η = effective GB viscosity
  - Stress is linear with velocity
  - There is an offset stress



Langdon, J. Mater Sci. 2006

Grain boundaries act like a Bingham fluid with viscous sliding

Link Between Superplasticity and Friction?

$$F_f = \tau A$$ ← Classic Bowden & Tabor friction formula

Expand $\tau = \tau_0 + \alpha P + \beta \varepsilon^{m\cdot}$

$F_f = \tau_0 A + \alpha F_N + \beta A \dot{\varepsilon}^m$

$\tau_f = \tau_0 + \alpha \sigma_N + \beta \varepsilon^{\dot{m}}$ ← fundamental shear strength of an interface

At $F_N = 0$

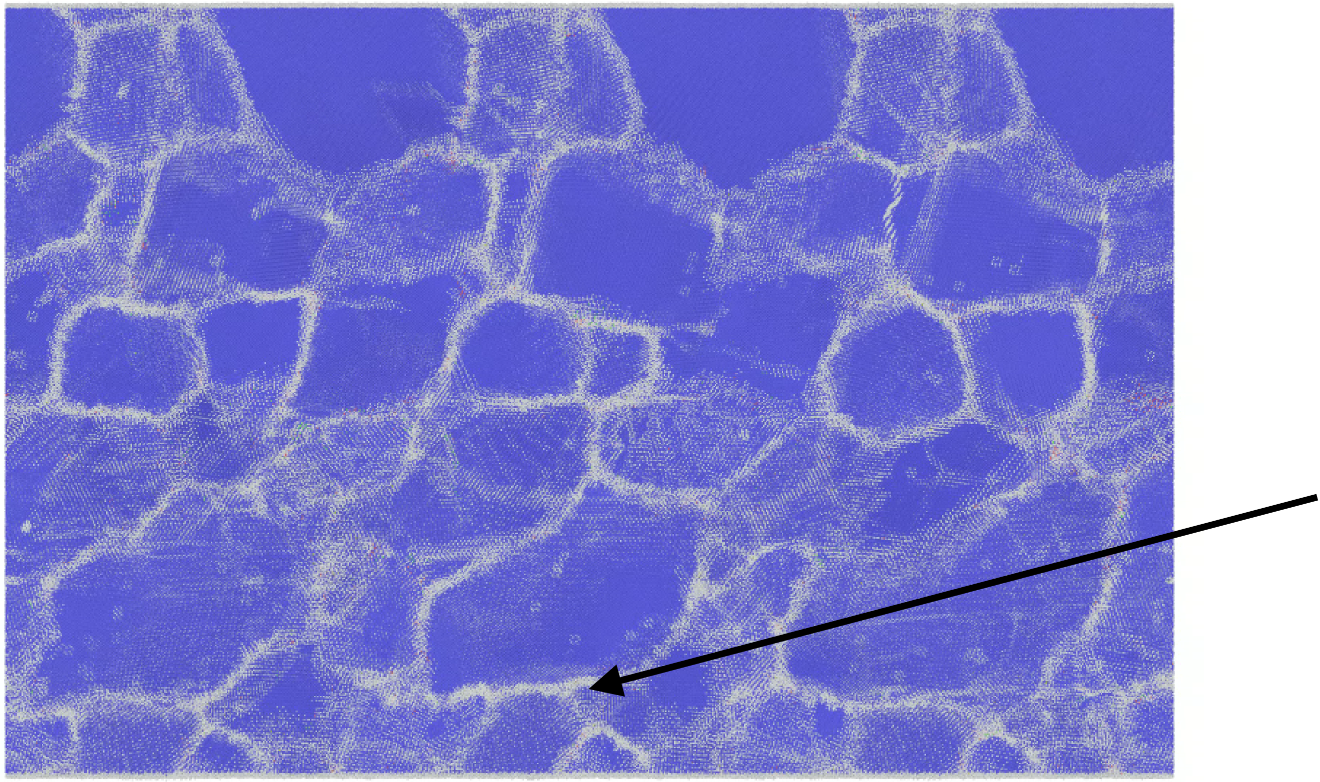
$\tau_f = \tau_0 + \beta \dot{\varepsilon}^m$

$Or: \dot{\varepsilon}^m = K(\tau_f - \tau_0)$ ← Superplasticity! (when m > 0.3)

- Extension of Bowden & Tabor's fundamental friction model
- Recovers superplasticity equations at $F_N=0$
- When pure GBS m= 1: $\tau_f = \tau_0 + \alpha\sigma_N + \gamma v$

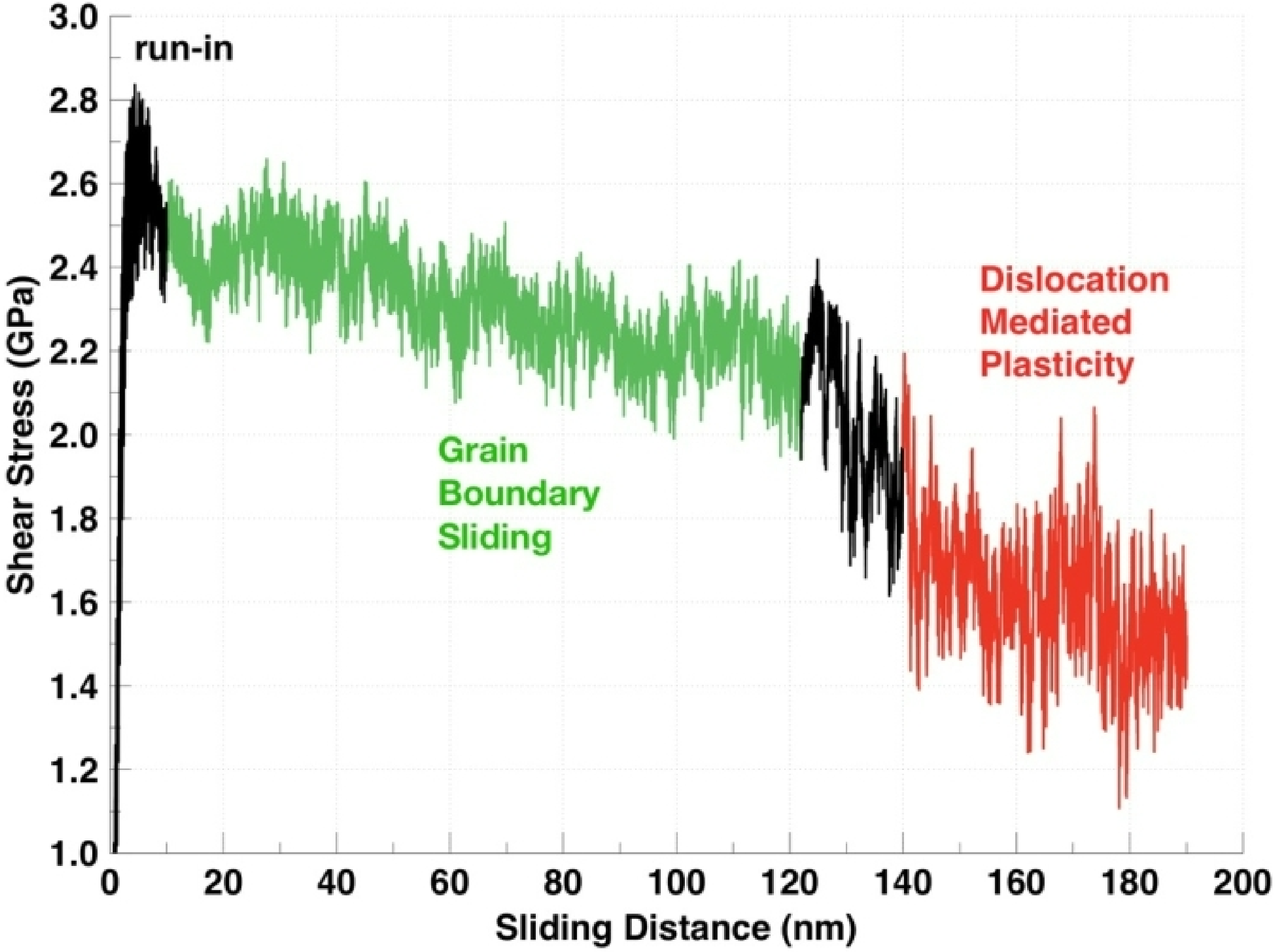
Pure GBS implies shear strength has a linear dependence on normal load and velocity with an offset stress

Evidence of GBS in MD simulations (Ta)


Grain boundary sliding here

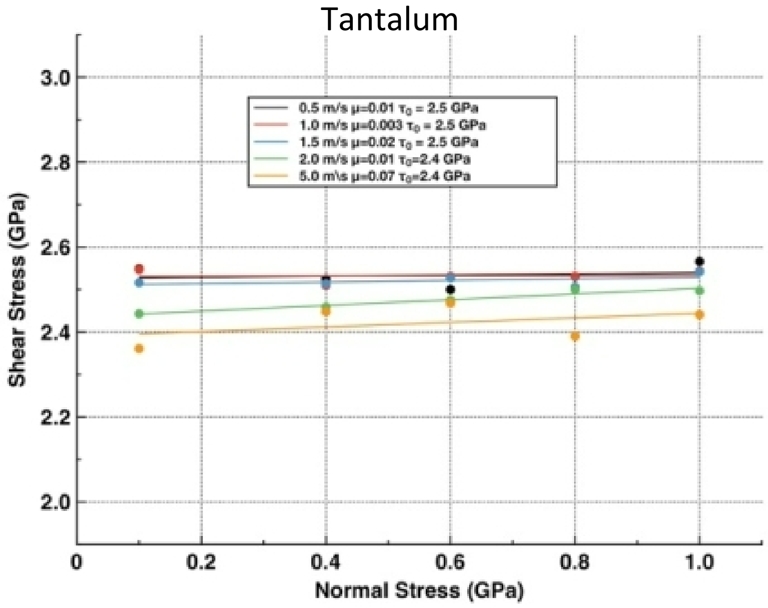
- Microstructure created with phase field
- Grains filled with BCC atoms to be ~10nm, randomly oriented
- Ravelo Ta potential (2013)
- Sheared at a range of velocities and normal loads
- Grains eventually grow, sliding transforms to dislocation mediated

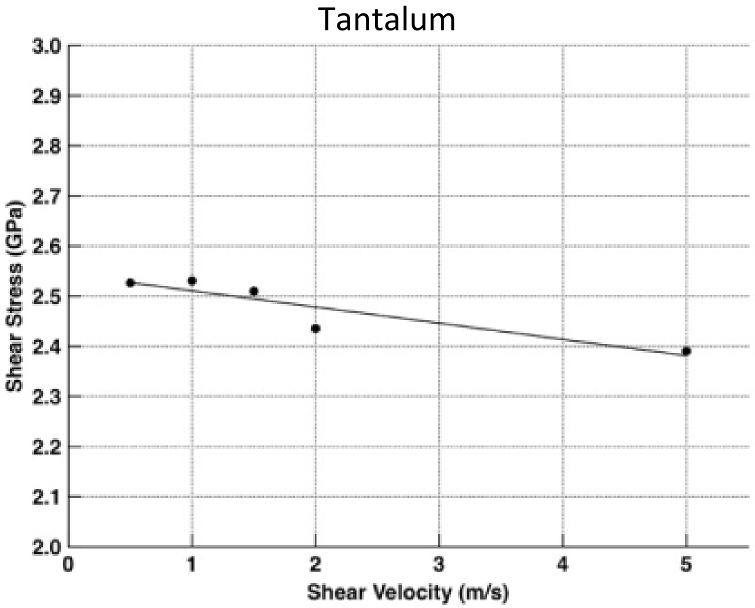
Stress is different between GBS and DMP



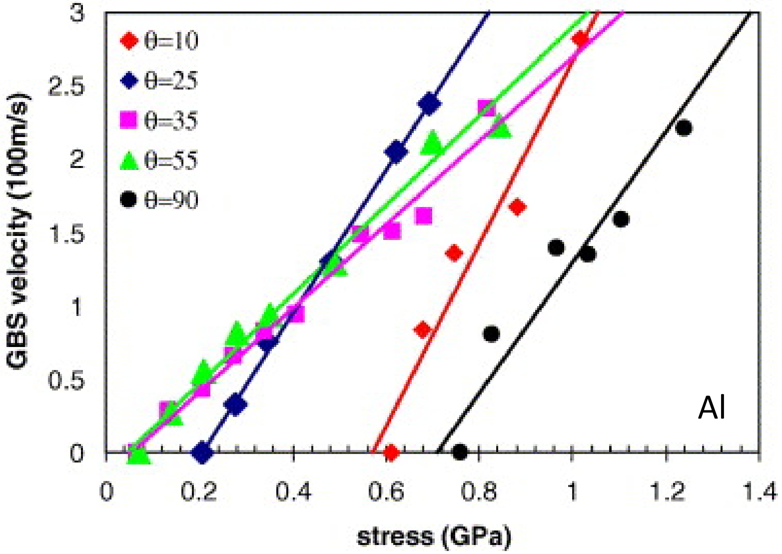
- Stress is *higher* during GBS
- Implies grain sizes
    - At/near peak for GBS (high stress)
    - Larger for DMP (lower stress)

Link Between GBS and Friction


Tantalum


Tantalum

- Simulations clearly show GBS
- Linear dependence of shear strength on velocity or strain rate
- Threshold stress (i.e. fundamental grain boundary stress) ~ 2.54 GPa
- Also seen in other metals
- What causes the stress?



