Bridging From Atomic Forces to Macroscopic Friction

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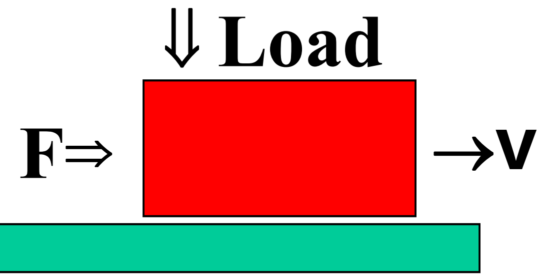
Non-linear Mechanics and Rheology of Dense Suspensions

KITP, Santa Barbara, Jan 22-26, 2018

With: L. Pastewka, T. Sharp, J. Monti, S. Akarapu, S. Cheng, G. He, S. Hyun, B. Luan, J. F. Molinari, M. H. Muser, L. Pei

Supported by NSF, AFOSR, European Commission

Friction Laws ?



Static friction F_s

→ minimum force needed to initiate sliding.

Kinetic friction $F_k(v)$

→ force to keep sliding at velocity v.

Typically, $F_k(v)$ varies only as log(v) and $F_s > F_k(v)$ at low v

Amontons' Laws (1699):

- Friction ∝ load → constant $\mu = F/\text{Load}$ (or $\mu = dF/d\text{Load}$)
- Friction force independent of apparent contact area A_{app}.

But: Amontons coated all surfaces with pork fat

$F \propto A_{app}$ for soft, flat solids, polymers, tape

μ often changes with load ⇒ friction for load ≤ 0

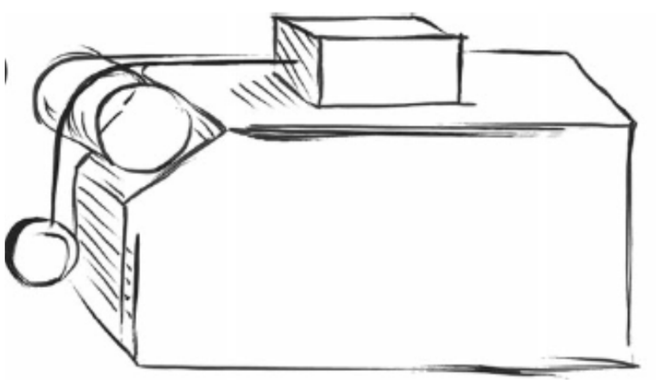
Friction depends on history (rate-state models)

Laws violated in nanoscale experiments & simulations

⇒ solids slide like fluids, fluids stick like solids

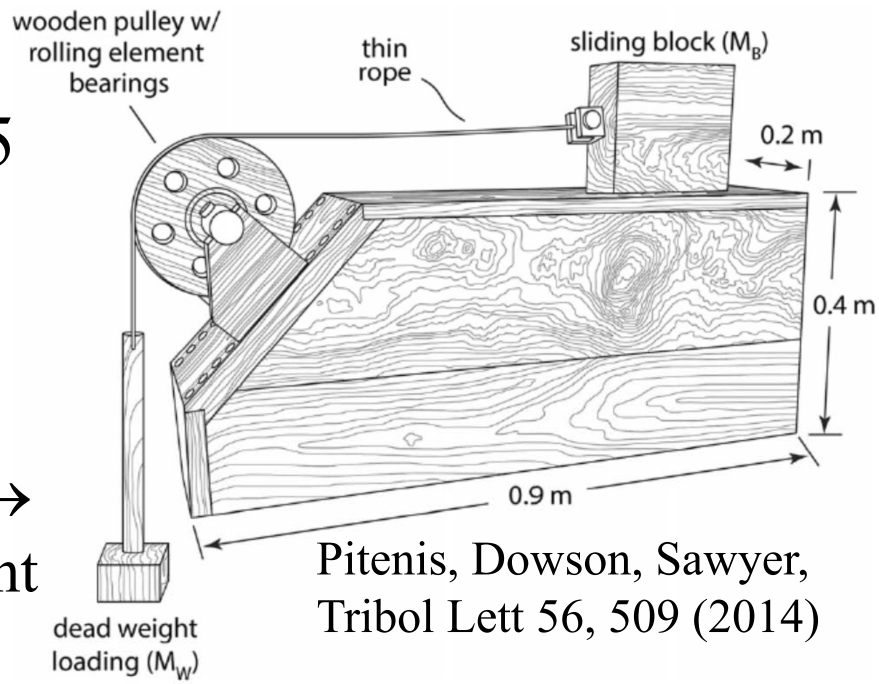
Friction Laws ?

Davinci's Experiments → μ=0.25

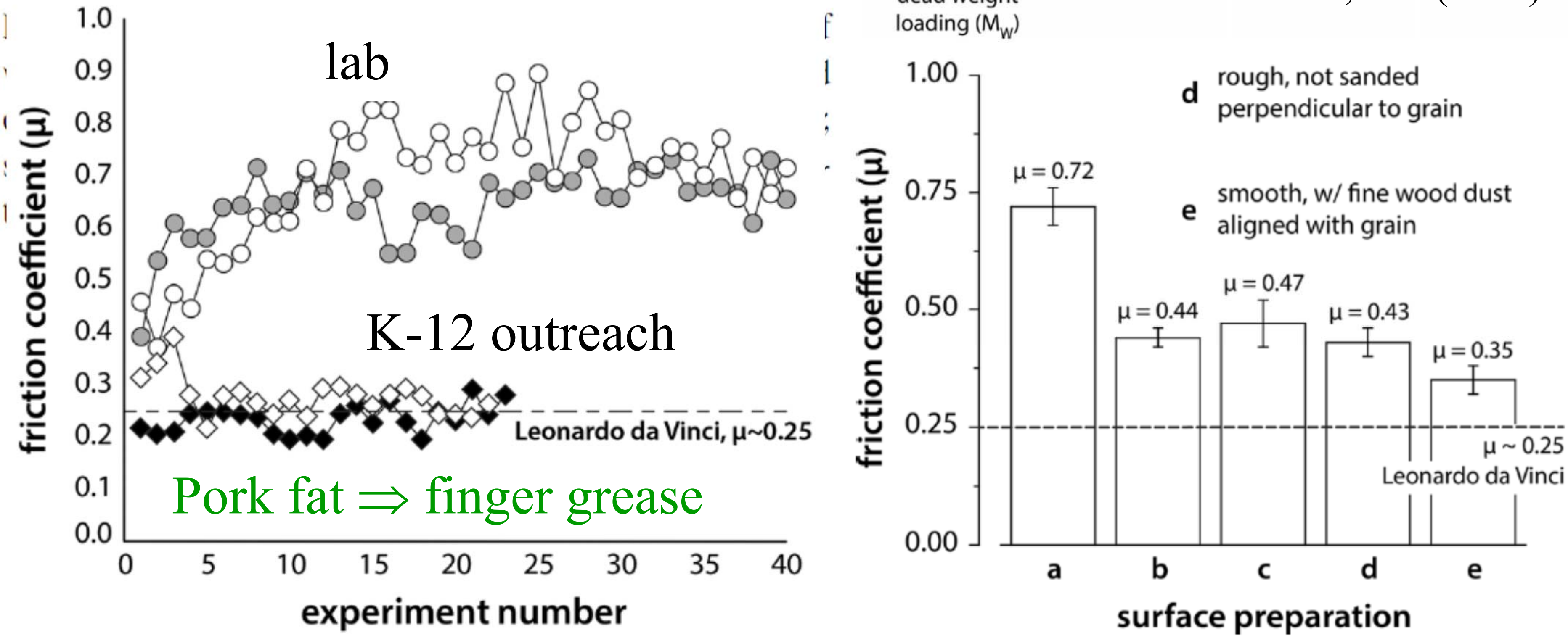


←DaVinci sketch

Modern → experiment



Pitenis, Dowson, Sawyer, Tribol Lett 56, 509 (2014)

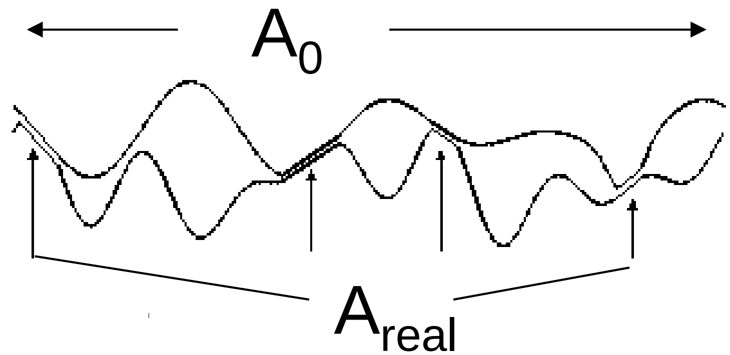


lab

K-12 outreach

Pork fat ⇒ finger grease

Friction Proportional to Real Area?



Common view since mid 1900's

Surfaces rough on many length scales and usually find $A_{real} << A_0$

Measurements and theory $\Rightarrow$ $A_{real} \propto$ Load in many cases

$\Rightarrow$ get Amontons' laws if constant shear stress τ_{shear}

$$\text{friction} = A_{real}\, \tau_{shear} \propto \text{Load}$$

Also explains many exceptions to Amontons' laws

- Adhesion $\Rightarrow$ A_{real} nonzero at zero load, still have friction
- Friction $\propto A_0$ for soft materials because $A_{real} \approx A_0$
- Friction $\propto A_{real}$ predicted by continuum theory for single asperities with radii from nm to mm
  - $\Rightarrow \propto N^{2/3}$ for non-adhesive solids (Hertz theory)
  - Bowden & Tabor – hard sphere on polymer

How Do Surfaces Interlock to Produce τ_{shear}?

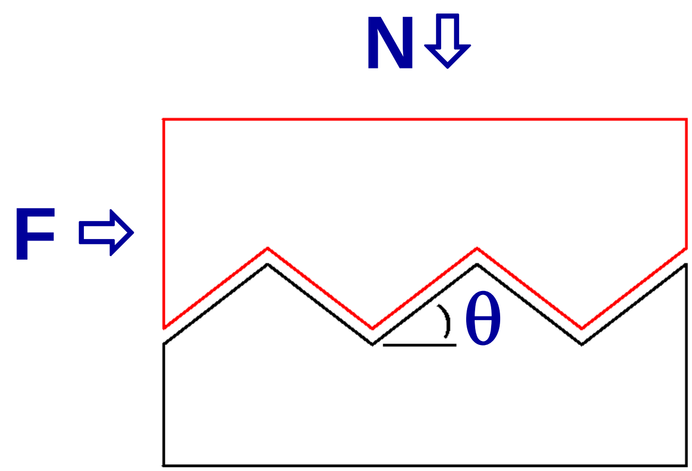
Geometric explanation (Amontons, Belidor, Parents, Euler, Coulomb)

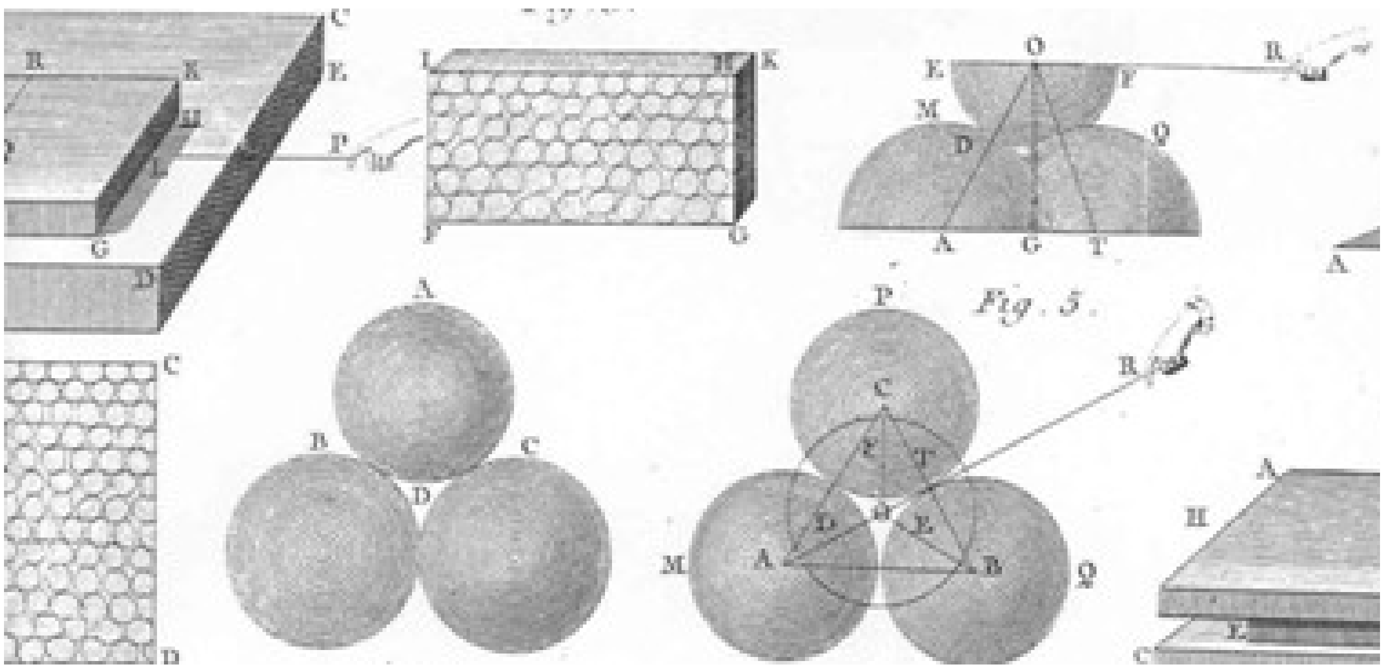
→ Surfaces are rough – mesh together

→ Friction = force to lift up ramp formed by bottom surface

→ $F=N \tan\theta \Rightarrow \mu=\tan\theta$

Belidor (1737) $\mu=1/3$ –
sliding of frictionless cannon balls - soil





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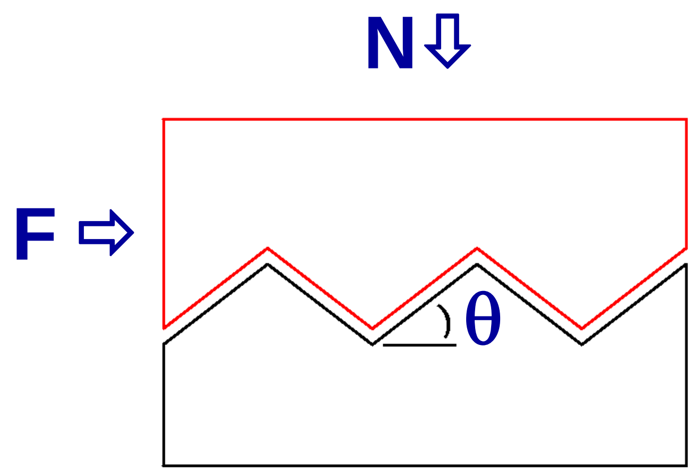
→ Friction = force to lift up ramp formed by bottom surface

→ F=N tanθ ⇒ μ=tan θ



Problems:

→ Most surfaces can't mesh

→ Roughening can reduce μ (hard disks)

→ Monolayer of grease changes μ not roughness

→ Once over peak, load favors sliding ⇒ kinetic friction=0

→ Friction proportional to apparent area not load in some cases

Static friction ⇨ Force to escape metastable state

How can two surfaces always lock together?

Kinetic friction ⇨ Energy dissipation as slide

Why is this correlated to static friction? Why does T matter?

Molecular Dynamics up to Micrometer Scales

Challenge: elastic interactions - long-range →need cube of size L^3
sound propagation time ~L. Compute time $\sim L^4$.