Qi and Krajewski, Acta Mat. 2006

When Grain Boundaries Aren’t Available, Amorphization Occurs

From Kaibyshev, Mat. Sci. & Eng., 2002:

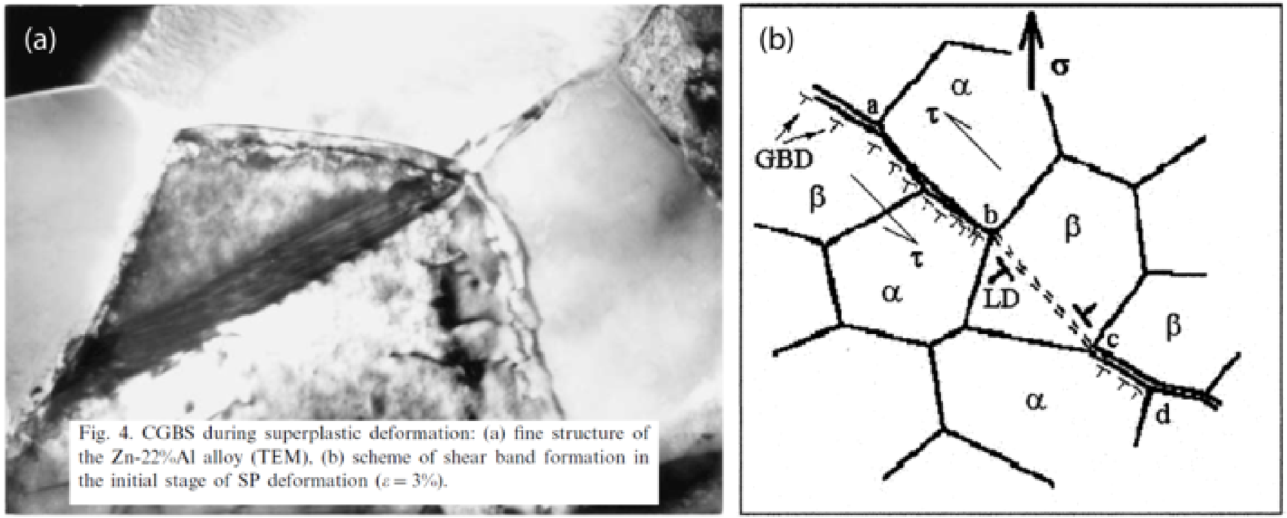
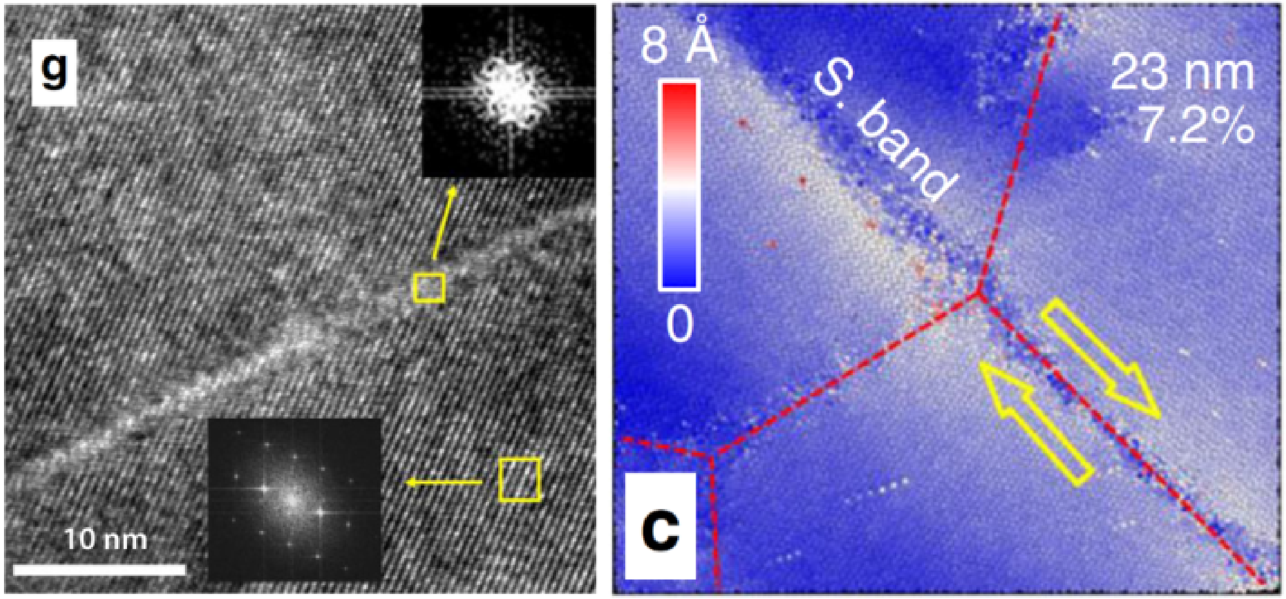


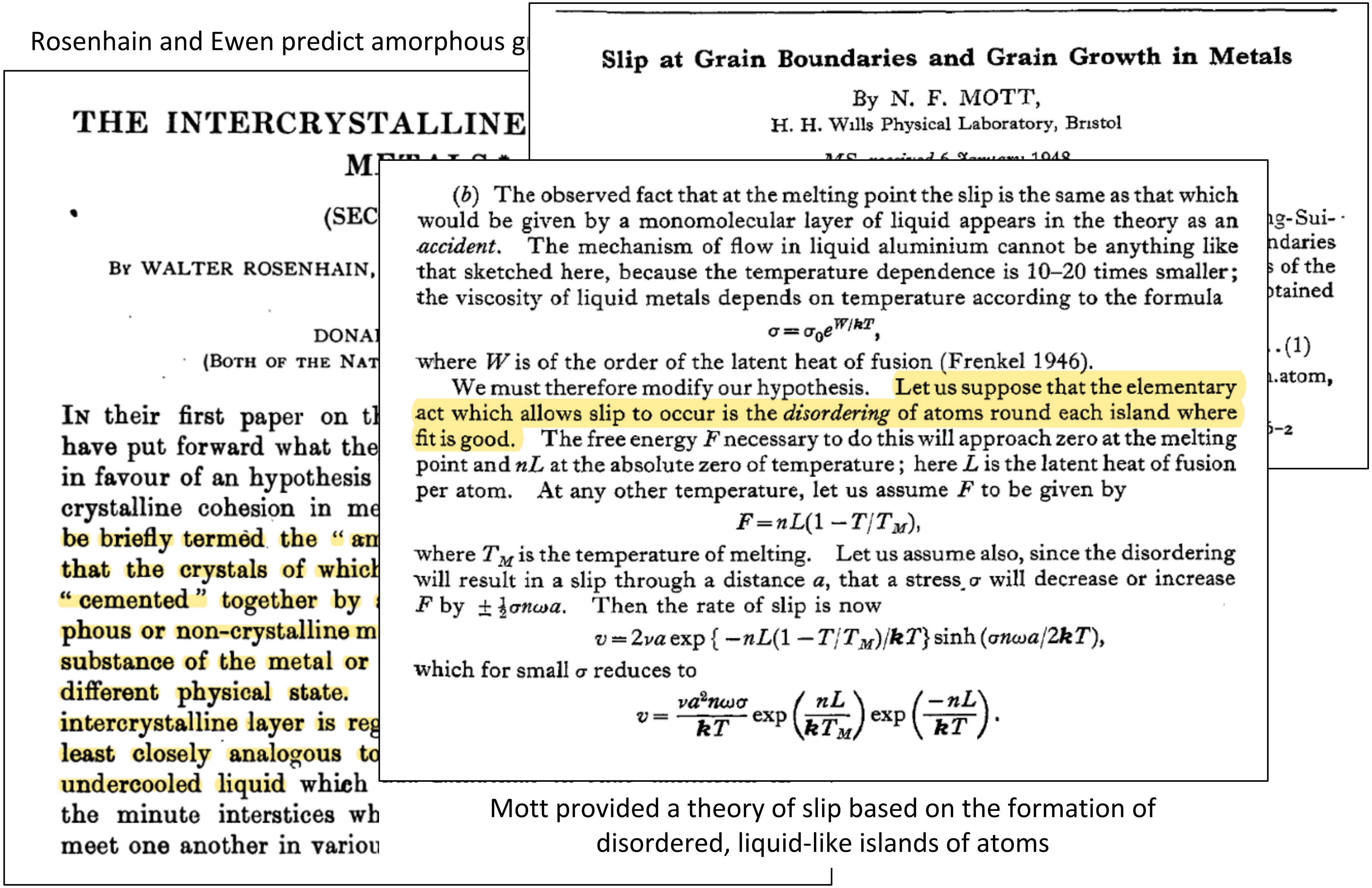
Fig. 4. CGBS during superplastic deformation: (a) fine structure of the Zn-22%Al alloy (TEM), (b) scheme of shear band formation in the initial stage of SP deformation ($\varepsilon = 3\%$).

From Luo, et al., Nat. Comm., 2019:



The Idea of Amorphization During Deformation is Over 100 Years Old!

Rosenhain and Ewen predict amorphous g



THE INTERCRYSTALLINE
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By WALTER ROSENHAIN,

DONA
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In their first paper on th
have put forward what the
in favour of an hypothesis
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"cemented" together by
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substance of the metal or
different physical state.
intercrystalline layer is reg
least closely analogous to
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Slip at Grain Boundaries and Grain Growth in Metals

By N. F. MOTT,
H. H. Wills Physical Laboratory, Bristol

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..(1)
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5–2

(*b*) The observed fact that at the melting point the slip is the same as that which would be given by a monomolecular layer of liquid appears in the theory as an *accident*. The mechanism of flow in liquid aluminium cannot be anything like that sketched here, because the temperature dependence is 10–20 times smaller; the viscosity of liquid metals depends on temperature according to the formula

$$\sigma = \sigma_0 e^{W/kT},$$

where W is of the order of the latent heat of fusion (Frenkel 1946).

We must therefore modify our hypothesis. Let us suppose that the elementary act which allows slip to occur is the *disordering* of atoms round each island where fit is good. The free energy F necessary to do this will approach zero at the melting point and nL at the absolute zero of temperature; here L is the latent heat of fusion per atom. At any other temperature, let us assume F to be given by

$$F = nL(1 - T/T_M),$$

where T_M is the temperature of melting. Let us assume also, since the disordering will result in a slip through a distance a, that a stress σ will decrease or increase F by $\pm\frac{1}{2}\sigma n\omega a$. Then the rate of slip is now

$$v = 2\nu a \exp\{-nL(1 - T/T_M)/\boldsymbol{k}T\} \sinh(\sigma n\omega a/2\boldsymbol{k}T),$$

which for small σ reduces to

$$v = \frac{\nu a^2 n\omega\sigma}{\boldsymbol{k}T} \exp\left(\frac{nL}{\boldsymbol{k}T_M}\right) \exp\left(\frac{-nL}{\boldsymbol{k}T}\right).$$

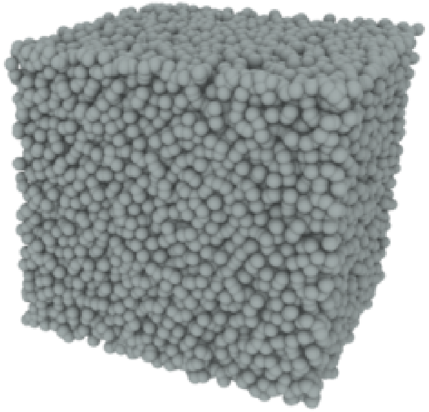
Mott provided a theory of slip based on the formation of disordered, liquid-like islands of atoms

Chandross and Argibay, Tribology Letters (2021).

What is the energetic cost for amorphization?

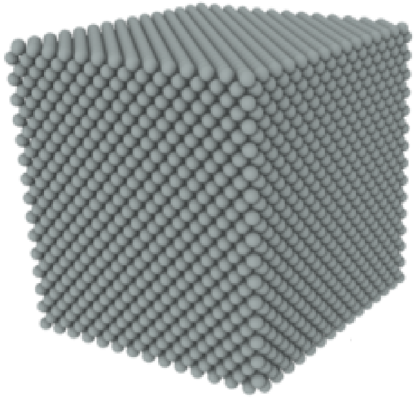
- Frenkel model of viscosity: $\dot{\varepsilon} = \dot{\varepsilon}_0 \, exp\left(-\frac{\Delta F - \tau V^*}{k_B T}\right)$
- Mott (1948): "… let us assume F to be given by $F = nL(1\text{-}T/T_m)$

amorphous solid



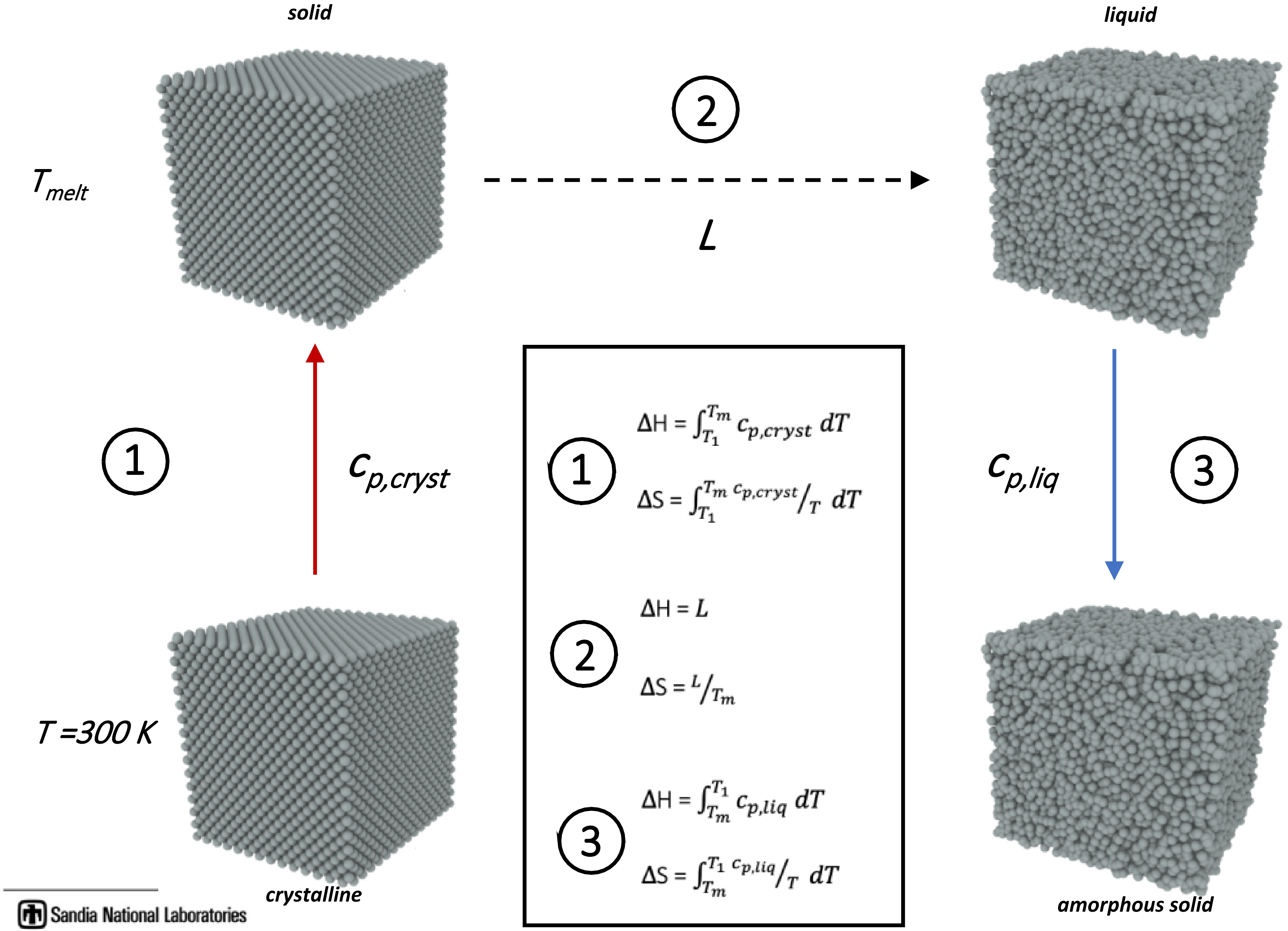
$$\dot{\varepsilon}_{tot} = \dot{\varepsilon}_{GBS} \, exp\left(-\frac{\Delta F \ - \ \tau V^*}{k_B T}\right)$$

crystalline



$\Delta \boldsymbol{F}$?

Calculation is similar to undercooled liquid



①

$$\Delta H = \int_{T_1}^{T_m} c_{p,cryst} \, dT$$

$$\Delta S = \int_{T_1}^{T_m} {}^{c_{p,cryst}}/_{T} \, dT$$

②

$$\Delta H = L$$

$$\Delta S = {}^{L}/_{T_m}$$

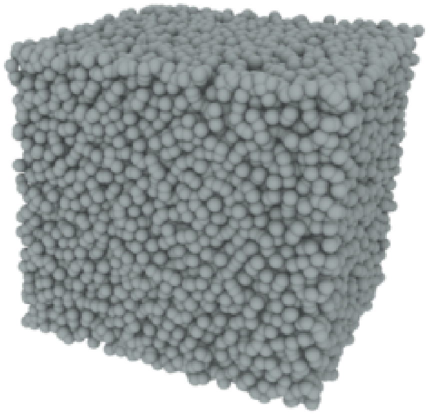
③

$$\Delta H = \int_{T_m}^{T_1} c_{p,liq} \, dT$$

$$\Delta S = \int_{T_m}^{T_1} {}^{c_{p,liq}}/_{T} \, dT$$

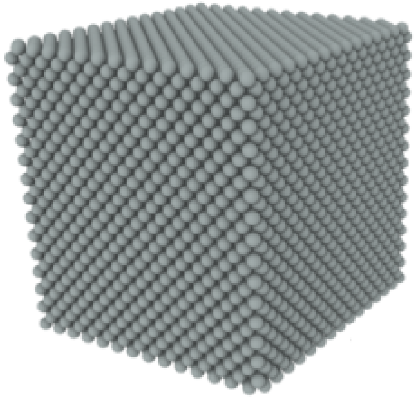
Energy Difference is Related to Heat of Fusion

amorphous solid



$$\Delta F = L\left(1 - \frac{T}{T_m}\right)$$

crystalline



$$\tau(d) = L\left(1 - \frac{T}{T_m}\right)\frac{\rho_L}{M}\left(\frac{d-\delta}{d}\right)^3 - \frac{kT}{b^3}$$

volume fraction of GB to crystal

heat of fusion

homologous temperature

amorphous metallic atomic volume

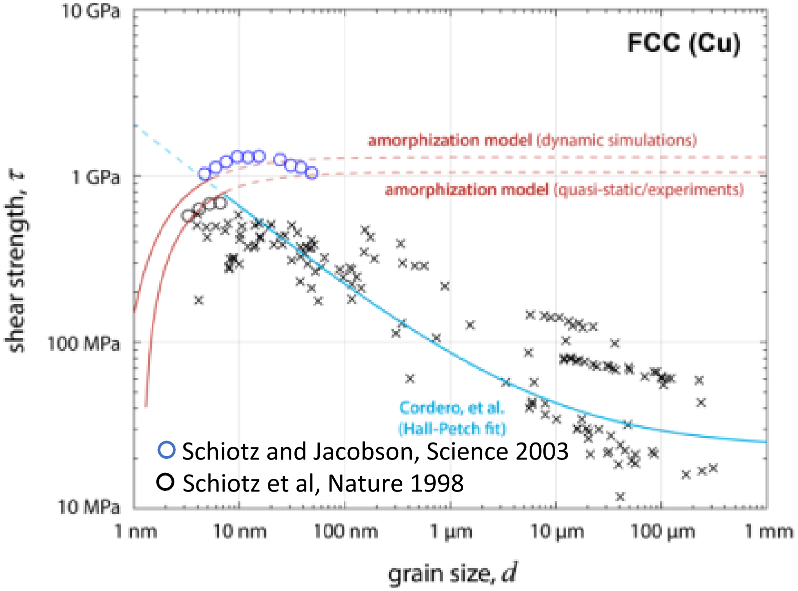
thermal energy

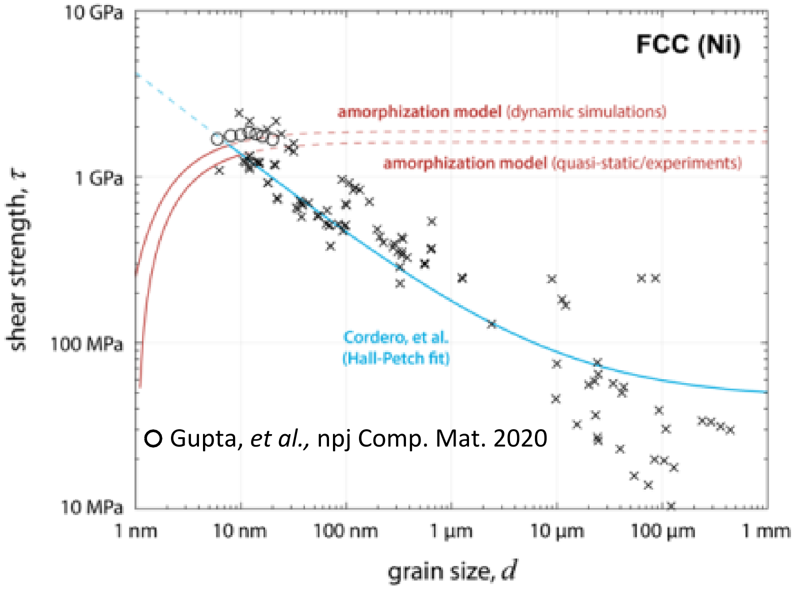
No adjustable parameters!