Use multiscale approach that scales as $L^2 \ln L$ for $L \sim 10^4$ atoms

At surface - molecular dynamics (MD) simulations of $\sim 10^8$ atoms

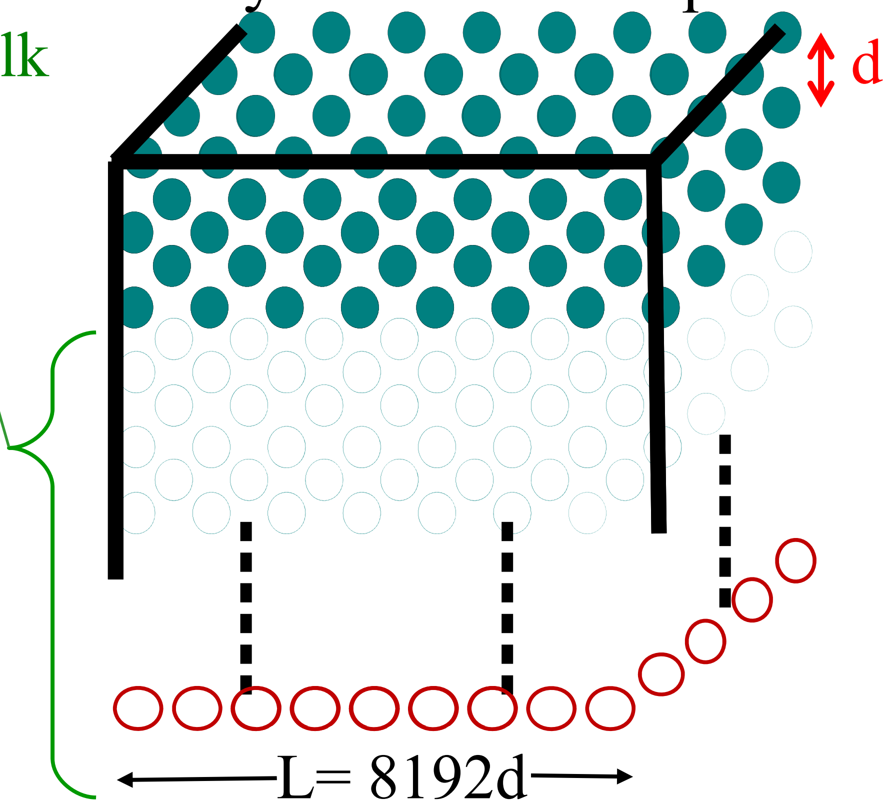
At depth where displacements are small only need linear response

→Use atomic Greens function in bulk
Seamless boundary conditions

Similar to Campana & Muser

Extended to long range interactions, analytic GF, multibody potentials
EAM, Stillinger-Weber, …

Periodic boundaries or semi-infinite

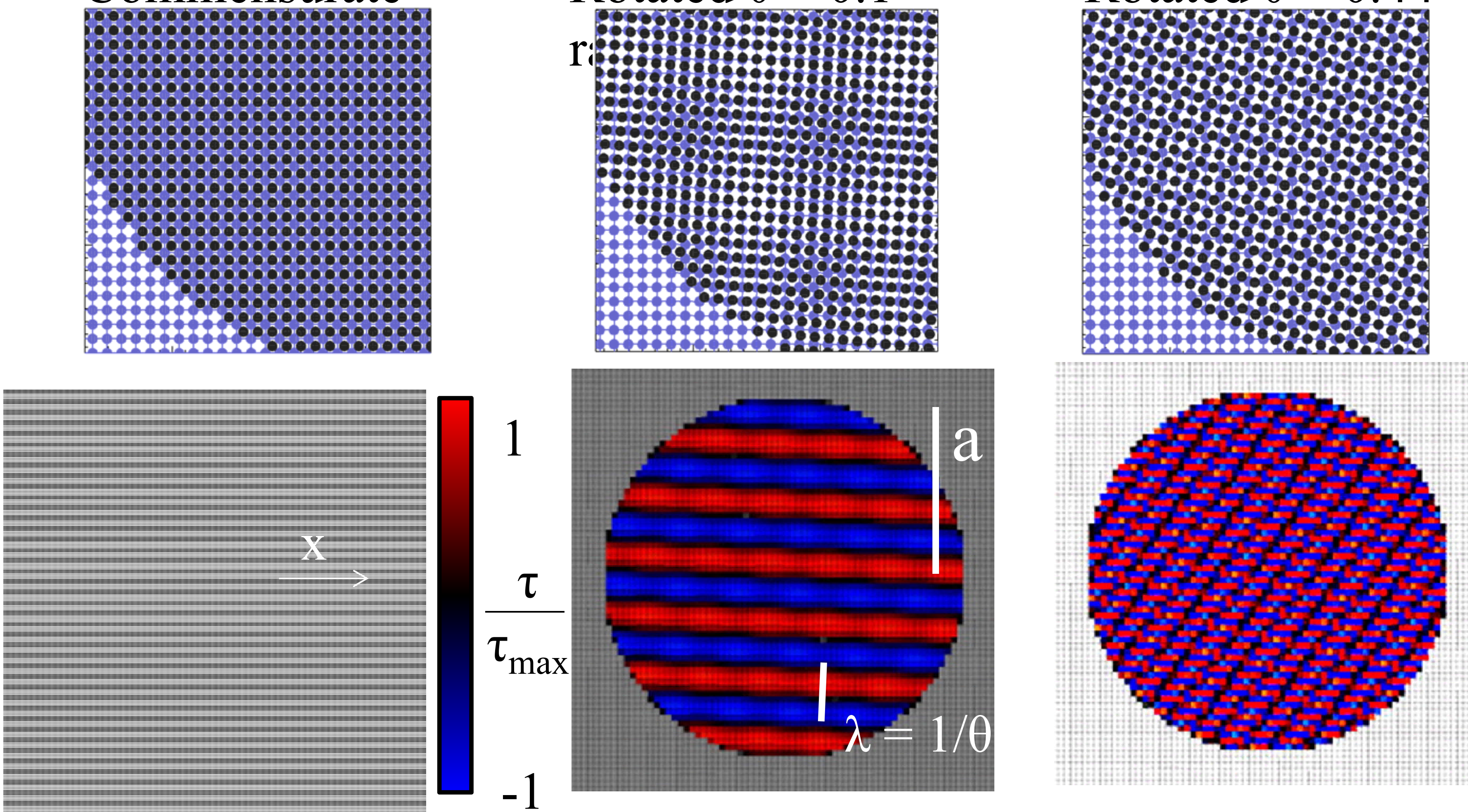


Campaña, Müser, *Phys. Rev. B* 74, 075420 (2006); Pastewka, Sharp, Robbins, *Phys. Rev. B*86, 075459 (2012)

What About Shear Stress in A_{real}?
Rigid Incommensurate Surfaces – No Net Friction!

Commensurate: Friction ∝ load for repulsive, ∝area for adhesive

Commensurate | Rotated θ = 0.1 | Rotated θ = 0.44



Structural Superlubricity – Rigid Surfaces

Hirano & Shinjo – Contacting crystals typically incommensurate,

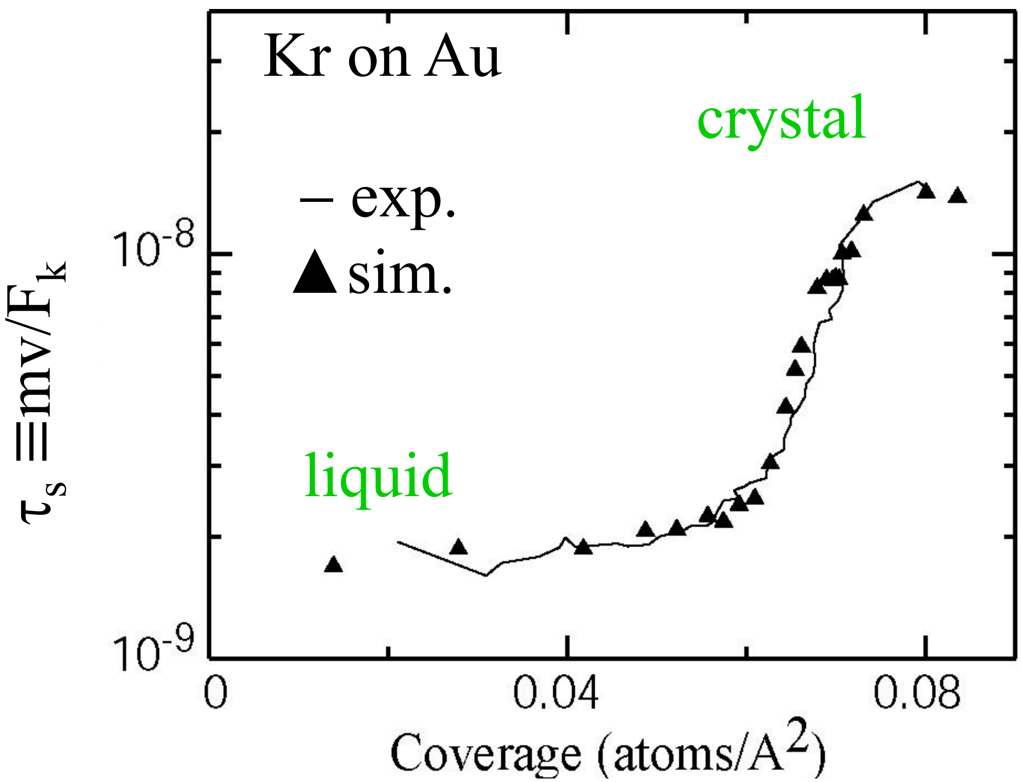
$\Rightarrow$No common period $\rightarrow$ lateral force averages to zero, $F_s=0$

Even identical surfaces become incommensurate if rotated

Consistent with many experiments & simulations

$F_s=0$ for incommensurate monolayers on substrate (Krim et al.)

Solids more slippery than fluid of same element



Friction proportional to velocity - $F_k=v\ m/\tau_s$

Cieplak, Smith, Robbins, Science **265**, 1209 (1994)

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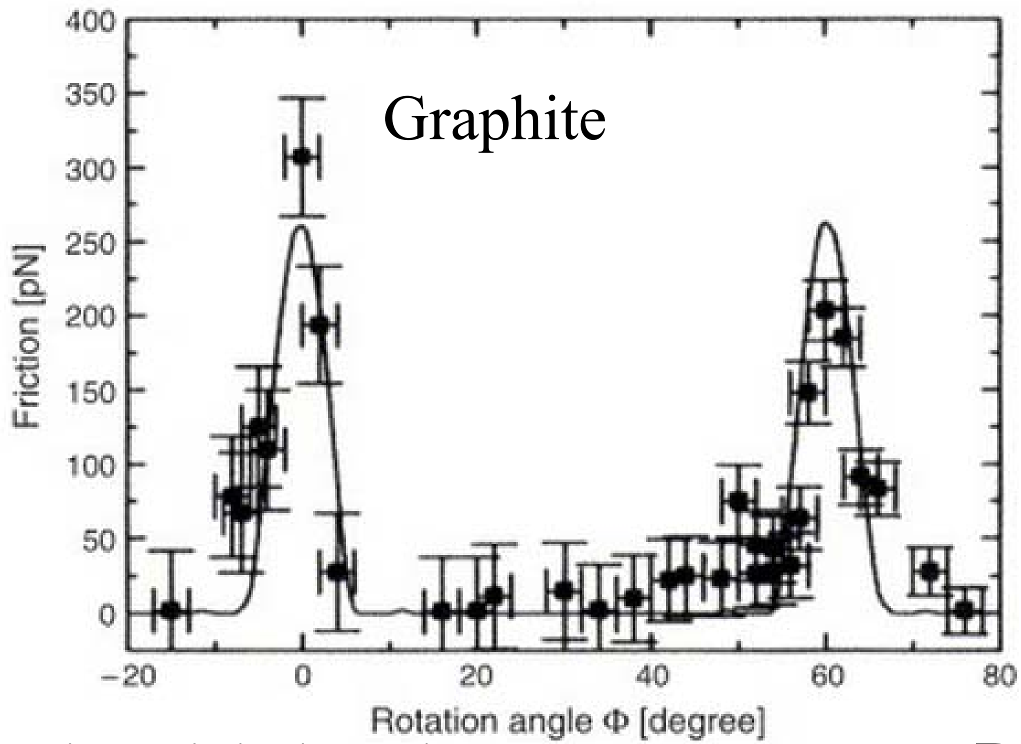
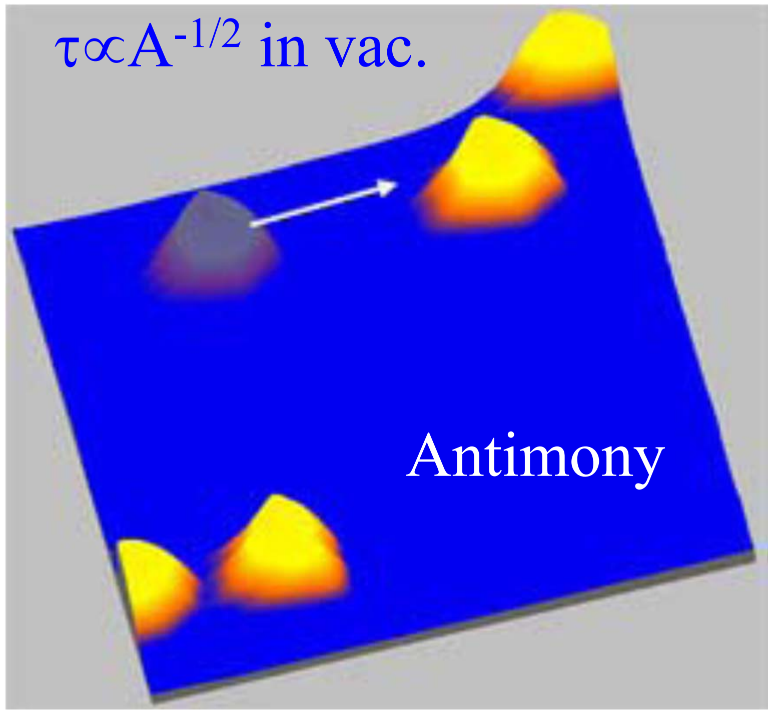
Consistent with many experiments & simulations *in vacuum*

F_s~0 for misaligned mica, graphite, MoS_2, antimony, adsorbed gas

[Hirano et al ‘91, Krim et al ‘90, Dienwiebel et al ‘04, Martin et al ‘93, Dietzl et al ’08]



Dienwiebel et al. ‘04



Dietzel et al. PRL 101, 125505, ‘08

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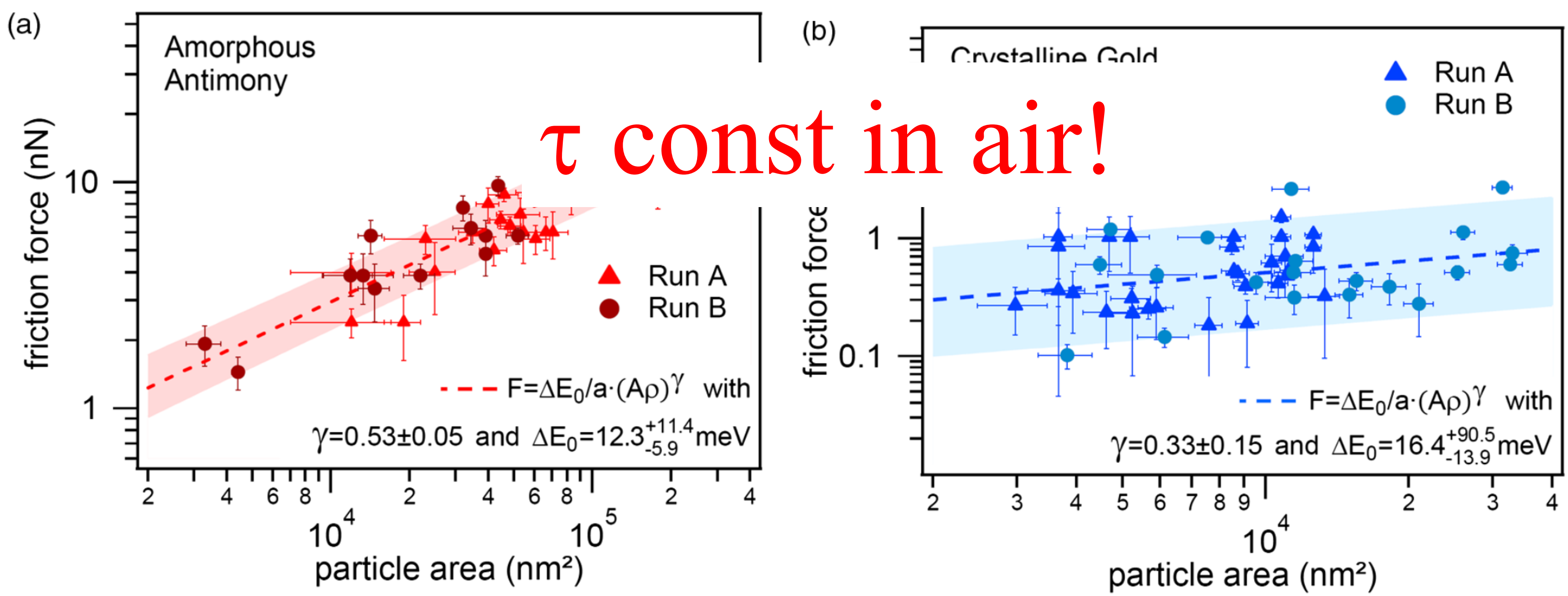
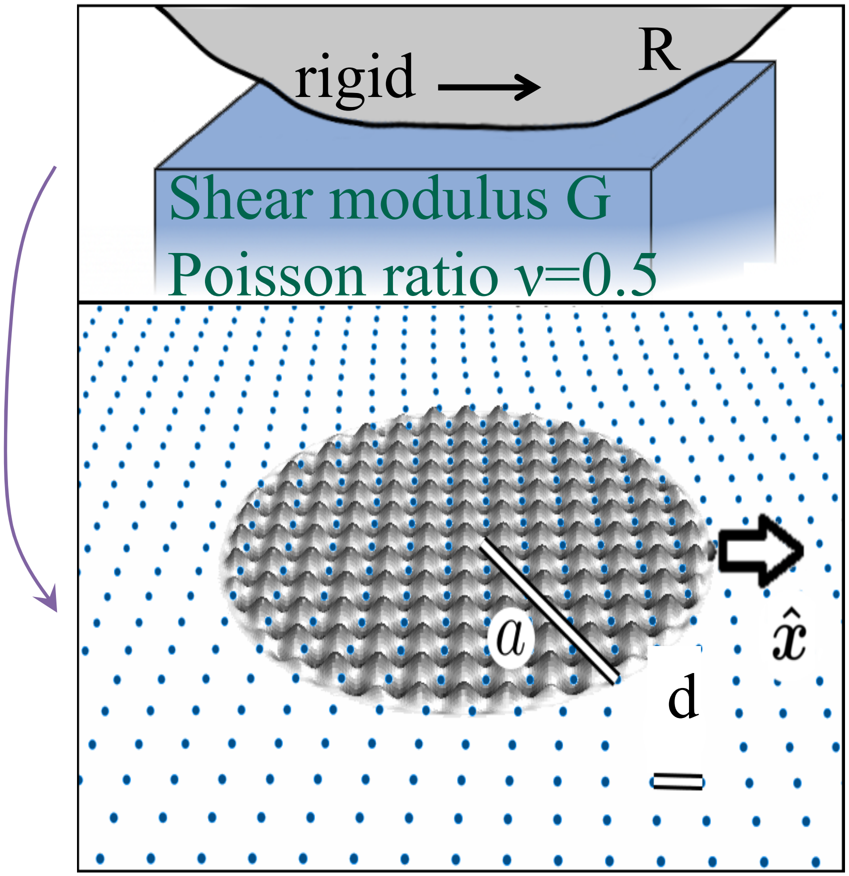
Dietzel et al. PRL 111, 235502 (2013)

$F \propto A^{1/2}$; $\tau \propto A^{-1/2}$ in vac. $F \propto A^{1/4}$ $\tau \propto A^{-3/4}$ in vac.



τ const in air!

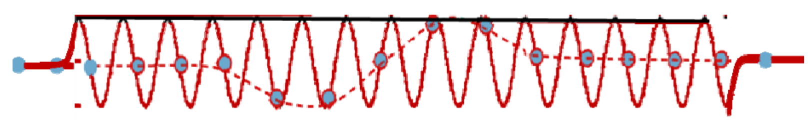
Elasticity Eliminates Structural Lubricity



Represent rigid surface with sinusoidal lateral force

$$f_x = f_0 \sin(2\pi x/d)$$
$$f_y = f_0 \sin(2\pi y/d)$$

"Adhesive model" $f_0 = \tau_{max} d^2$



Similar behavior for full sphere on flat simulation ⇒ linear response not influenced by curvature

Slide corrugation potential quasi-statically, minimize the energy

Vary ratio of stiffness G to interfacial shear stress τ_{max}

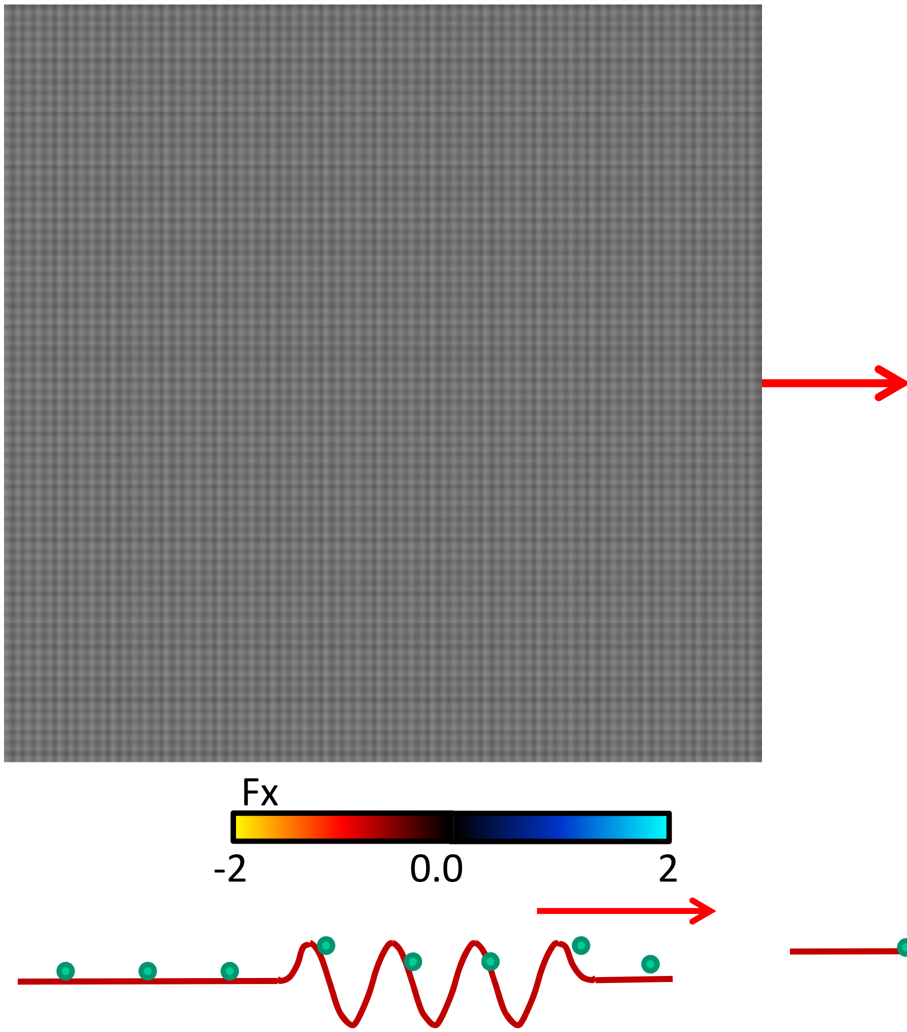
Key length = interfacial dislocation core size $b_{core} = dG/\tau_{max}$

Minimum lateral distance over which can change registry by d

Commensurate Slides via Dislocations at Large a/bcore

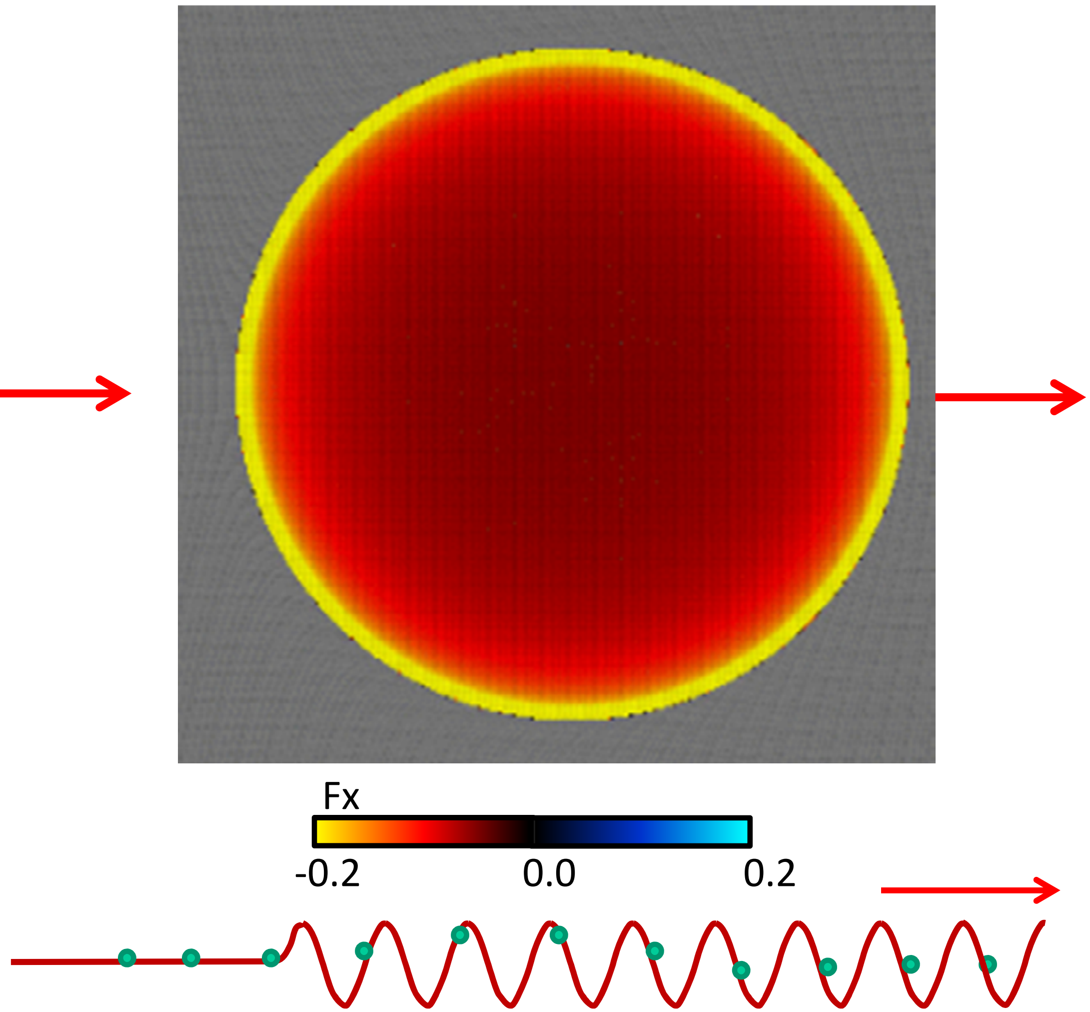
Small – coherent

a = 30 d b_{core} = 128 d



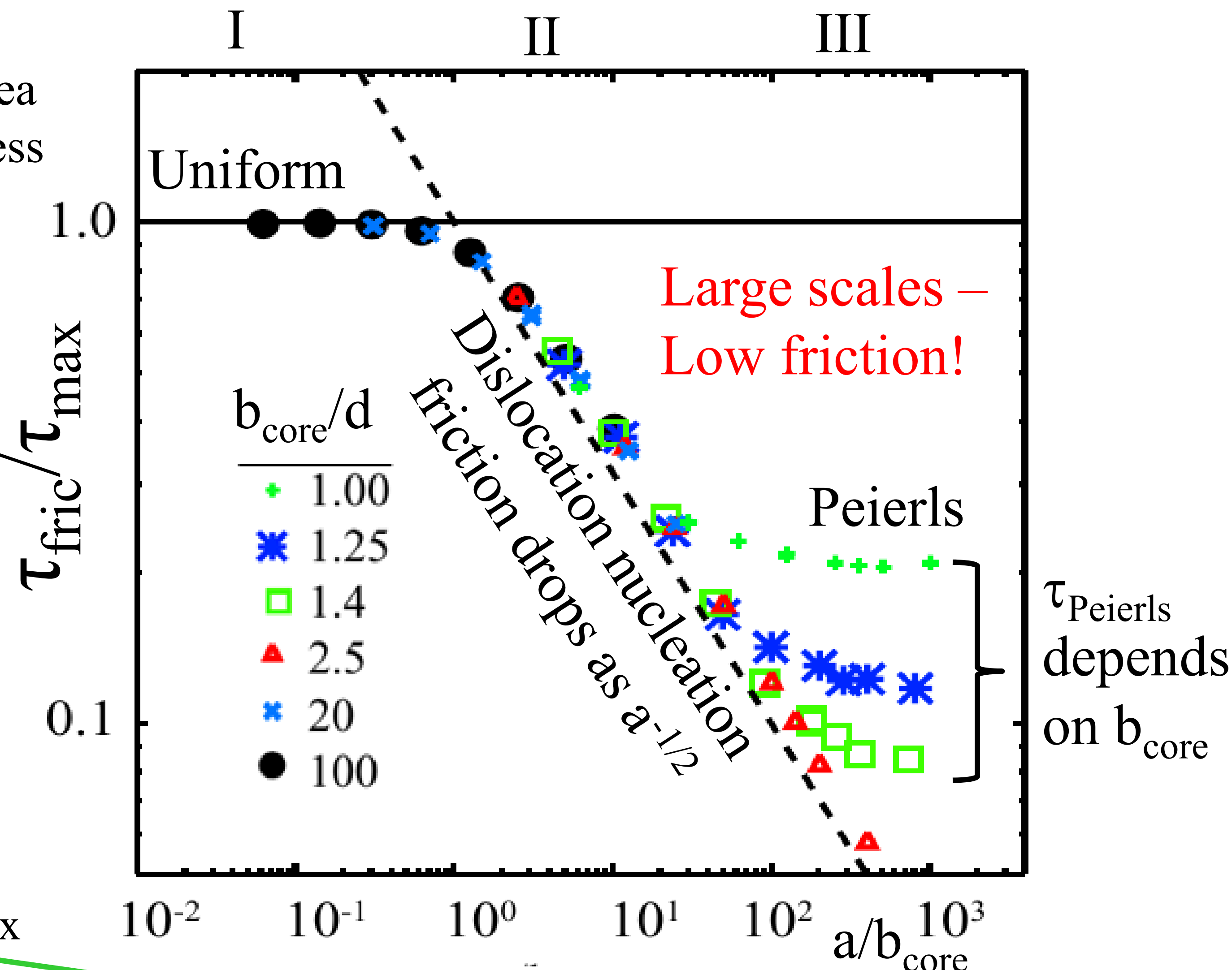
Large – dislocation assisted

a = 126 d b_{core} = 1 d



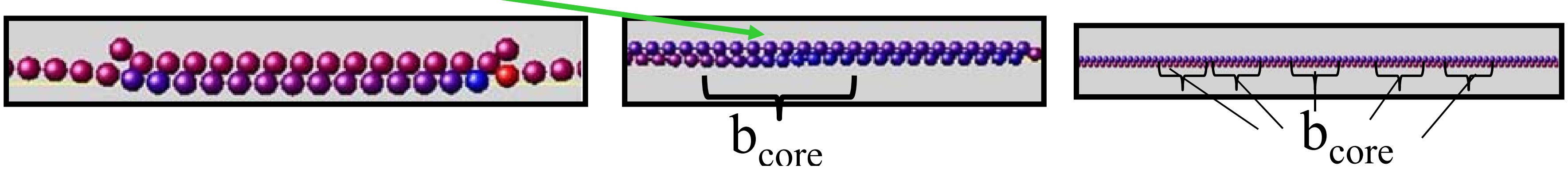
Commensurate Adhesive Case: Three Friction Regimes

τ_{fric} – Total static friction per area
τ_{max} – Max local stress
a – contact radius
b_{core} – core size
d – atomic spacing
G – shear modulus