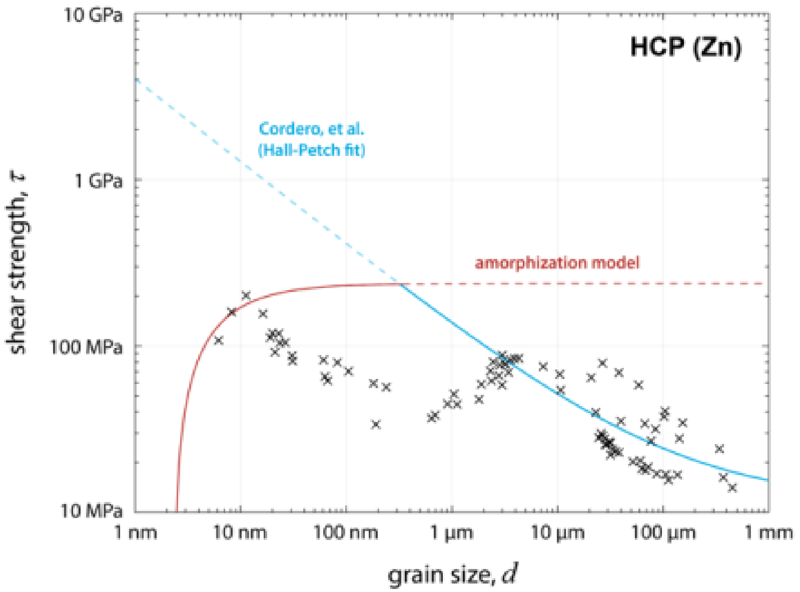
Chandross and Argibay, Phys. Rev. Lett. 2020

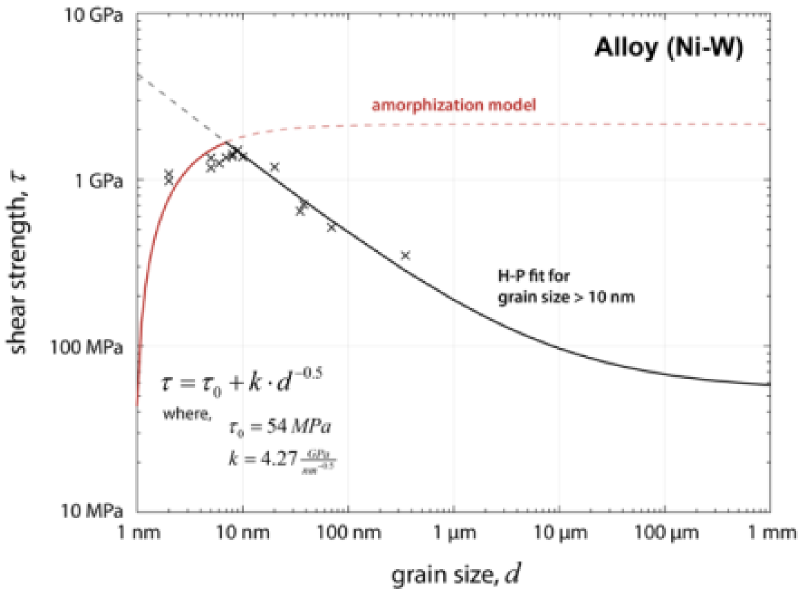
Model Works for a Variety of Metals

x Cordero, *et al.*, Int. Mat. Rev. *2016*





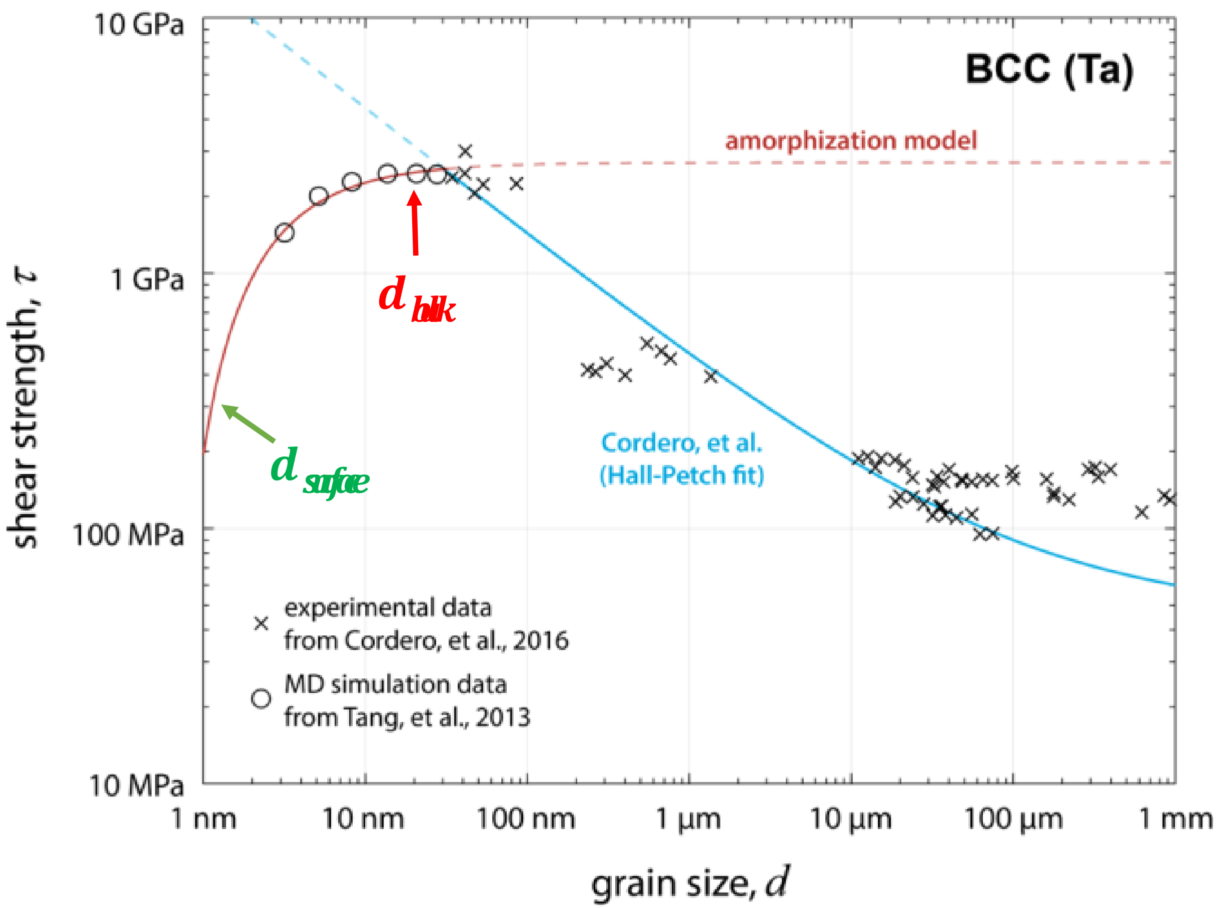




Chandross and Argibay, Phys. Rev. Lett. 2020

No adjustable parameters!

Minimum Friction Coefficient for Metals

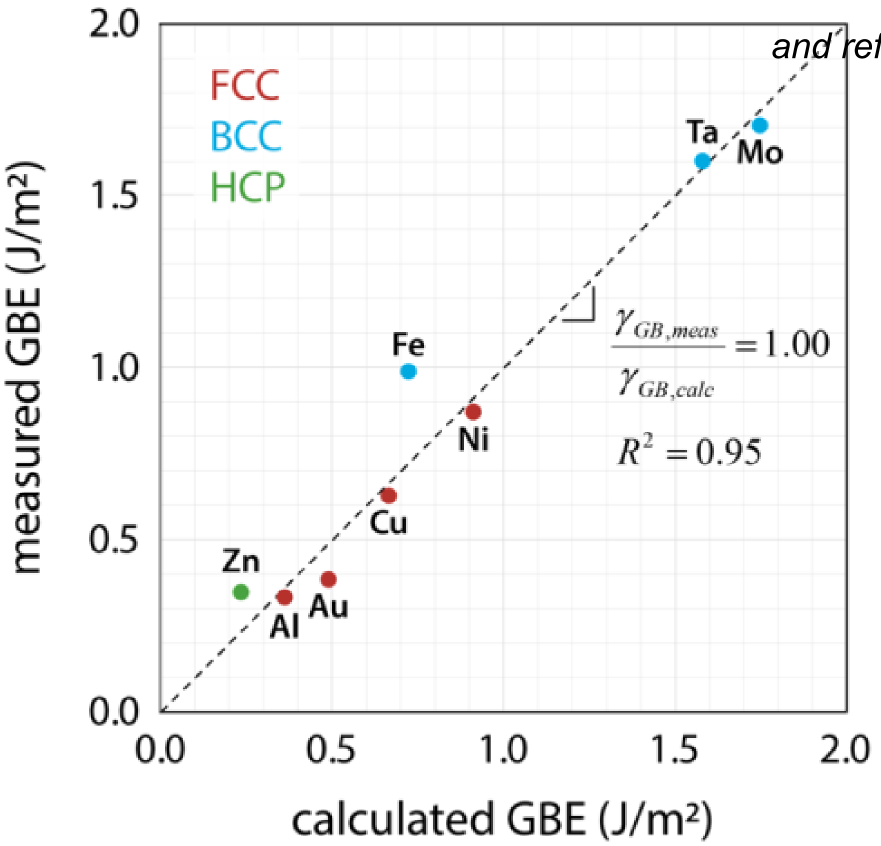


Bowden & Tabor: $\mu = \frac{\tau}{H} \xrightarrow{\text{Tabor}} \mu = \frac{\tau}{3 \cdot \sigma_Y} \xrightarrow{\text{Von Mises}} \mu = \frac{\tau\left(d_{surface}\right)}{3\sqrt{3} \cdot \tau\left(d_{bulk}\right)}$

Minimum at $d_{surface}$ at amorphous limit, d_{bulk} at peak => $\mu_{min} = 0.16$

Another Prediction: Grain Boundary Energy

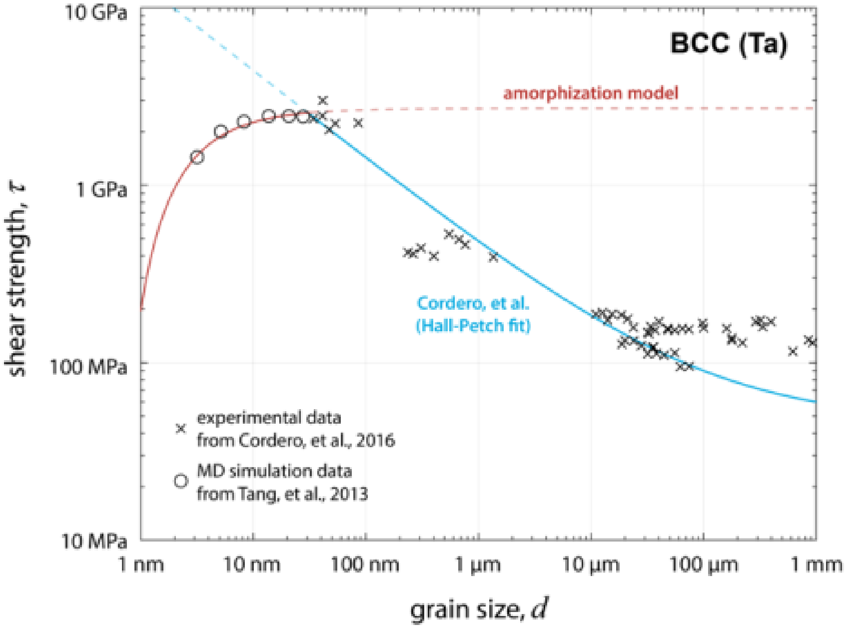
Chandross and Argibay, Phys. Rev. Lett. 2020
and references therein



- Amorphization related to creation of new high-angle grain boundaries
- Implies a relationship between amorphization energy and GBE
- Similar discussion in Shvindlerman and Gottstein, *Grain Boundary Migration in Metals* (2009)