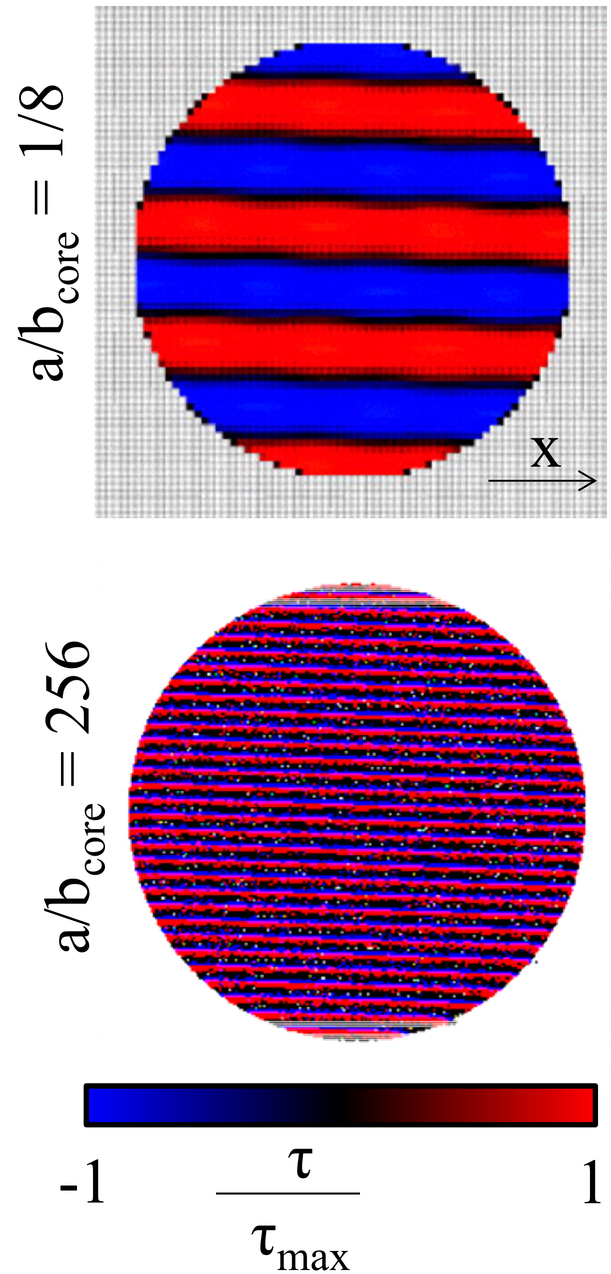


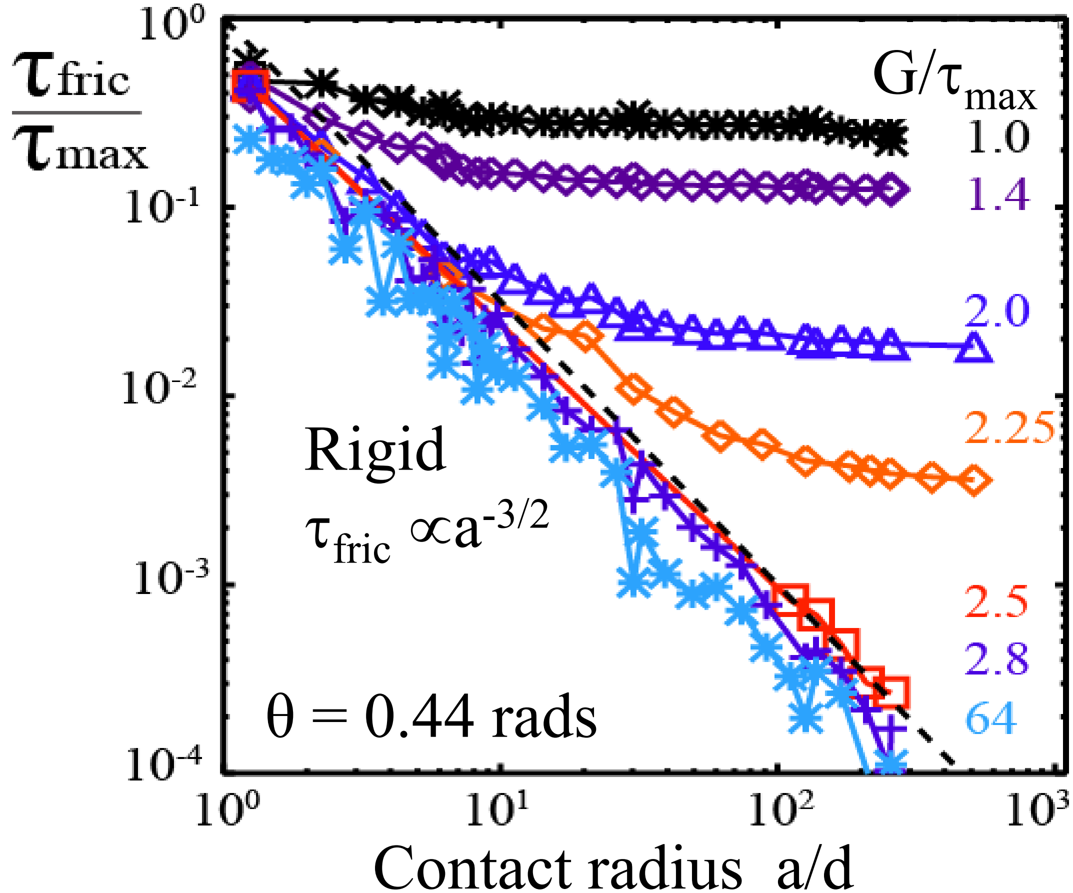
Agrees with scaling of Hurtado, J. A. & Kim, K.-S. 1999 *Proc. R. Soc. Lond* A **455**, 3363–3384.

$b_{core} \equiv dG/\tau_{max}$



Elasticity → Breakdown of Structural Superlubricity





τ_{fric} – Static friction force per area

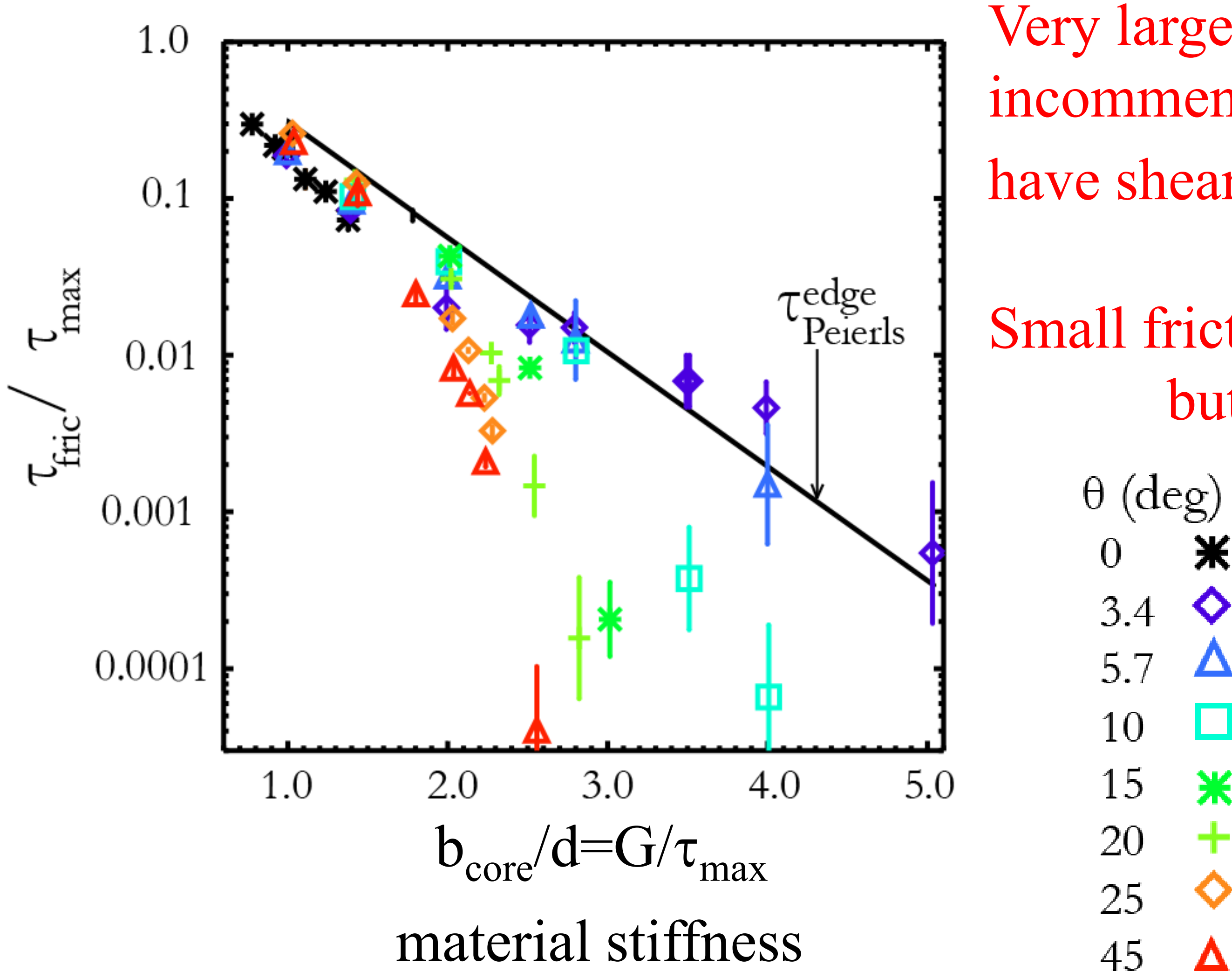
τ_{max} – max traction parameter, d – atomic size

$b_{core} = dG/\tau_{max}$ – dislocation core size

Large a/d, $\tau_{fric} = \tau_{Peierls} \propto G \exp[-2\pi G/\tau_{max}]$

Static friction → Peierls Stress as $a/b_{core} \to \infty$

Single dislocation $\tau^{edge}_{Peierls} \propto G \exp[-2\pi b_{core}/d]$ measured separately

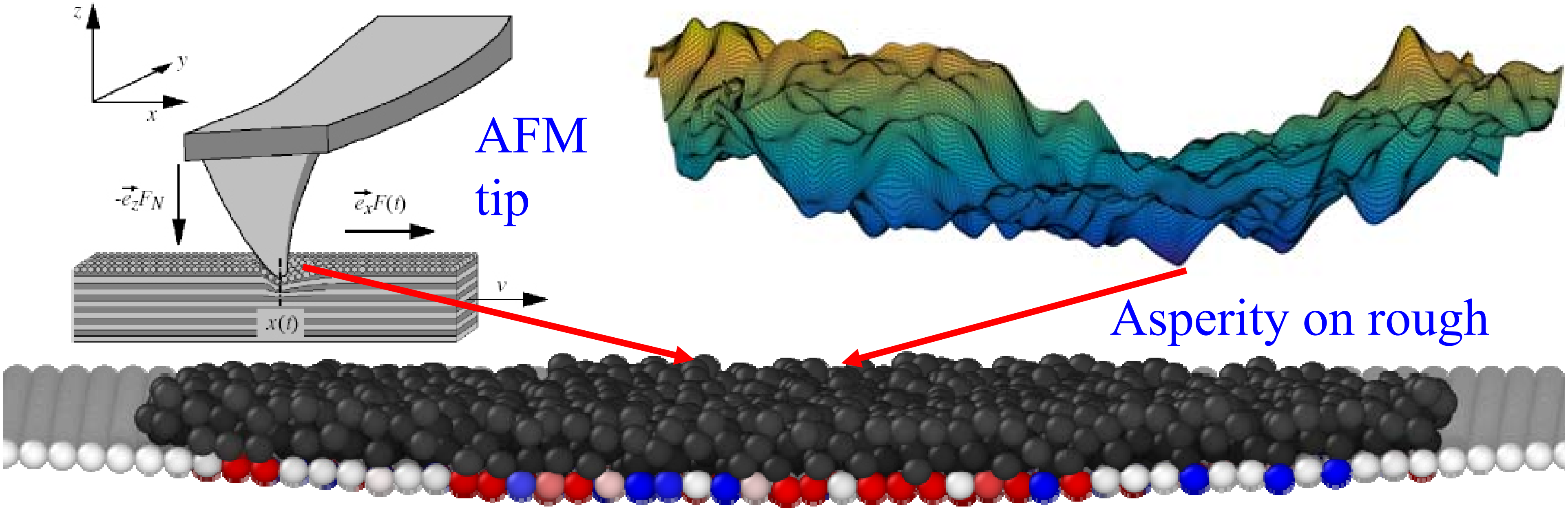


Very large commensurate and incommensurate contacts both have shear stress $\sim\tau^{edge}_{Peierls}$

Small friction for large b_{core} but finite, not zero

Phys Rev B93, R121402 (2016)

What About Disordered Surfaces?



Imry-Ma argument – Compare deformation and locking energies

Deform on scale L, get interfacial energy ~ $\tau\sqrt{L^{d-1}}$, d=dimension

Cost of deformation on scale L: $GLq^2L^{d-1} = GL^{d-2}$ with q=1/L

For d=2, disorder wins at large L: $\tau\sqrt{L} > G$ –raindrops on windows

For d=3 ⇒ same scaling at large L: $\tau L \sim GL$ - marginal dimension

Expect pinning at exponentially long scales, friction $\propto \tau \exp(-\frac{cG}{\tau})$

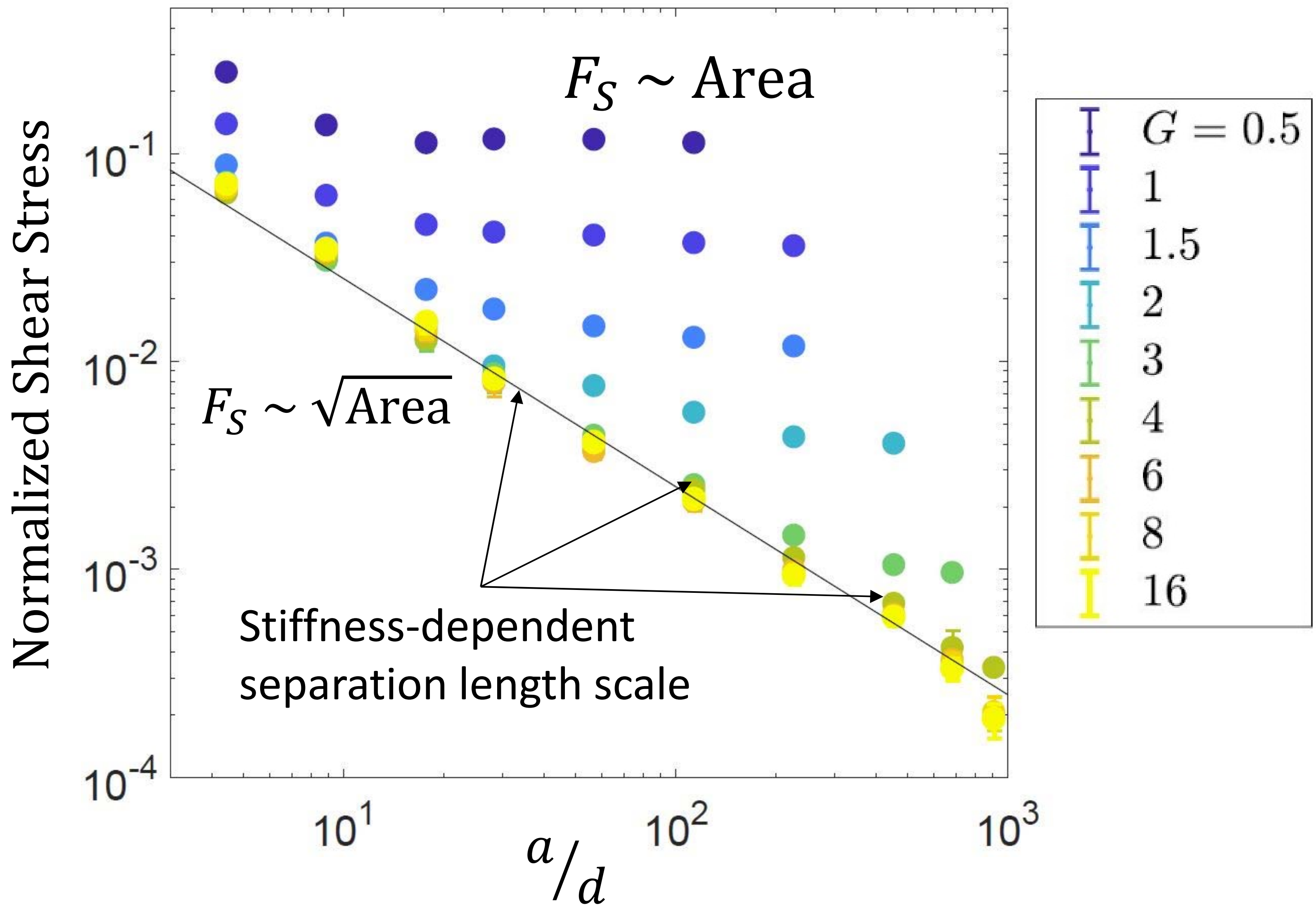
⇒ Similar to exponential scaling for Peierls stress!