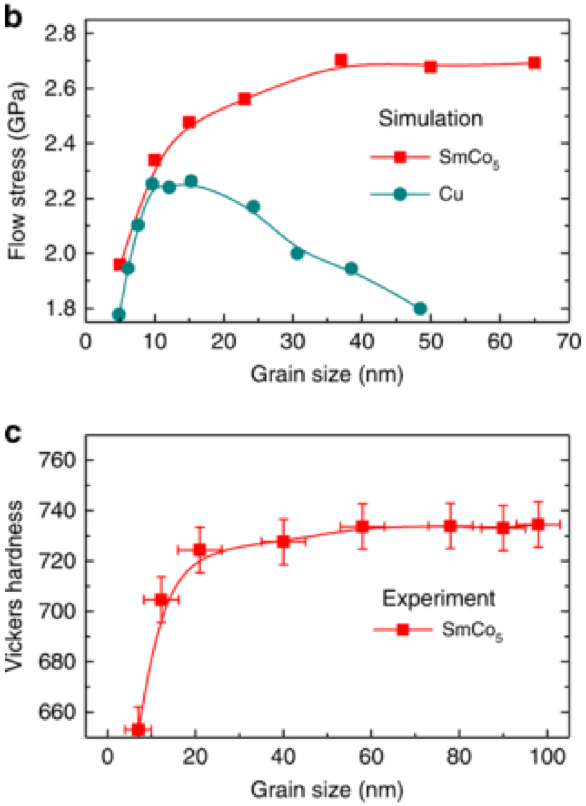
The Plateau Seems to be Real

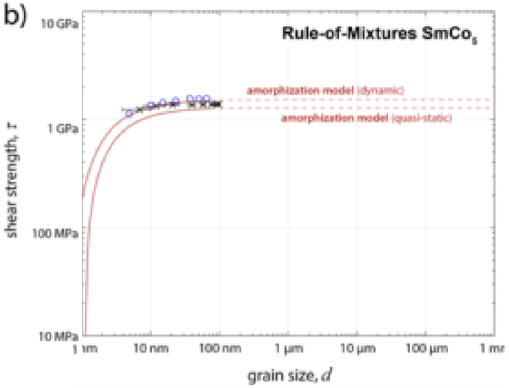
Hinkle, et al., *Phys. Rev. Mater.* 2020



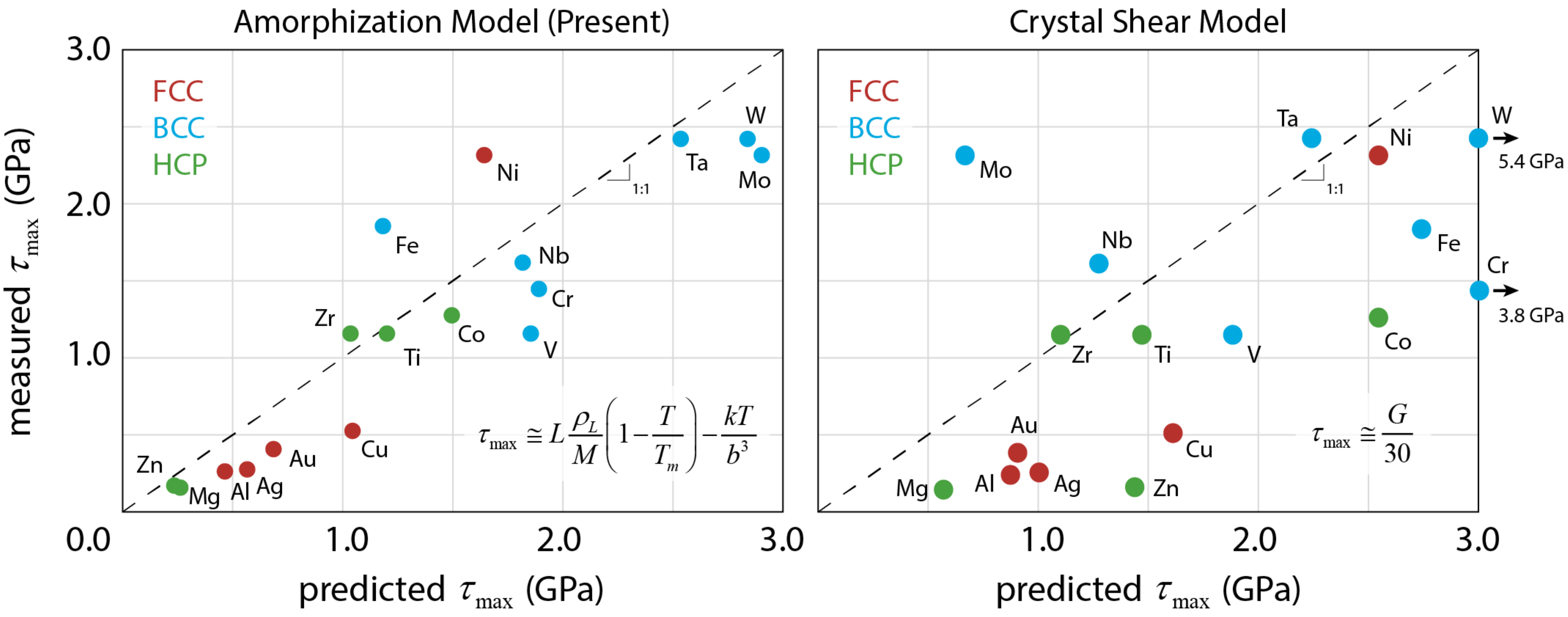
- Plateau in the inverse-HP region is clear in the model
- Experiments show this as well
  - $SmCo_5$: Luo, et al., *Nature Comm.* 2019
  - Ni: Gupta, *et al.,* npj Comp. Mat. 2020
- Implies a maximum achievable strength

Luo, et al., *Nature Comm.* 2019





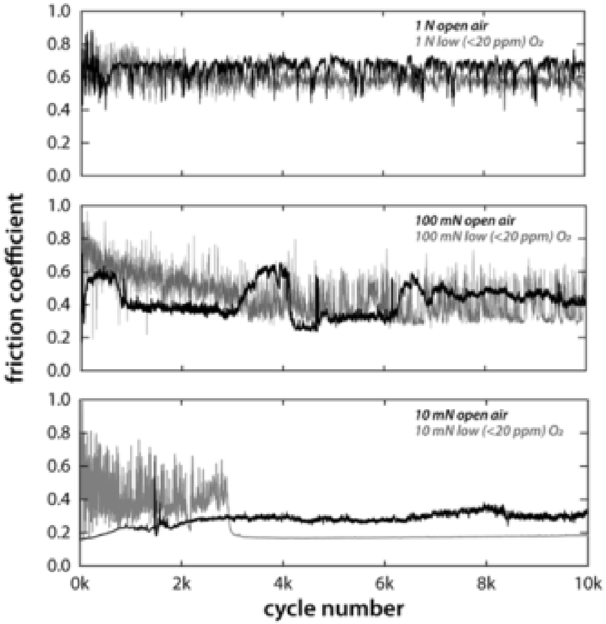
Prediction: Ultimate Strength of Pure Metals



- Maximum strength is at the peak of the HP curve (at crossover with amorphization curve)
- Very close to asymptote from our model
- Implies asymptote should relate to maximum strength
- The ”standard” value of G/30 does a poor job

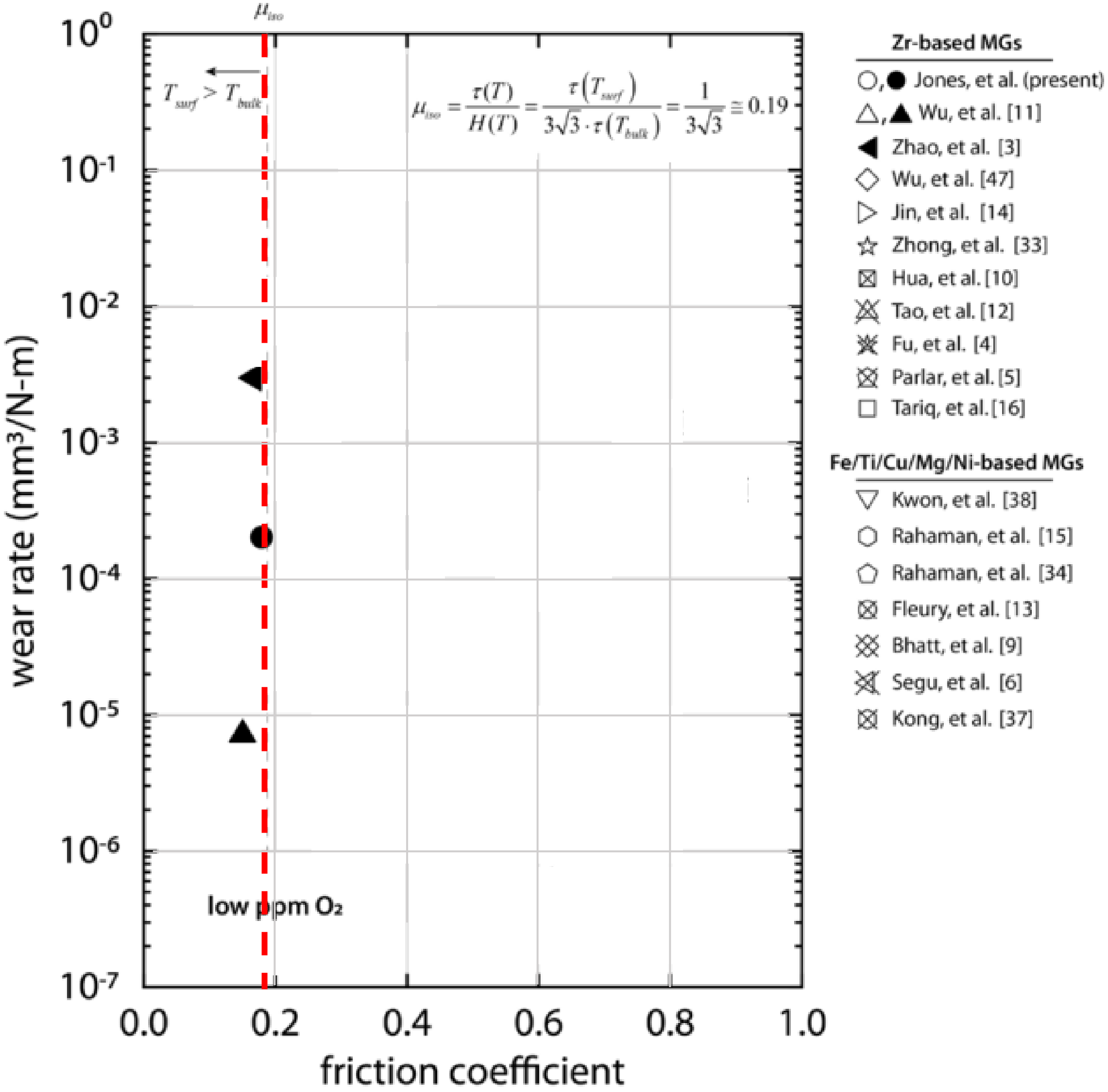
Chandross and Argibay, Phys. Rev. Lett. 2020
and references therein

Prediction: Friction of amorphous alloys



- Oxidation affects friction in metallic glasses
- Use Bowden and Tabor relation again
- Surface strength is the same as bulk strength
- Predicts $\mu \cong 0.19$ *without oxidation*

$$\mu_{iso} = \frac{\tau(T)}{H(T)} = \frac{\tau\left(T_{surf}\right)}{3\sqrt{3}\cdot\tau\left(T_{bulk}\right)} = \frac{1}{3\sqrt{3}} \cong 0.19$$



Jones, *et al.*, Tribology Letters (2020)

Conclusions

- GBS is linked to inverse H-P and low friction
  - Experiments and simulations
    - Pure metals (Cu, Ni…)
    - Alloys (NiW, $SmCo_5$…)

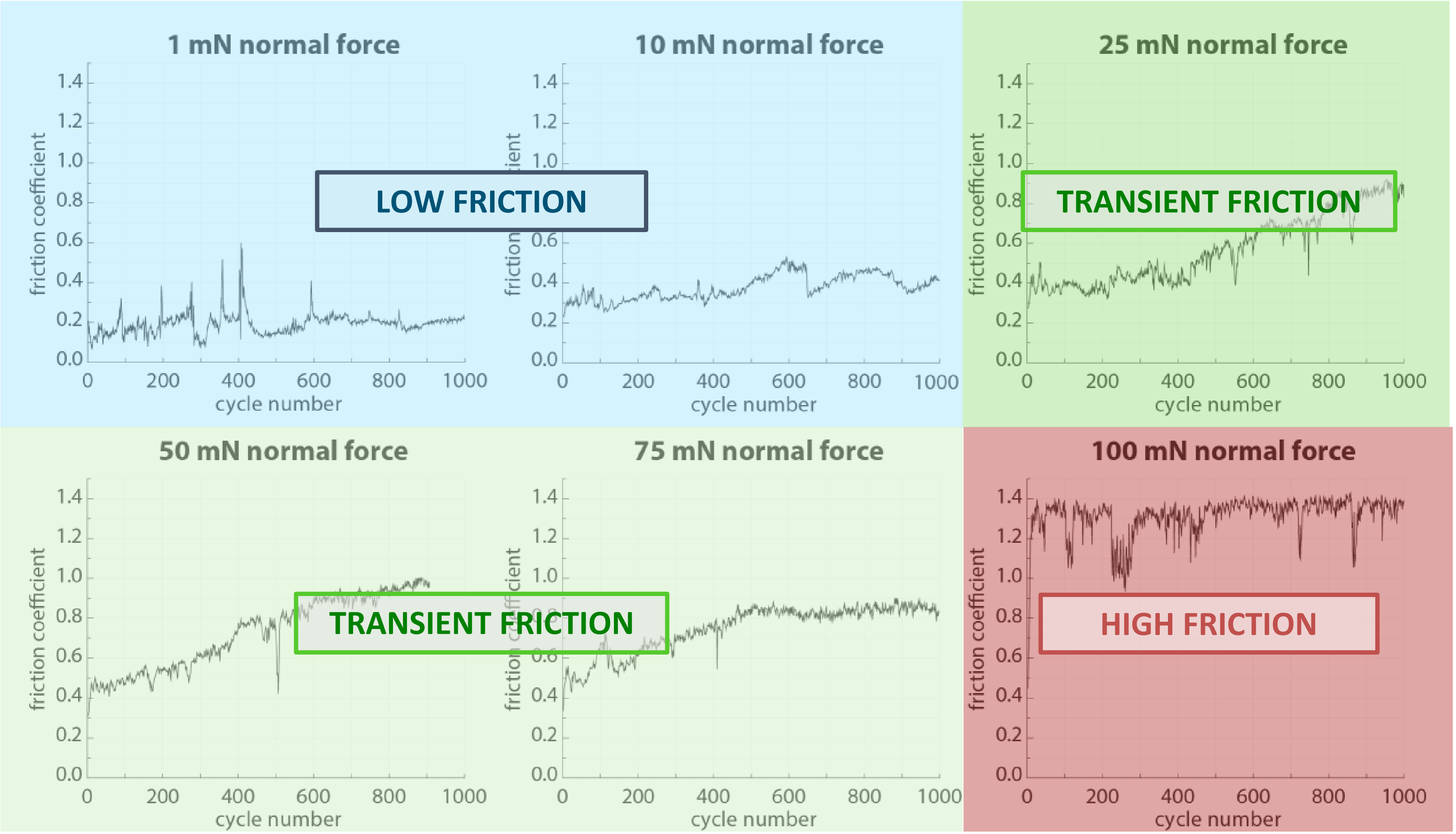
- Tribological experiments maintain inverse H-P regime
  - High strain rates
  - Repeated contact

- Link to superplasticity
  - Linear strain rate dependence
  - Implies new potential for friction models

- GBS can be described as viscous flow
  - Stress is related to fundamental bond strength
  - Enables predictions of strength and friction

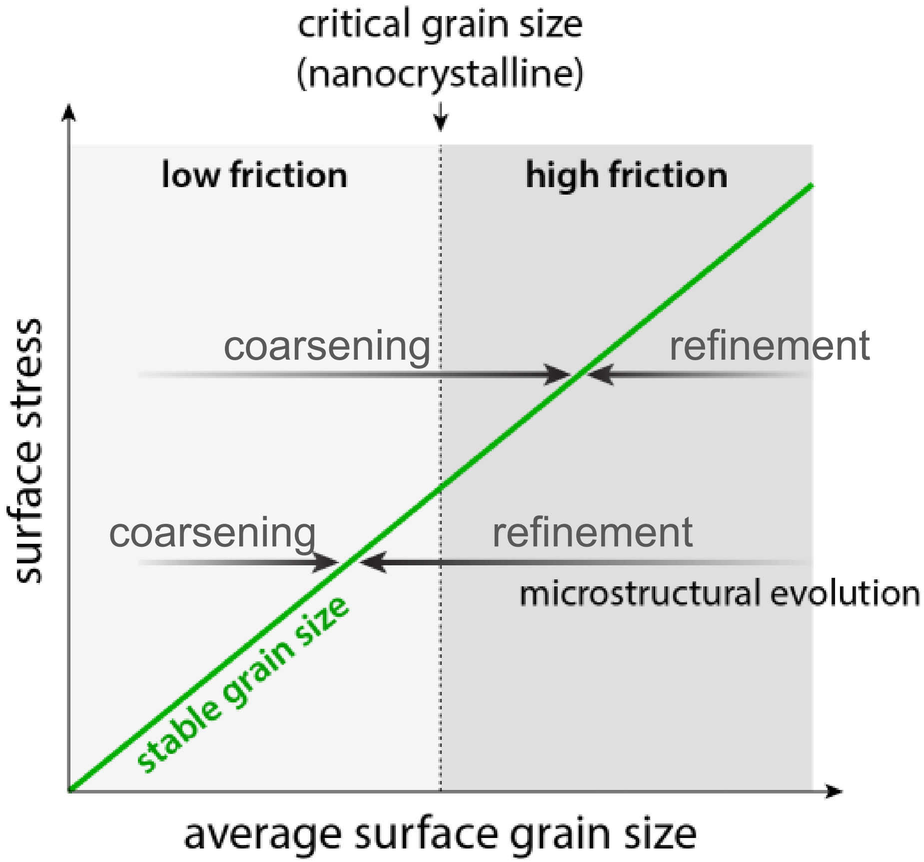
What do we know? Friction depends on applied load

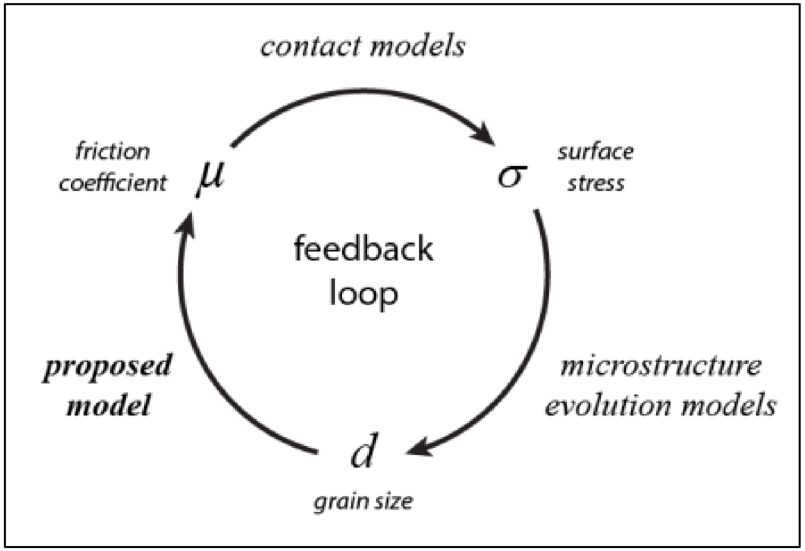
(Pure Au in dry N_2)



Three different friction regimes, with transitions.

Proposed stress-dependent steady-state (asymptotic) grain size



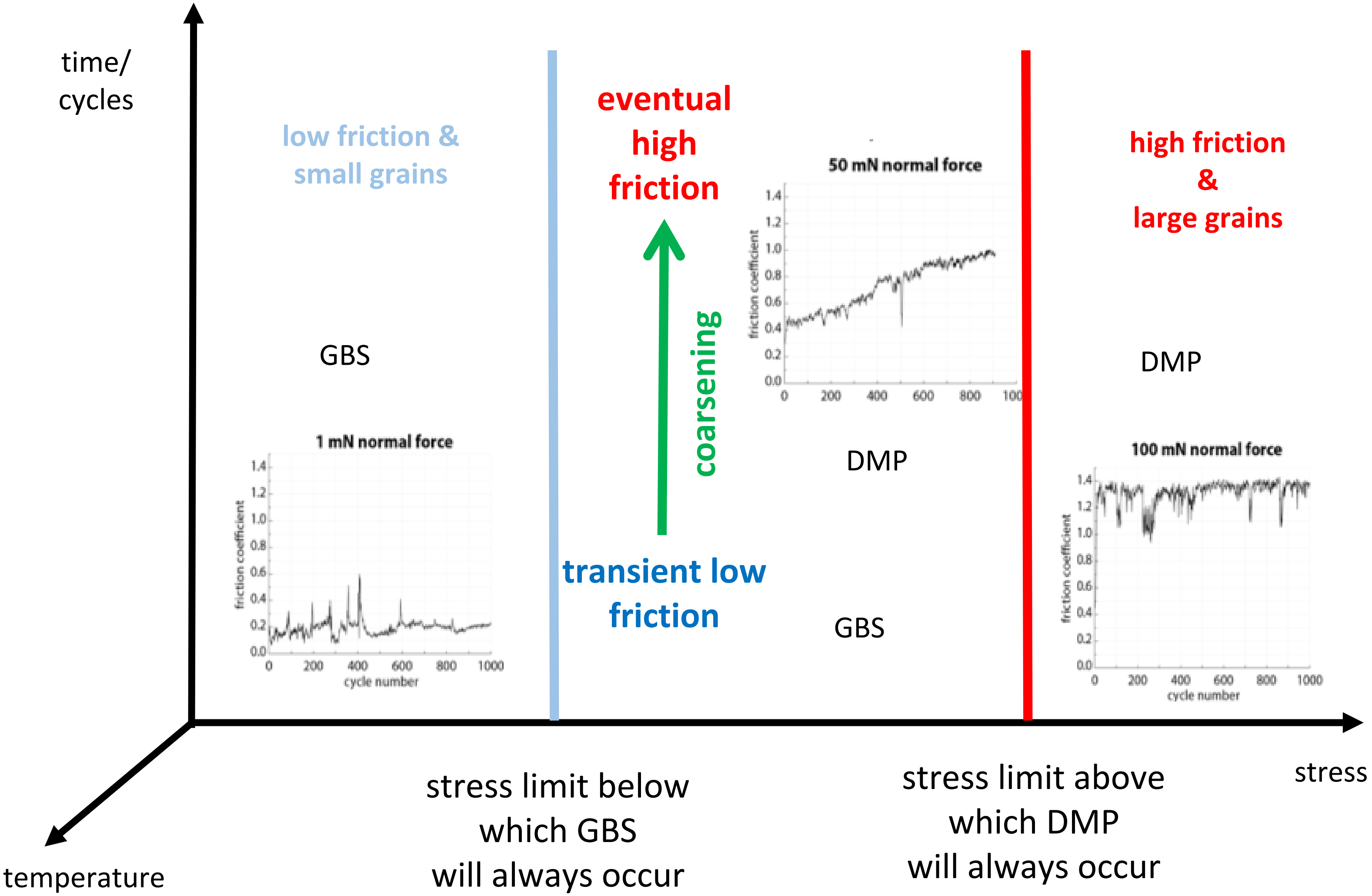


- Effective refinement from recrystallization (Zener & Holloman, 1944; McQueen et al., 1967)
- Known in rocks and ice cores (Derby et al., 1992)
- Recently extended to metals under severe plastic deformation (Pougis et al., 2014)