Analytic work: Persson & Tossati, Volmer & Natterman, Caroli & Nozieres, Müser

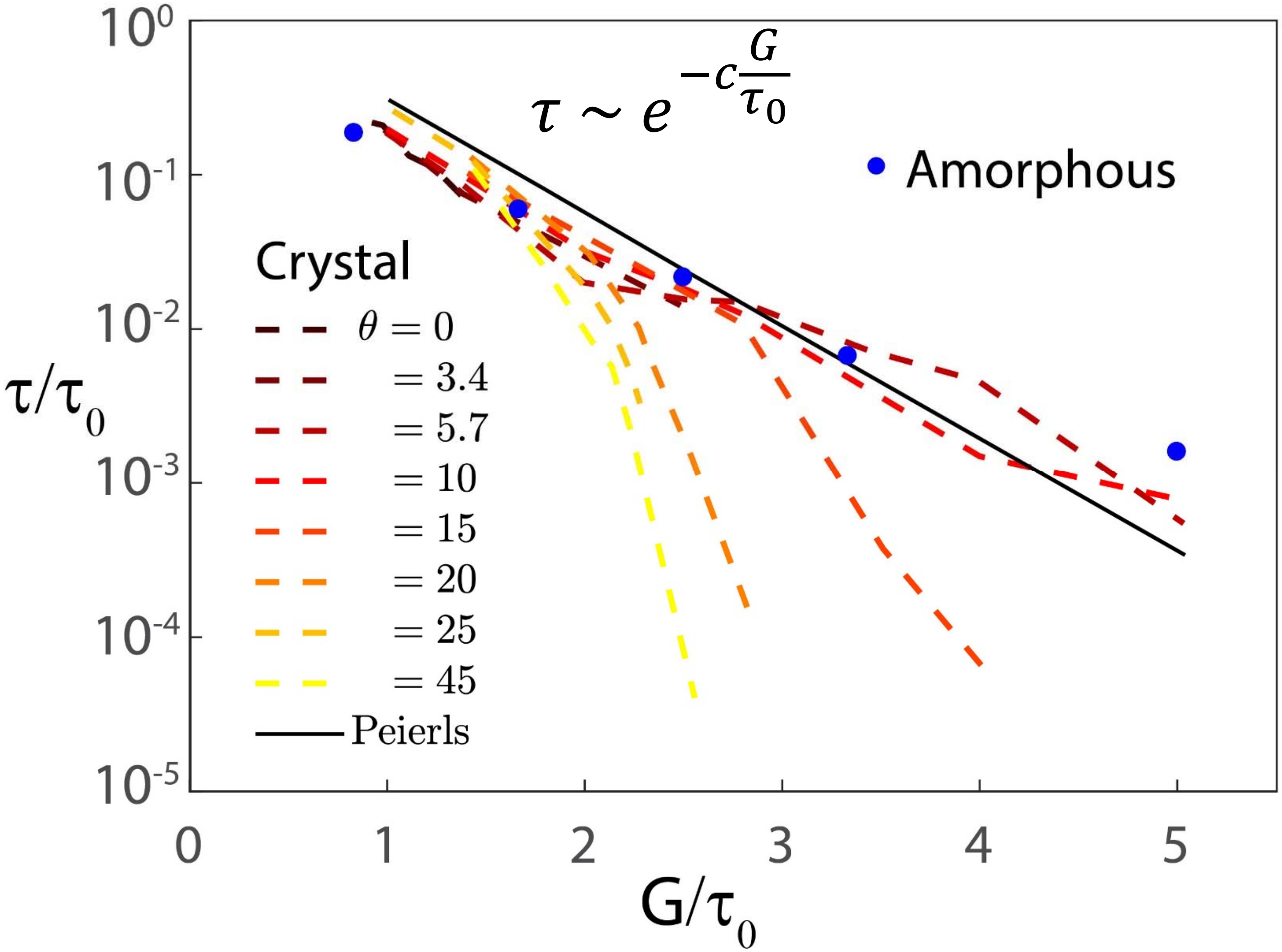
Large Contacts ⇒ Constant Shear Stress

Rigid – Stress scales with 1/a

Elastic- Stress saturates at stress that drops exponentially with G



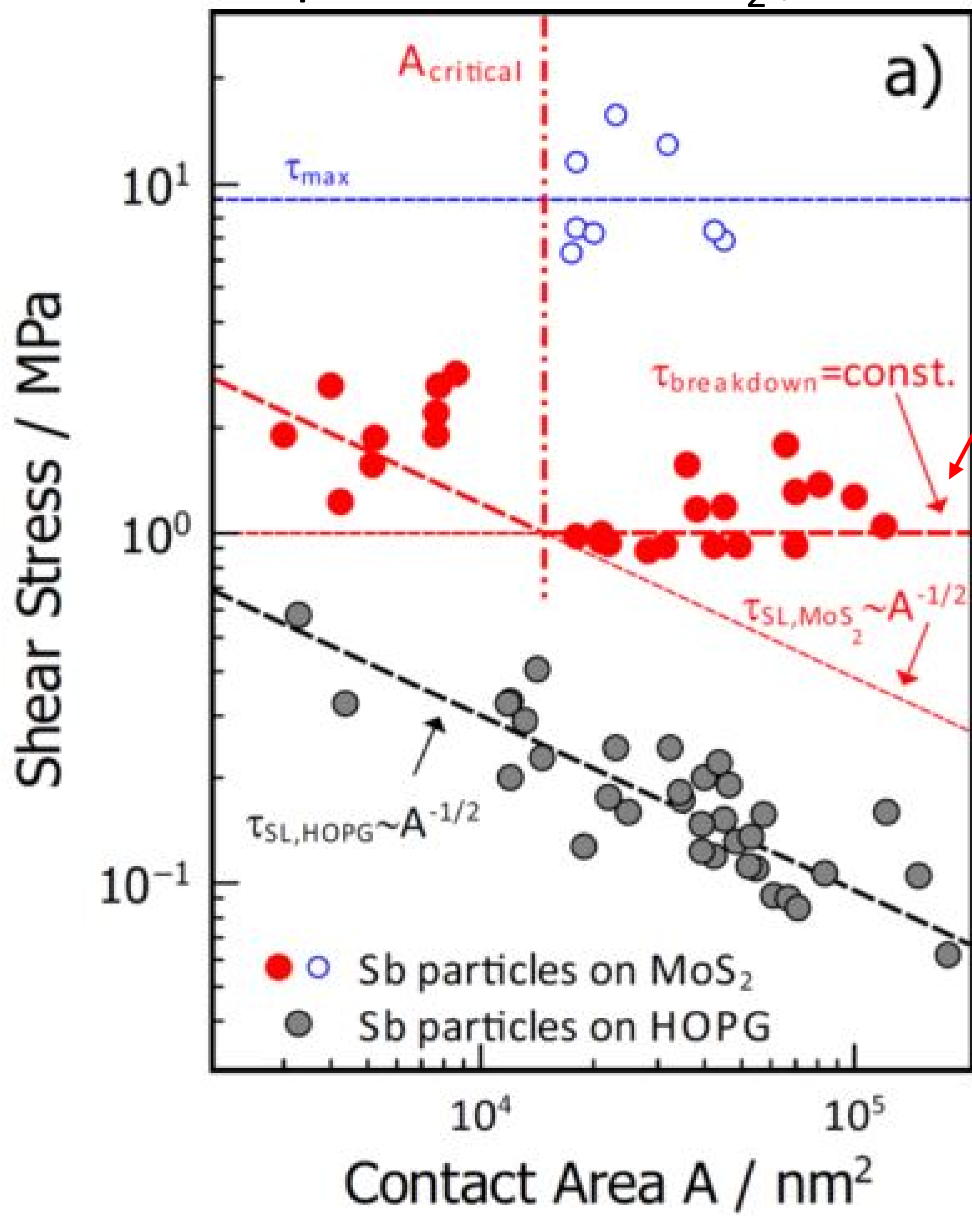
Same for Amorphous, Commensurate, Incommensurate



Incommensurate, commensurate and amorphous surfaces all have similar friction at large scales – drops exponentially with G

Experimental Measurements: Dietzel 2017

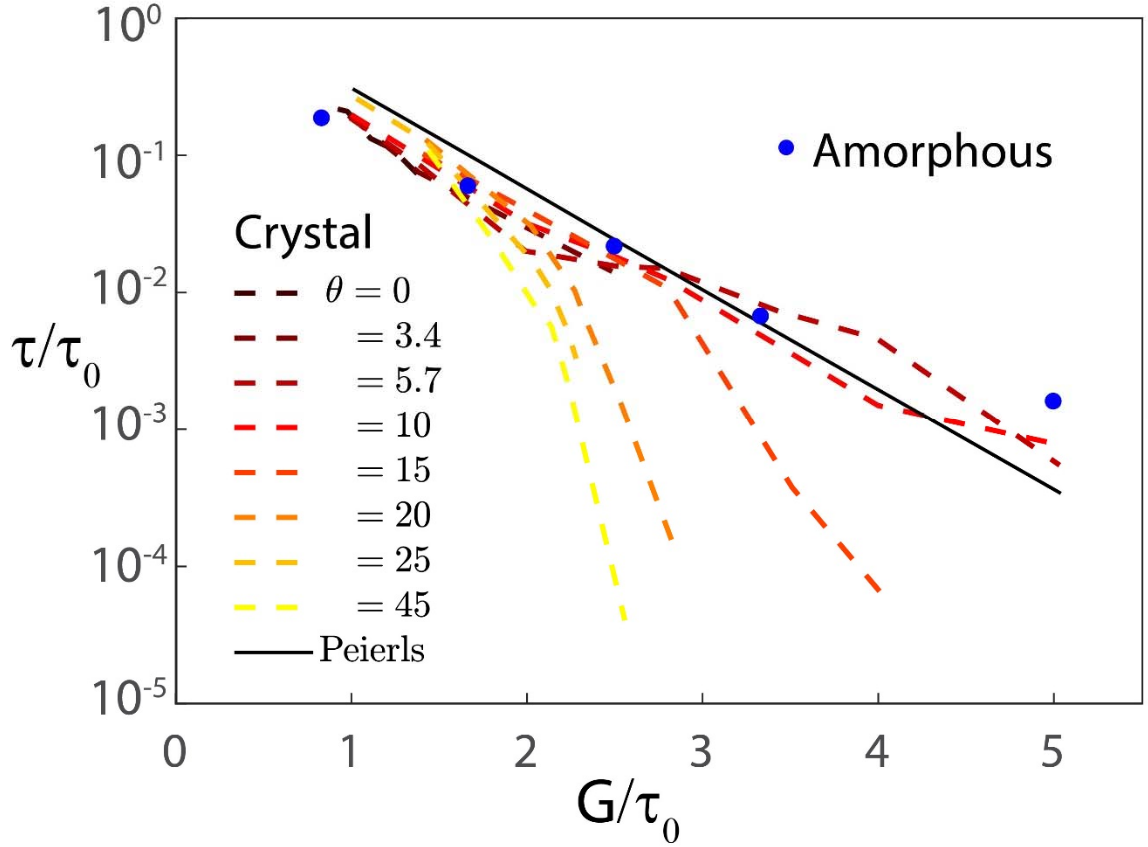
Amorphous Sb on MoS_2 , HOPG



- See saturation at large areas for MoS_2.
- Radius ~56nm~150d
- Larger chemical interaction energy leads to better frictional locking than for HOPG

What Should Length Scale of Crossover Be?

FCC crystal – two identical surfaces G/τ_0~ 2.2 scales ~ 10nm
Graphite, MoS_2 have low shear strength between planes very high stiffness within planes – expect much larger G/τ_0
Potential contribution to performance as solid lubricants



Conclusions: Scale Dependence In Single-Asperity Contact

Simulate rigid tips on flat elastic crystal

$a > 10^3$ d ~1μm and R up to 10^5d, d=atomic spacing

Tip is commensurate, incommensurate or amorphous

Local friction – constant stress or local Amontons's law

Three regimes of sliding:

1) Small contacts: rigid, smooth sliding, F_{kin}~0

   F_{stat} large only for commensurate

2) Intermediate: a > interfacial dislocation width

   ⇒sliding through dislocations at decreasing F_{stat},

   stick-slip motion, F_{kin}/F_{stat} rises

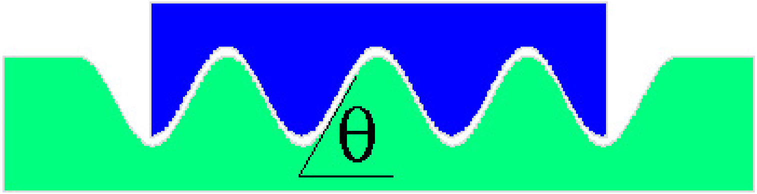
3) Large contacts: Elasticity leads to scale independent friction stress for adhesive local friction

   Elasticity leads to rising friction in repulsive contacts

Friction not zero but very weak for very large stiffness

IF surfaces are clean and elastic

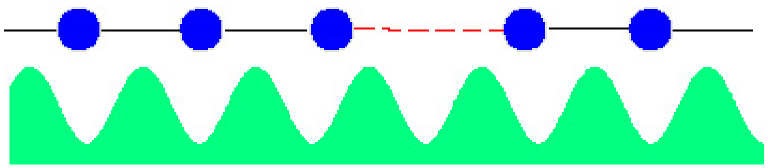
Friction Mechanisms in Contacts



Geometrical Interlocking: $F=N \tan \theta$

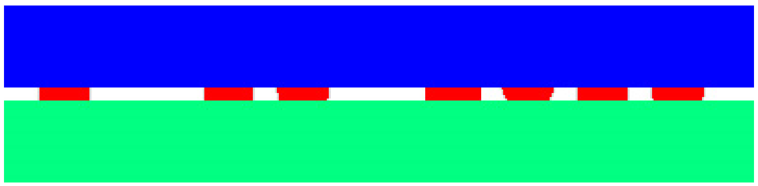
Unlikely to mesh, F goes up as smooth

Kinetic friction vanishes



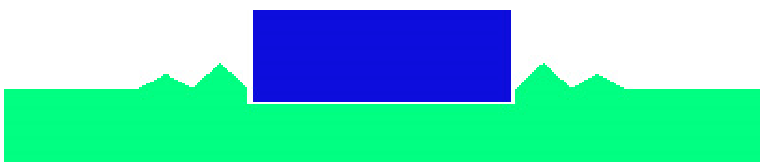
Elastic Metastability:

Marginal dimension - exponentially weak in disorder or lateral coupling



Mixing or Cold-Welding

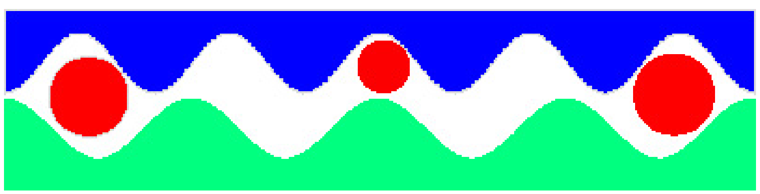
Most likely for clean, unpassivated surfaces in vacuum



Plastic Deformation (plowing)

Load and roughness dependent

⇒High loads, sharp tips



Mobile third bodies → "glassy state"

hydrocarbons, wear debris, gouge, …

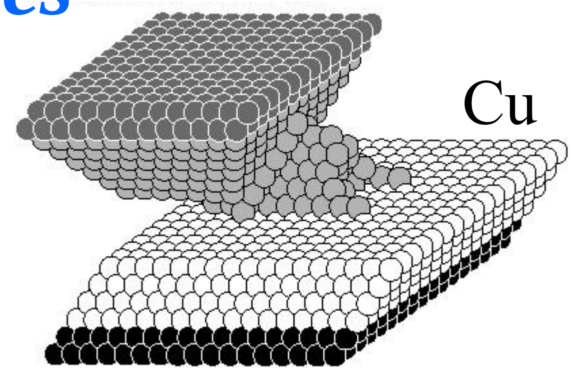
Glass seen in Surface Force Apparatus,

Robust friction mech. on many scales

Welding at Interfaces

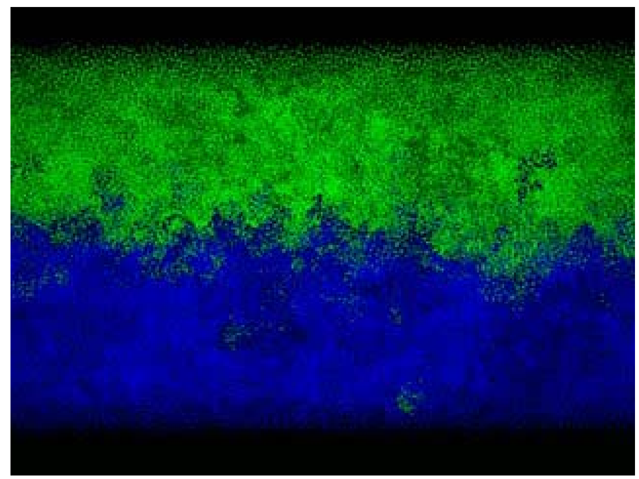
Metals weld in vacuum conditions
- Scale, orientation dependence