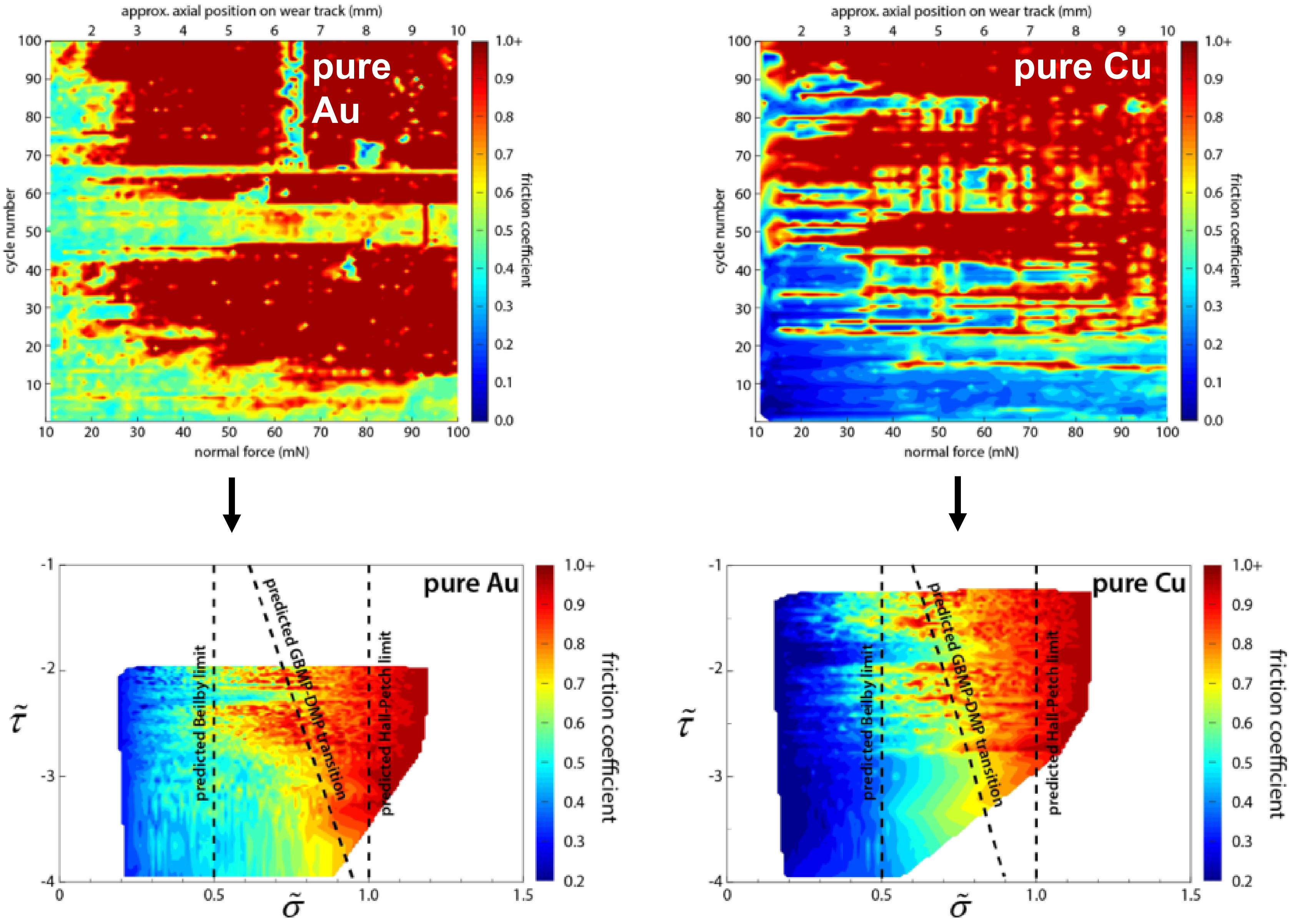
Argibay, et al., ***J. Mat. Sci. (2017)***

Generalized Friction Map for Metals

Argibay, Chandross, Cheng, Michael; J. Mater. Sci. (2017)

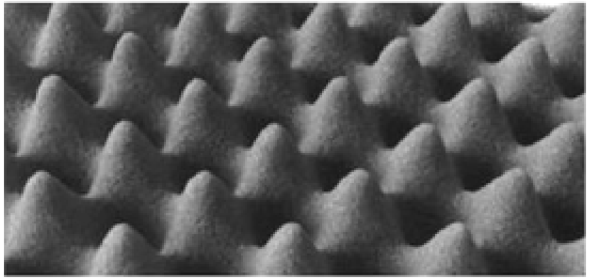


Model Predicts Stress Limits Well

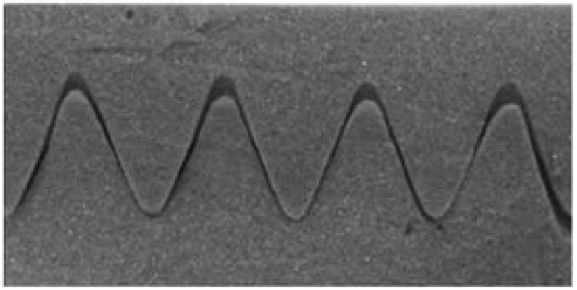


The Mechanism Behind High and Low Friction in Metals

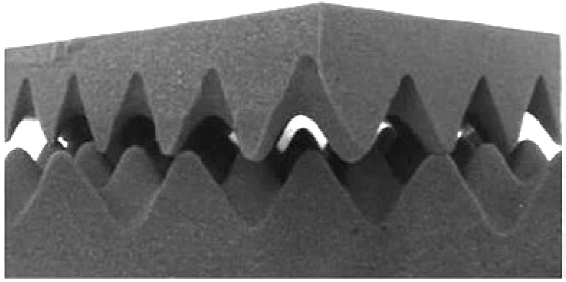
Atomic lattices have periodicity



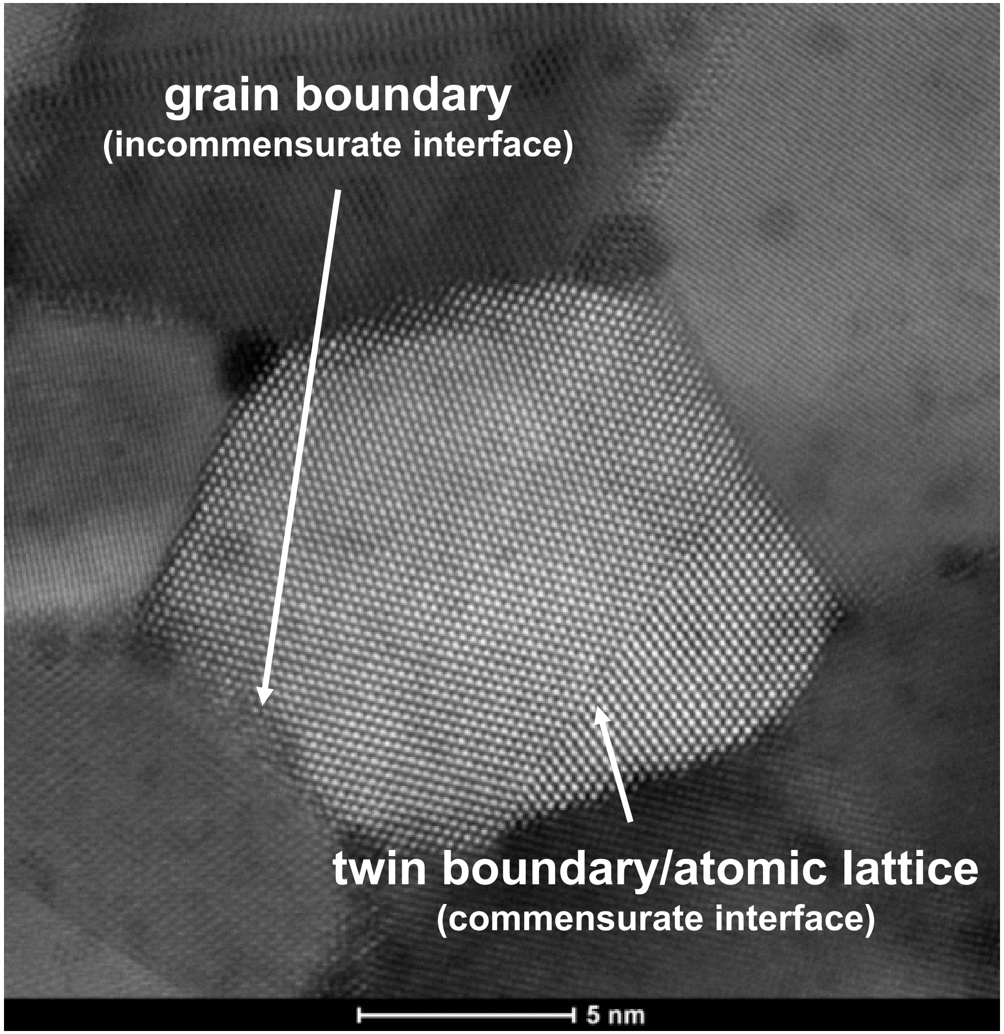
Commensurate interface
(higher energy barrier/higher μ)



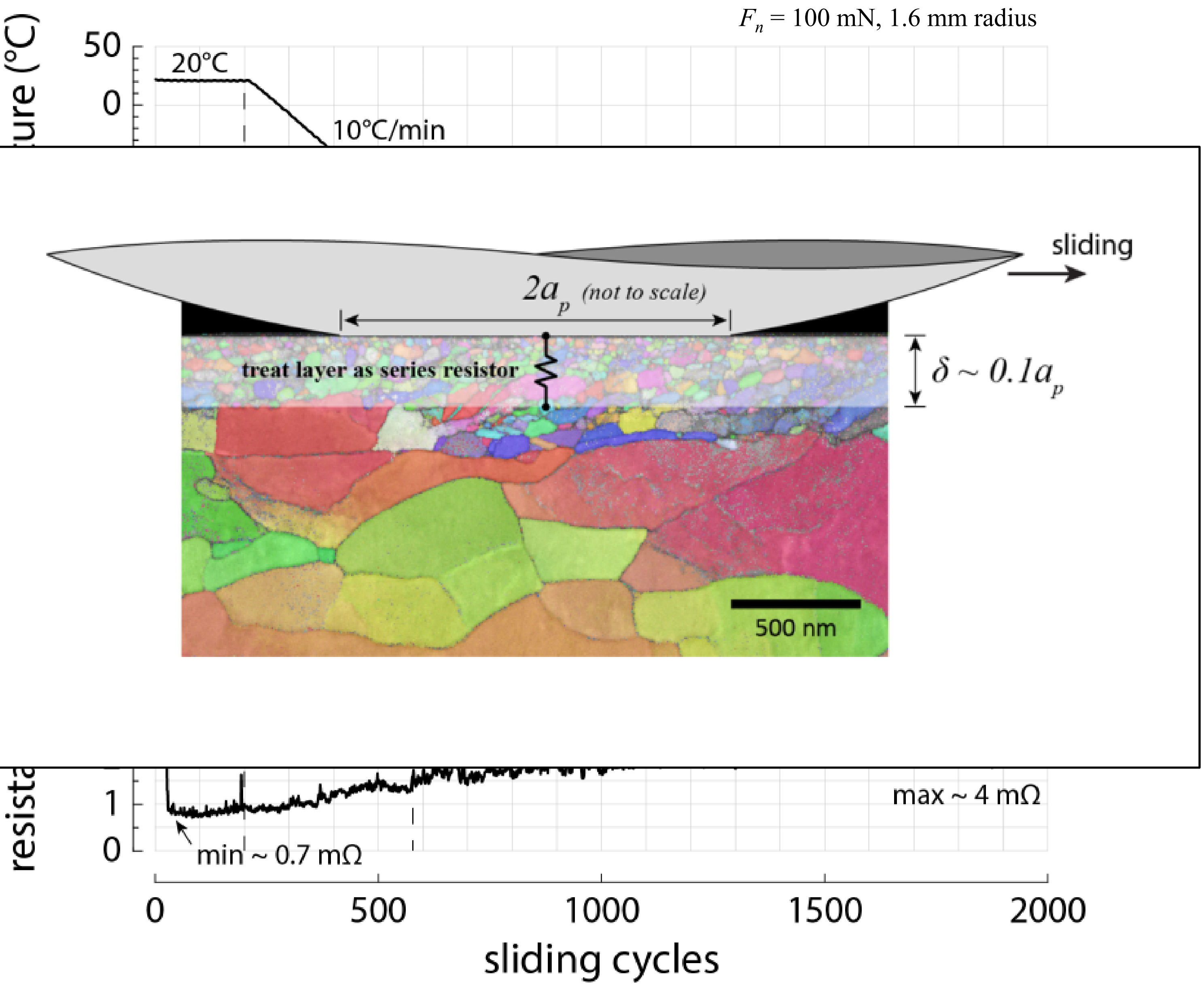
Incommensurate interface
(lower energy barrier/low μ)



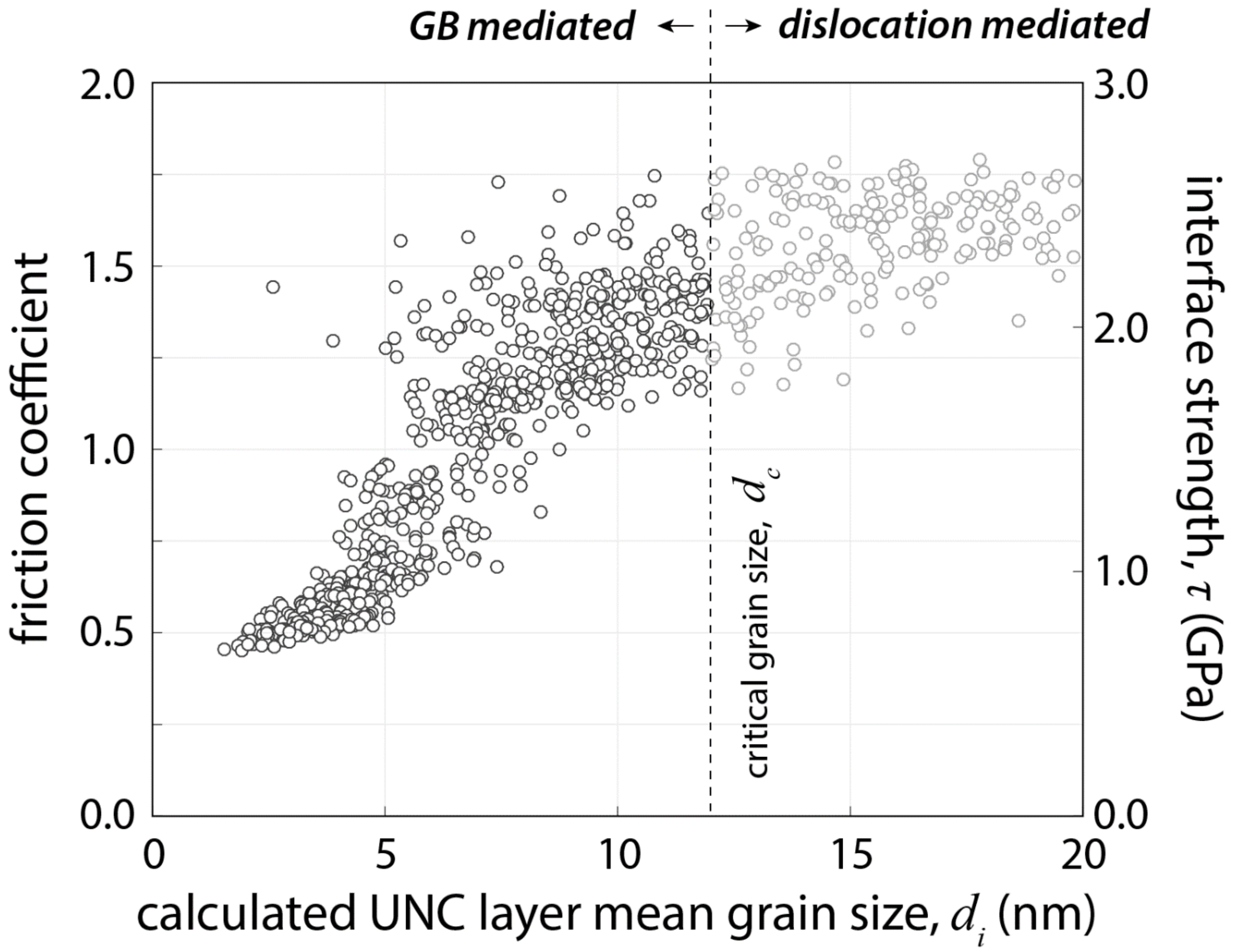
High resolution TEM



Evidence for GBS as a Low Friction Mechanism

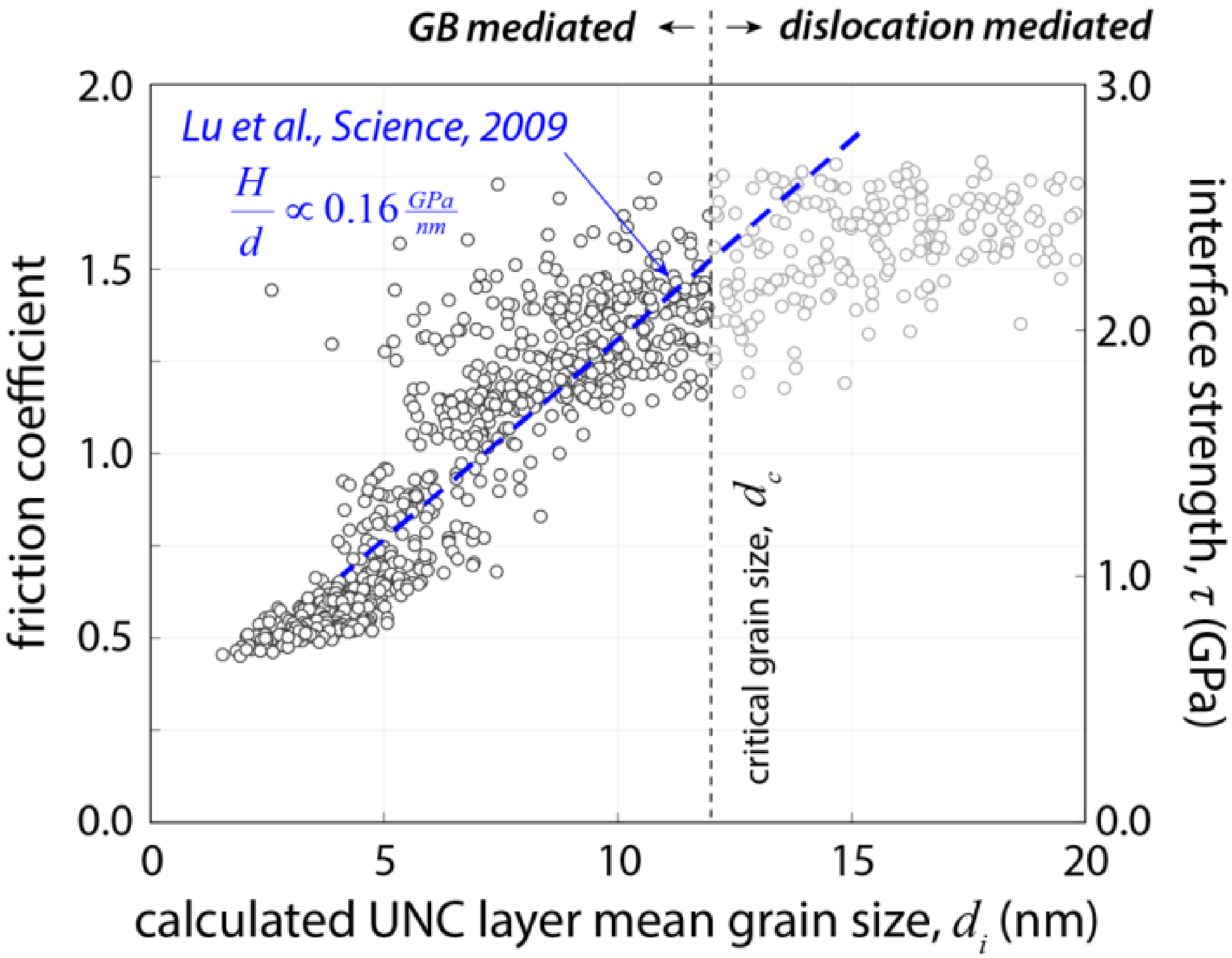


Direction Connection between Friction and Grain Size



Direction Connection between Friction and Grain Size

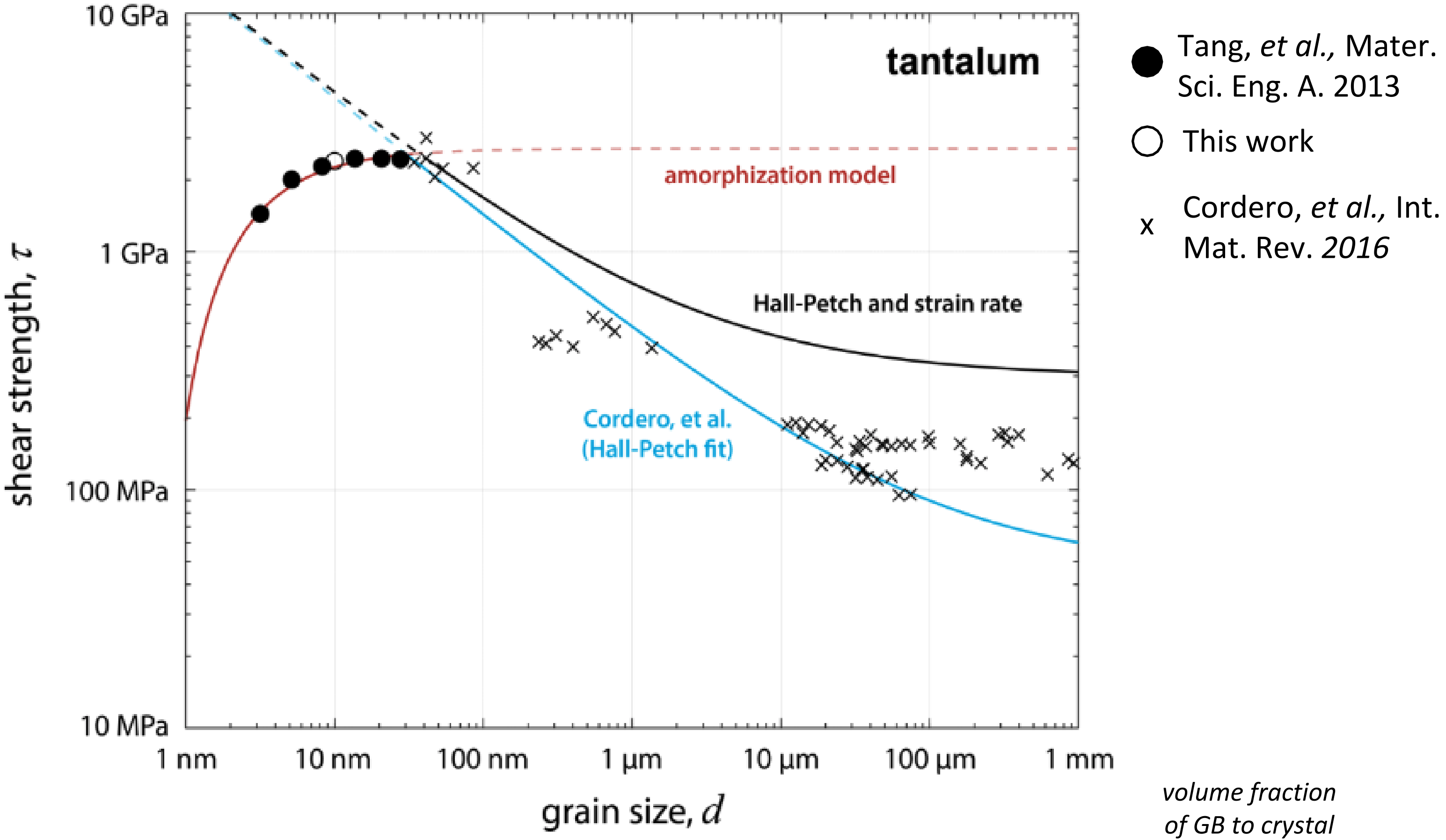
Chandross, et al. *Scripta Mat* .(2017)



- Grain size dependent friction
- Inverse H-P linked to low friction
- Implies tribology can be used to study inverse H-P behavior of metals

Grain Size Dependent Strength of Metals

Hinkle, et al., *Phys. Rev. Mater.* 2020



Amorphization model:

Chandross and Argibay, Phys. Rev. Lett. (2020)

No adjustable parameters!

$$\tau(d) = L\left(1 - \frac{T}{T_m}\right)\frac{\rho_L}{M}\left(\frac{d-\delta}{d}\right)^3 - \frac{kT}{b^3}$$

volume fraction of GB to crystal

heat of fusion

homologous temperature

amorphous metallic atomic volume

thermal energy