Sørensen, Jacobsen & Stoltz, Phys. Rev. B 1996
Bowden and Tabor for many metal pairs
Landman, Fujita, Matsukawa, …



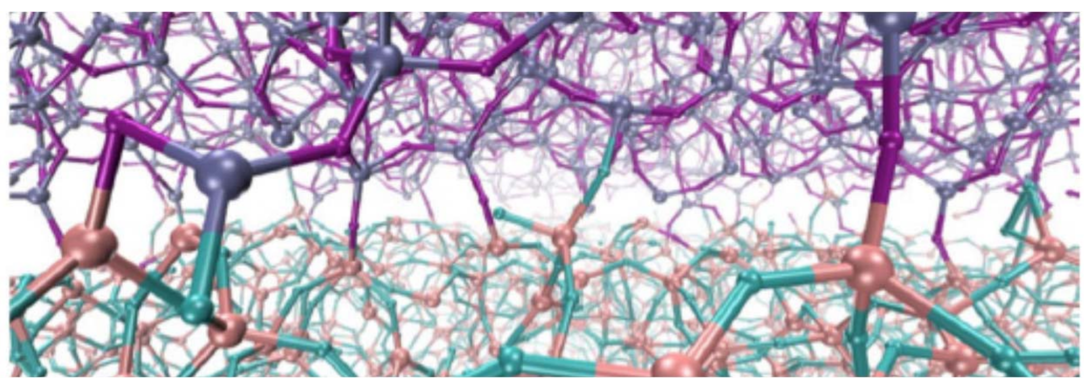
PMMA in Fineberg experiments
– energy release ~ fracture energy

Strength of polymer weld depends on contact time and pressure - ~ 2 entanglements ⇒bulk
Ge, Pierce, Perahia, Grest, Robbins
PRL 110, 098301 (2013); Macromol (2014)



Thermally activated covalent bonding of silica: friction ~log(time)

Li, Liu, Szlufarska,
Trib. Lett. 56: 481 (2014)
Li, Tullis, Goldsby, Carpick
Nature 480, 233 (2011)



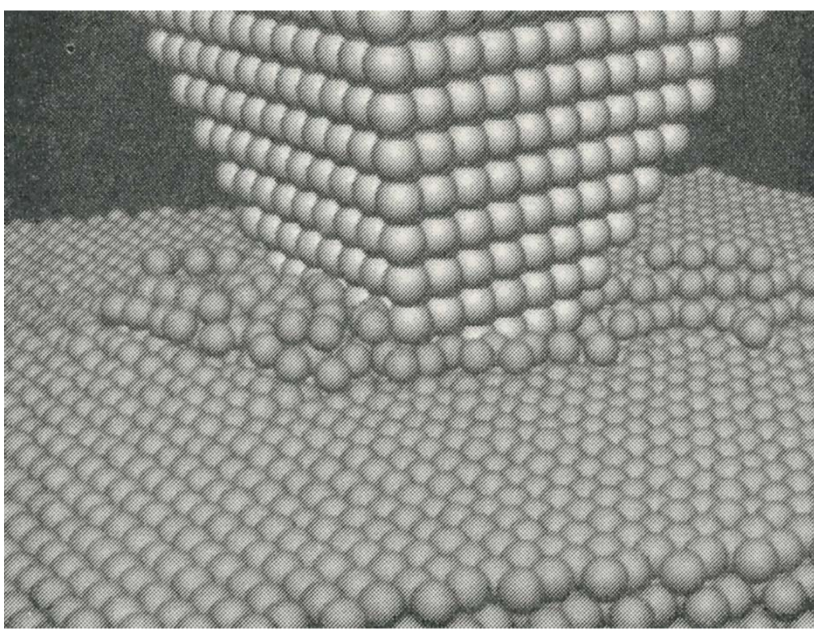
Friction from Plastic Deformation

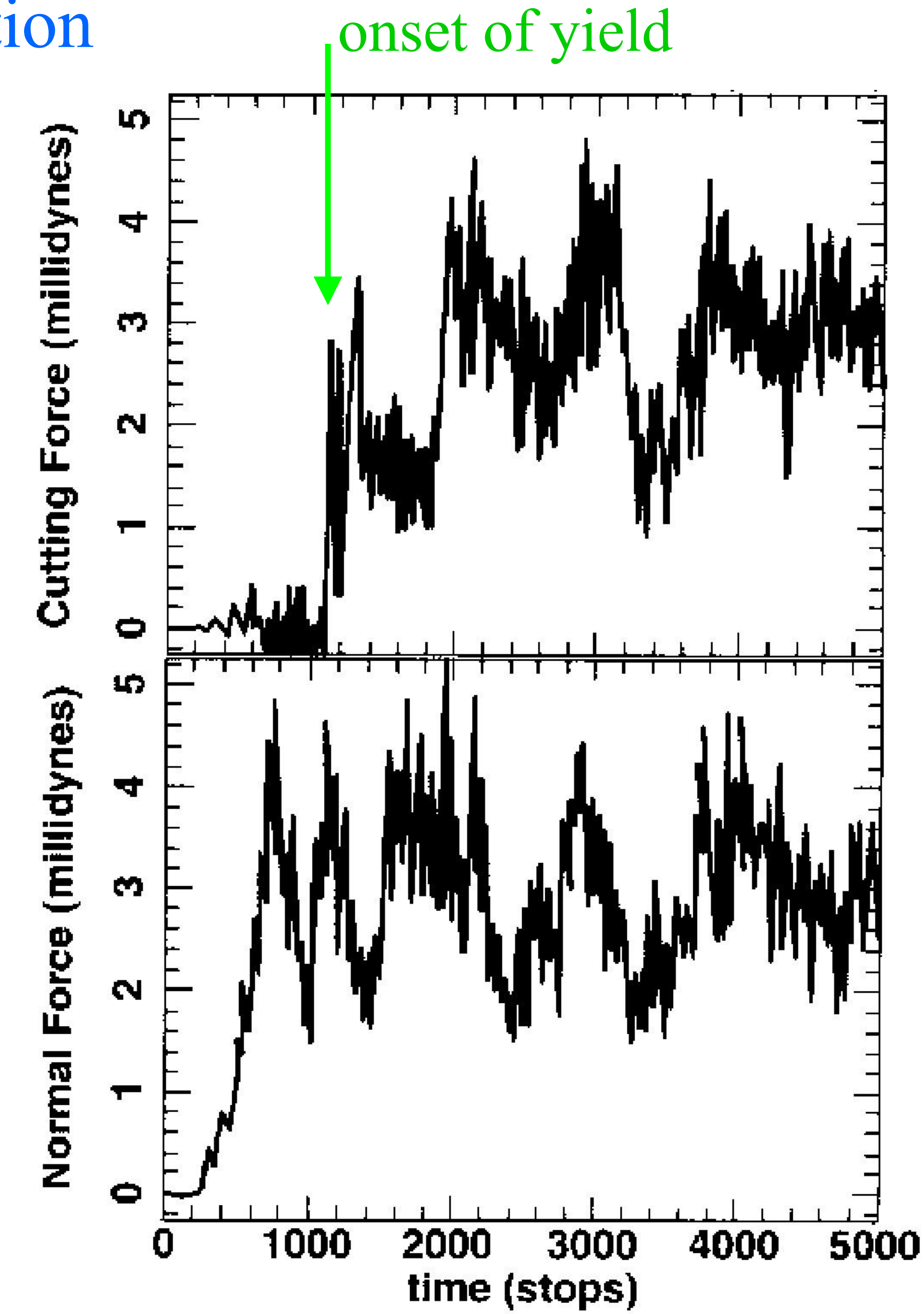
Belak and Stowers, Fundamentals of Friction, 1992

Many other examples: Molinari, Szlufarska, …

No sliding friction (cutting force) until plastic deformation occurs

Geometry dependent





Glassy "Pork Fat" Layer Leads to Amontons' Laws

Molecules adsorbed from air, wear debris, elastomer segments, and other mobile "third bodies" lock surfaces together, $F_s \neq 0$

Glass: $\tau_s = \tau_0 + \alpha\, p \Rightarrow F_s = \tau_0\, A_{real} + \alpha\, N$ (He, Müser, Robbins, Science '99)

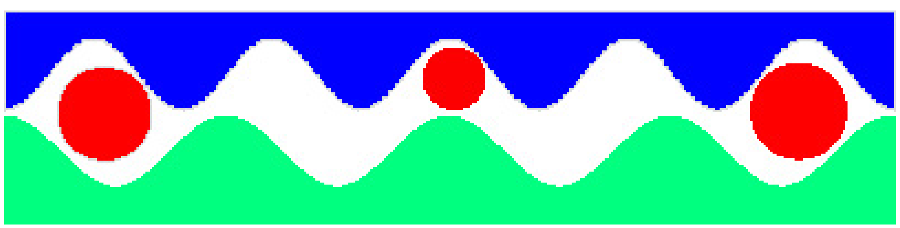
⇒ can explain Amontons's laws without a constant τ_{shear}

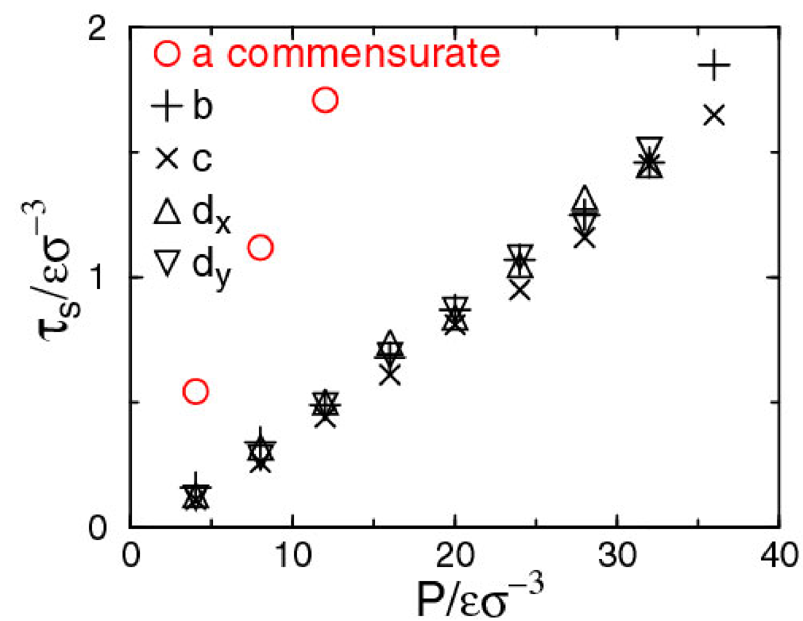
⇒ $\alpha \sim \mu$ only depends on molecular geometry: polymers ~0.1 to 0.2

Reflects slope of ramp formed by adsorbed molecules

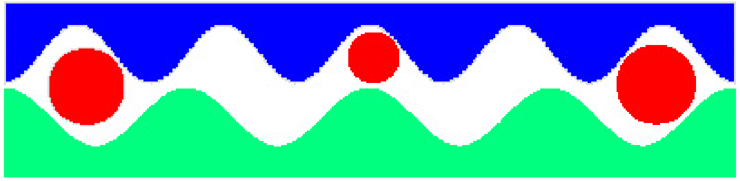
⟹ Ramp keeps rearranging so always uphill

⇒ Thermal activation model explains why kinetic friction near static and rises like $(k_B T/V^*) \log(v)$ with atomic scale volume V^*





3rd Body Leads to Amontons



Molecules adsorbed from air, wear debris, elastomer segments, and other mobile "third bodies" lock surfaces together, $F_s \neq 0$

Find $\tau_s=\tau_0 + \alpha\, p \Rightarrow F_s=\tau_0\, A_{real} + \alpha\, N$ (He, Müser, Robbins, Science '99)

$\Rightarrow$ can explain Amontons's laws without a constant τ_{shear}

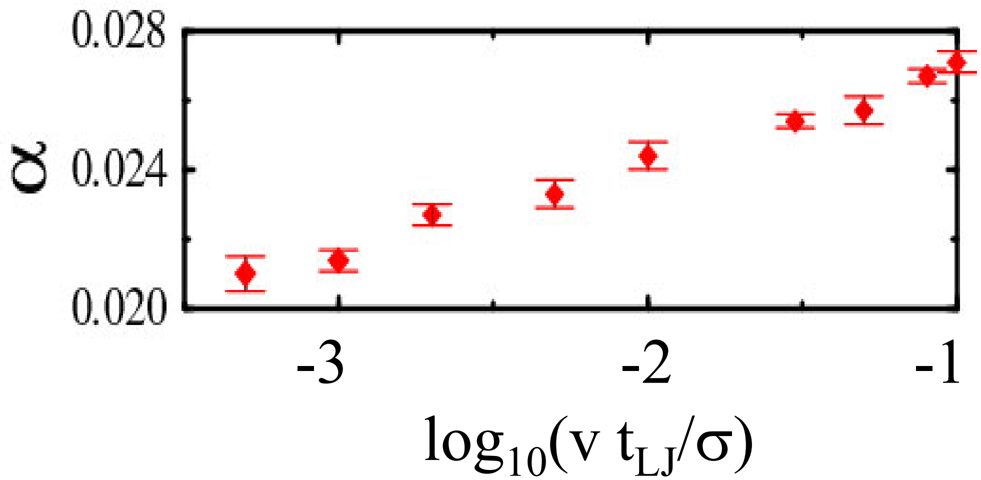
$\Rightarrow$ $\alpha \sim \mu$ is indep. of many parameters not controlled in experiment

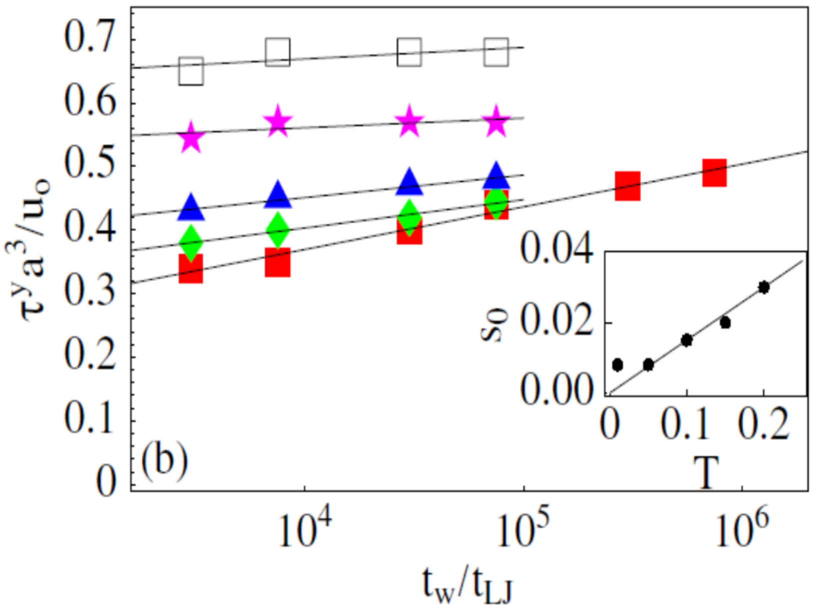
Reflects slope of ramp formed by adsorbed molecules

$\Longrightarrow$ Ramp keeps rearranging so always uphill

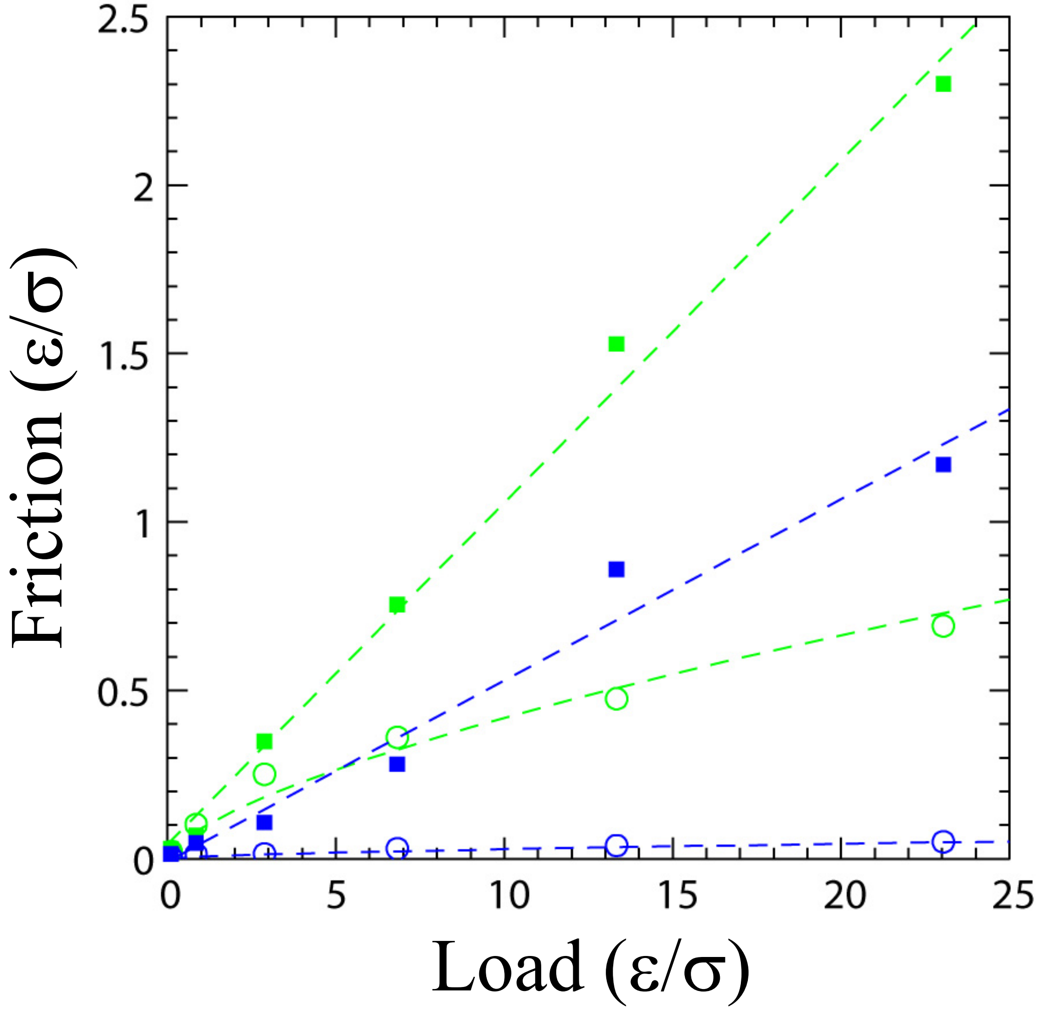
$\Rightarrow$ Thermal activation and aging give rate-state dependence:

$\mu-\mu_0=A \ln(v)+ B \ln(t_w)$





Adsorbed layers give F ∝ load for AFM tips and decrease variability of friction with tip geometry

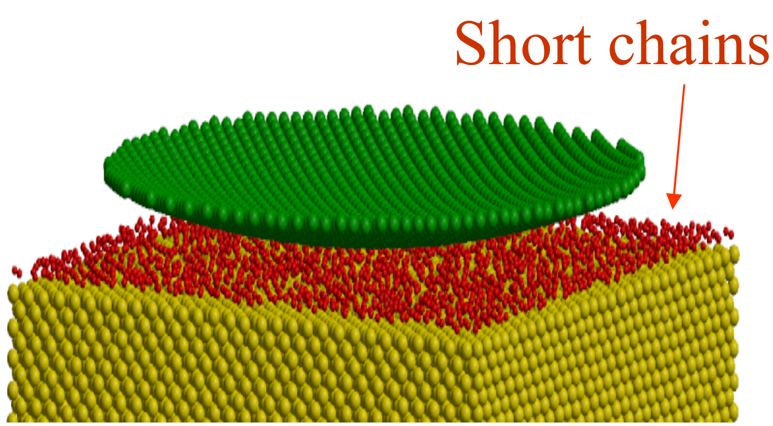


■ amorphous with adsorbed layer

■ incommens. with adsorbed layer

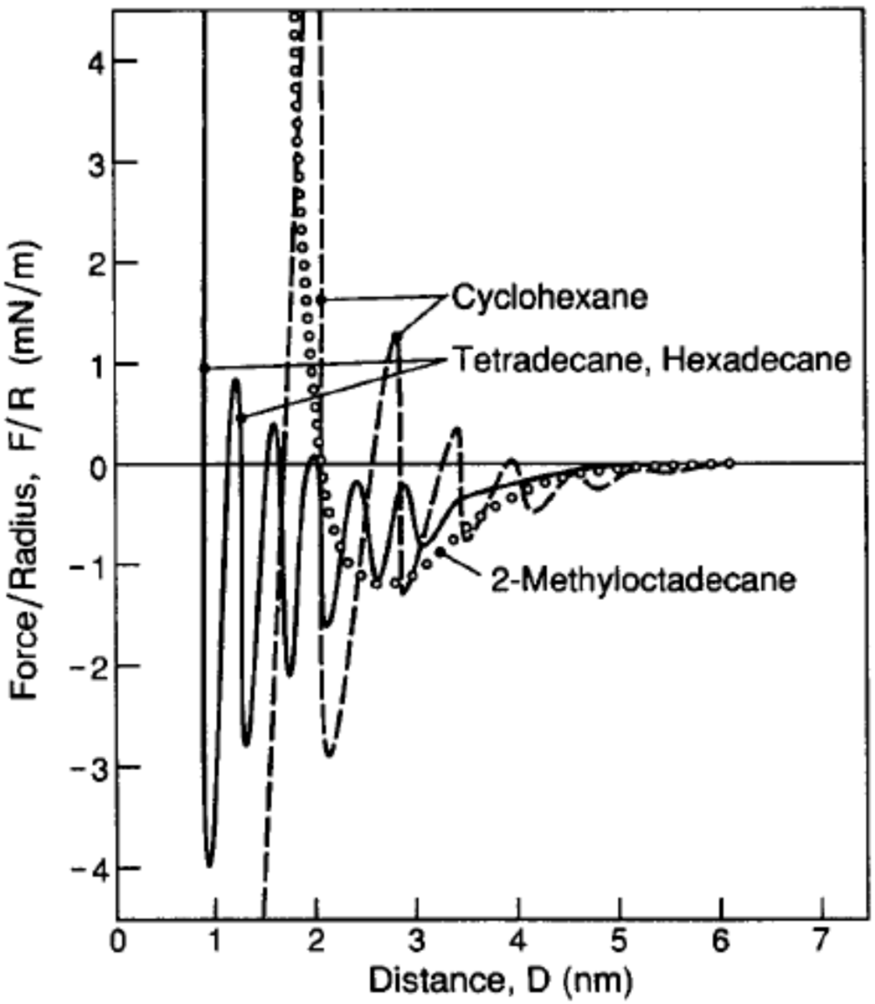
○ bare amorphous

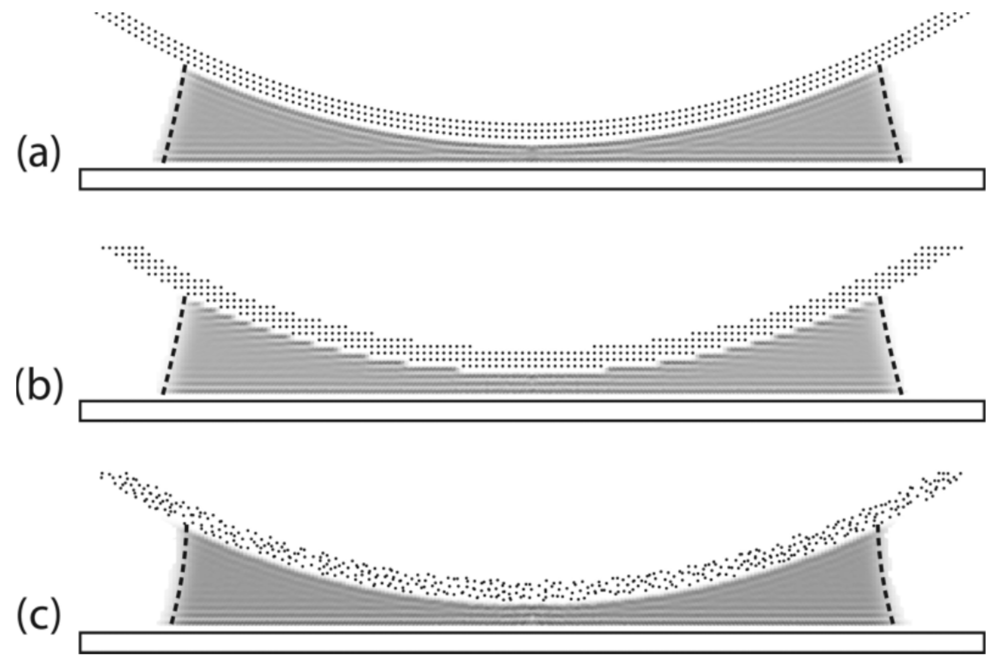
○ bare incommens.



Surface Force Apparatus Measurements

Simple fluids confined between mica plates – flat over ~100μm
See layered structure – period = molecular diameter
Gee, McGuiggan, Israelachvili J. Chem. Phys. 93, 1895 (1990)
Also seen by Jacob Klein, Steve Grannick, Susan Perkins, …





Cheng & Robbins PRE89, 062402 (2014)

Surface Force Apparatus Measurements

Simple fluids confined between mica plates – flat over ~100μm

Many act like solids when a few layers thick – up to ~2.5nm

May have constant μ or stress S

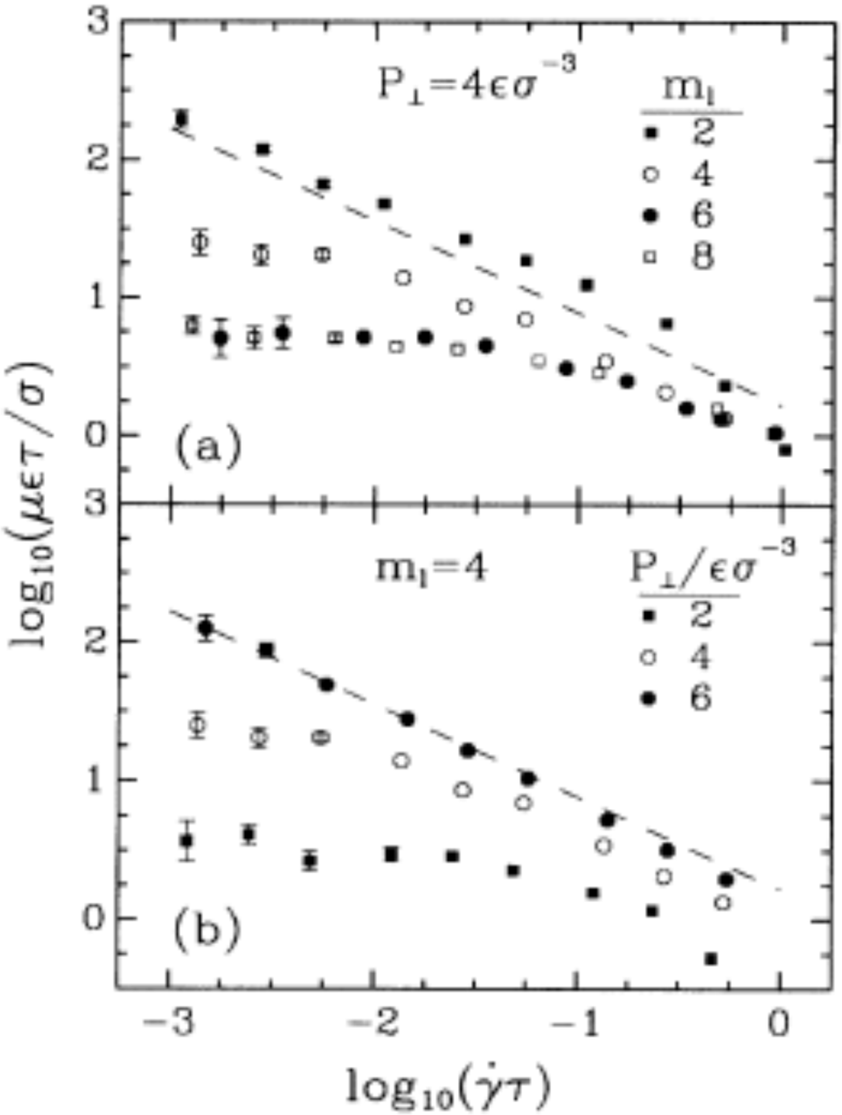
Also glass transition seen

in simulations with decrease

in # layers m or increase in p

Thompson, Grest, Robbins,

PRL 68, 3448 (1992)



Surface Force Apparatus Measurements

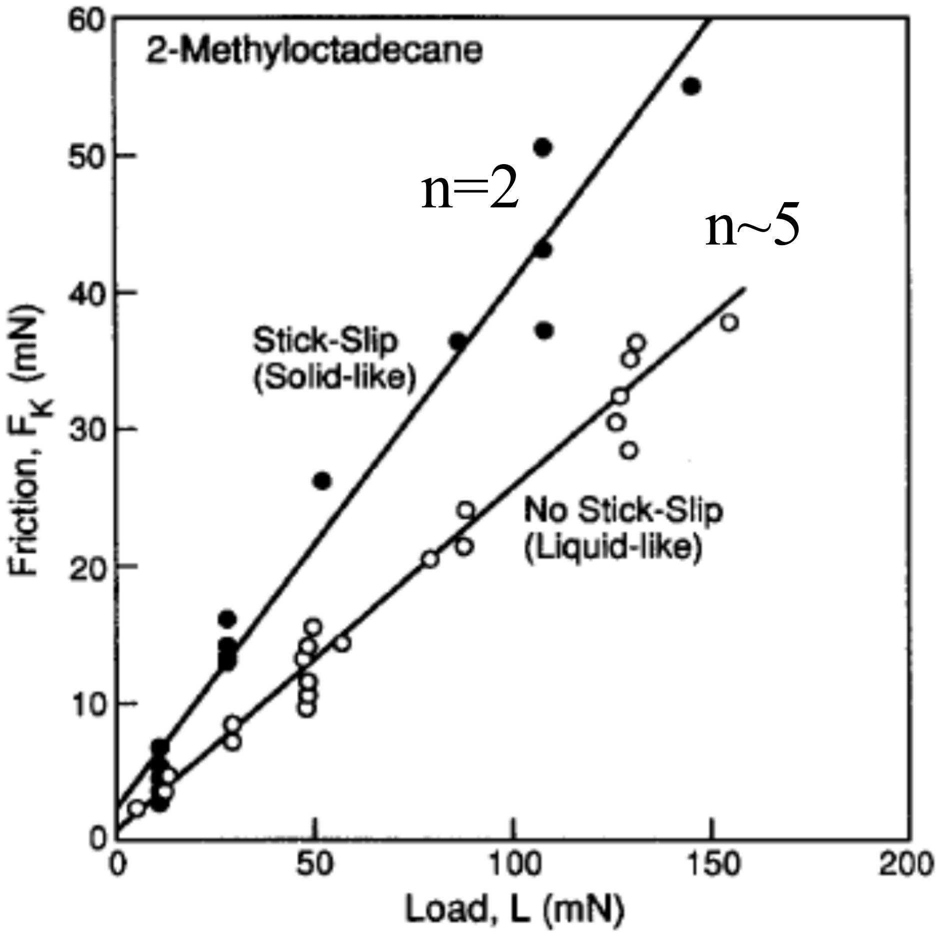
Simple fluids confined between mica plates – flat over ~100μm

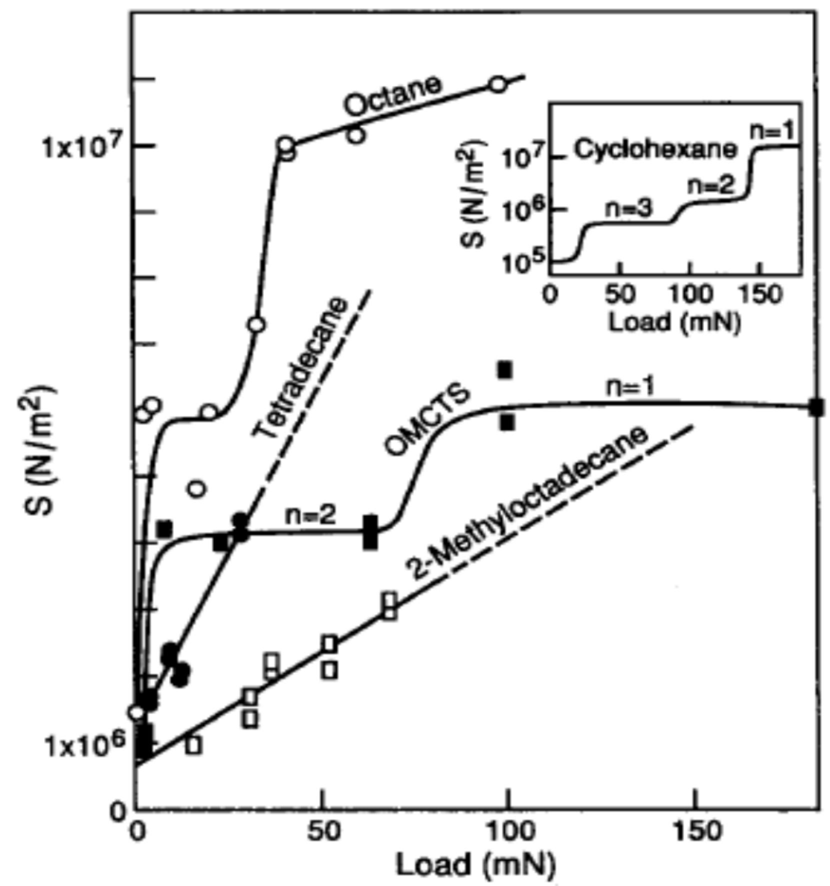
Many act like solids when a few layers thick – up to ~2.5nm

May have constant μ or stress S ~ yield stress of glass

Gee, McGuiggan, Israelachvili J. Chem. Phys. 93, 1895 (1990)

Also seen by Jacob Klein, Steve Grannick, Susan Perkins, …

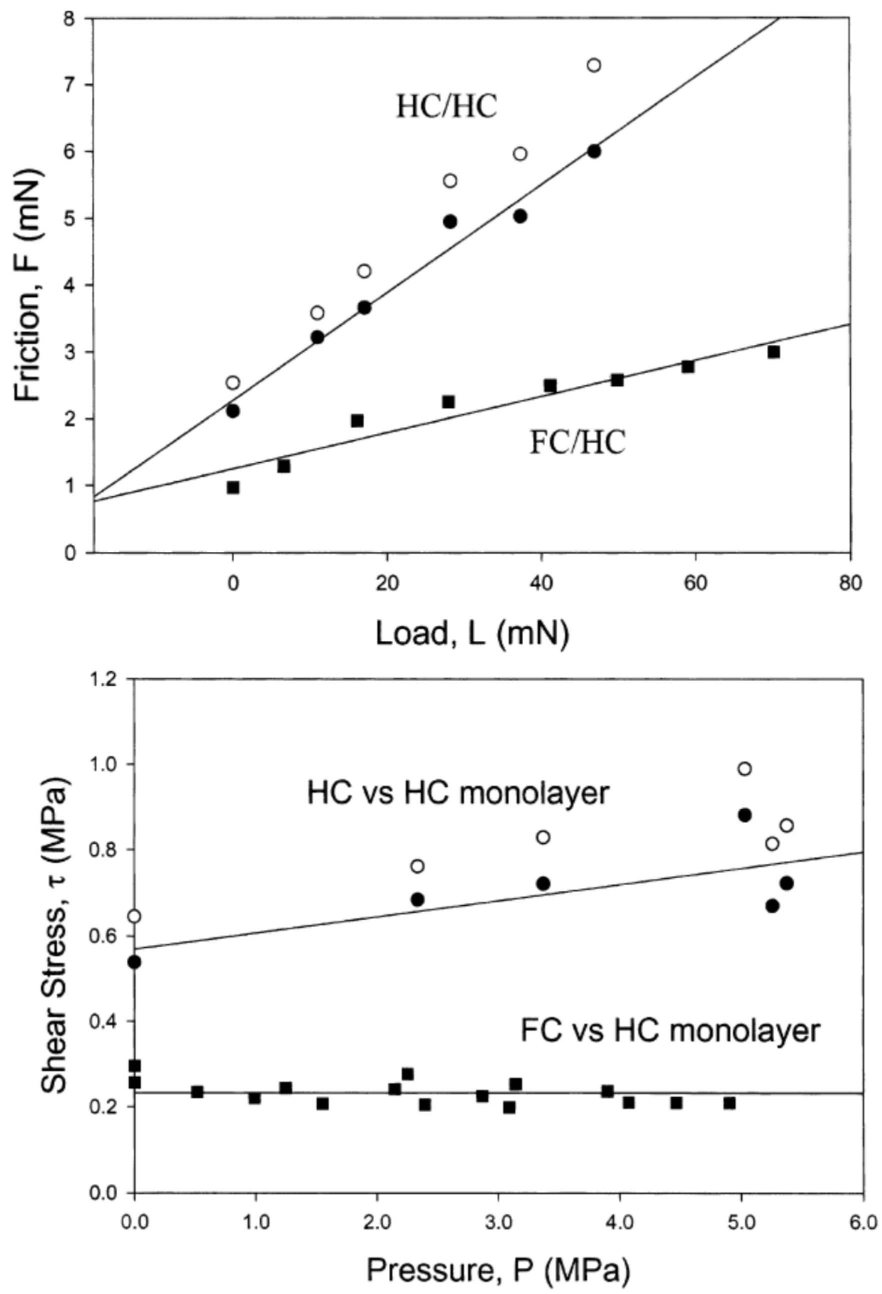




Surface Force Apparatus Measurements

Hydrocarbon (HC) and fluorocarbon (FC) monolayers
Better fit to constant shear stress than constant μ

McGuiggan, J. Adhesion 80, 395 (2004)



Surface Force Apparatus Measurements

Purely repulsive interactions tend to give friction $\propto$ load

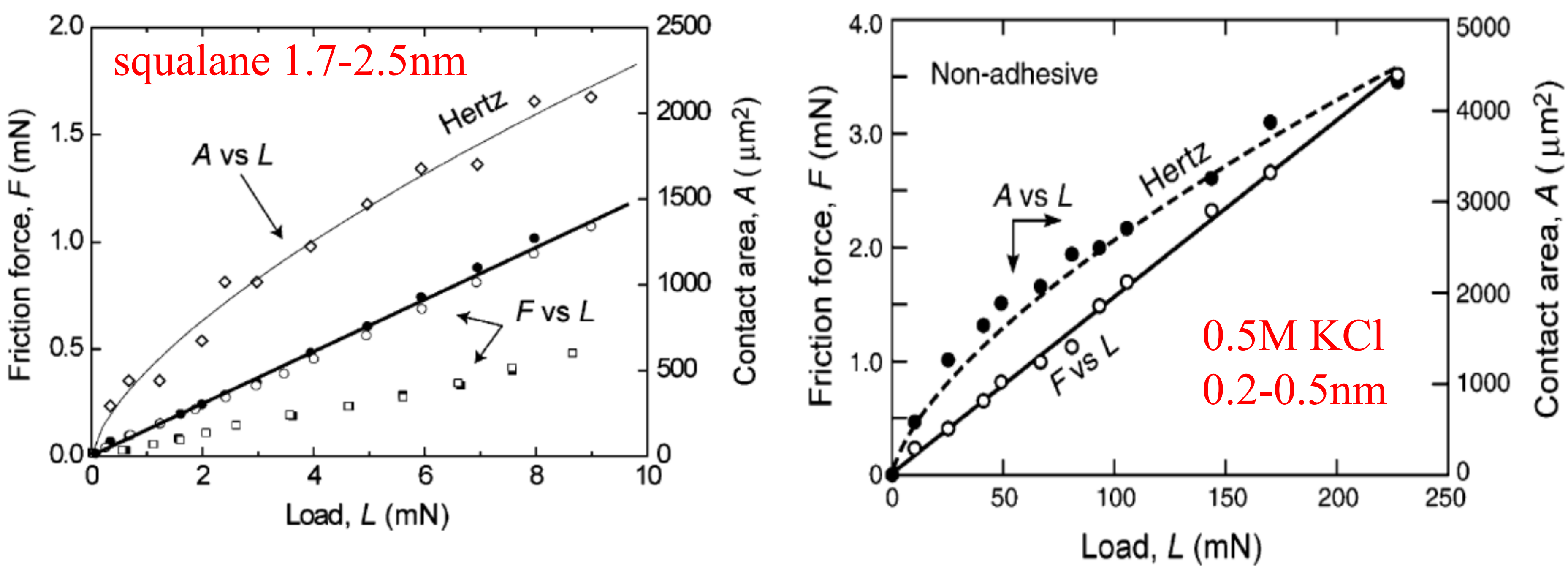
small adhesive τ_0: $\tau_s = \tau_0 + \alpha\ p \Rightarrow F_s = \tau_0\ A_{real} + \alpha\ N$

Squalane glassy to 3-5 layers

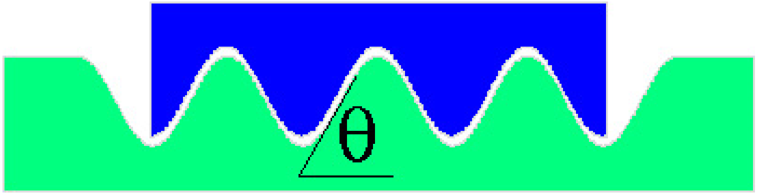
Water with double layer – μ~0.02 with 1-2 water layers,

KCl from 0.01 to 0.5M; pressure 10-50MPa

Gao, Luedtke, Gourdon, Ruths, Israelachvili, Landman, J. Phys. Chem. B108, 3410 (2004)



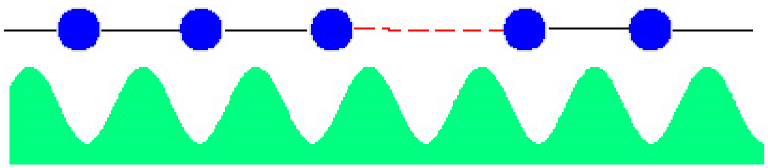
Friction Mechanisms in Contacts



Geometrical Interlocking: F=N tan θ

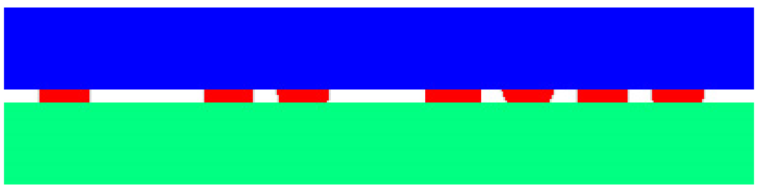
Unlikely to mesh, F goes up as smooth

Kinetic friction vanishes



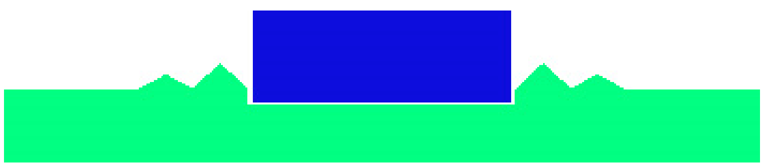
Elastic Metastability:

Marginal dimension - exponentially weak in disorder or lateral coupling



Mixing or Cold-Welding

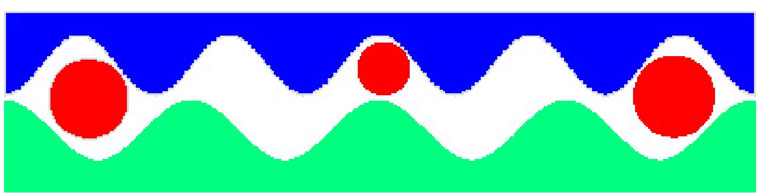
Most likely for clean, unpassivated surfaces in vacuum



Plastic Deformation (plowing)

Load and roughness dependent

⇒High loads, sharp tips



Mobile third bodies → "glassy state"

hydrocarbons, wear debris, gouge, …

Glass seen in Surface Force Apparatus,

Robust friction mech. on many scales

Surfaces Often Rough on Many Scales – Self-Affine
Archard ⇒ Bumps on Bumps on Bumps

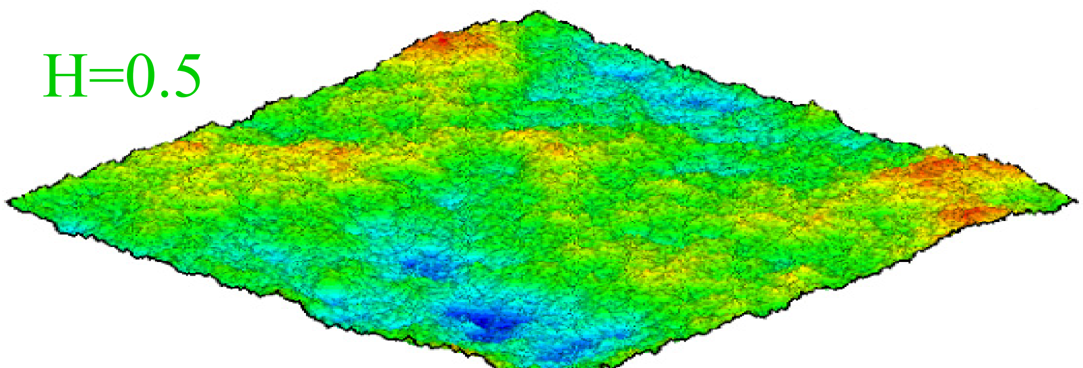
Elastic surfaces – Area $\propto$ Load – constant pressure

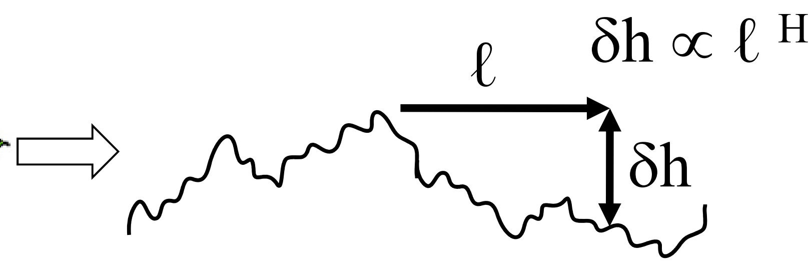
Key surface property = h'_{rms} = rms slope of surface

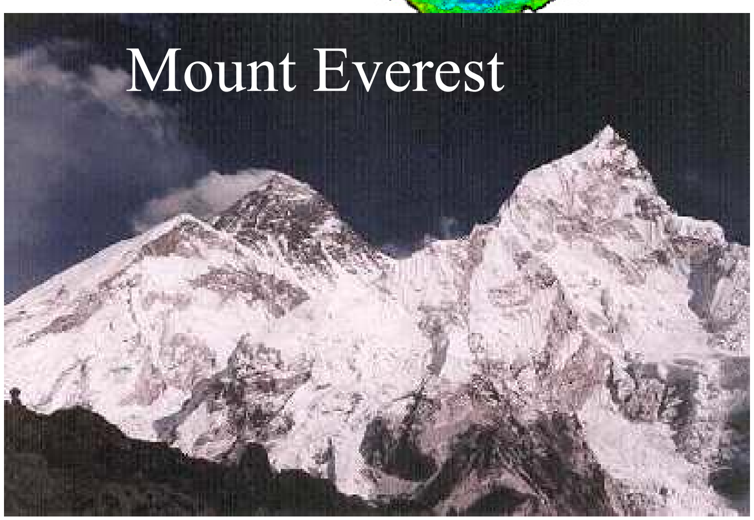
Repulsive contacts - $p_{rep} = E'\, h'_{rms}/\kappa_{rep}$; $E' = E/(1-\nu^2)$

Adhesion - $p_{att} = w/\Delta r$; w=energy/area, Δr range

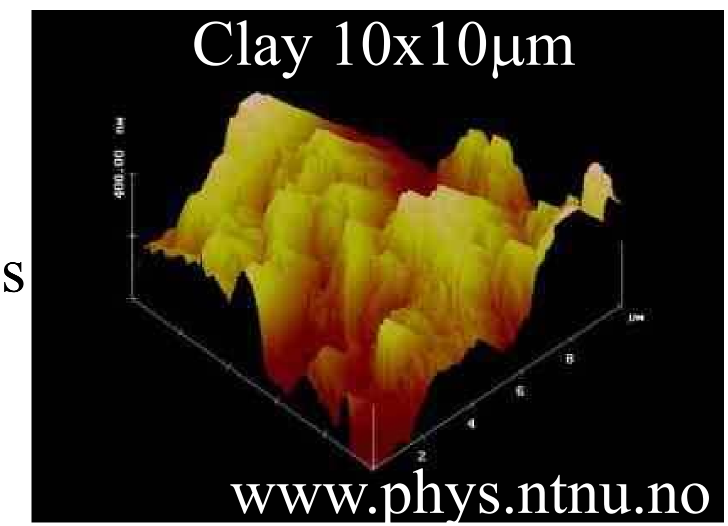
H=0.5







Examples with H=0.8



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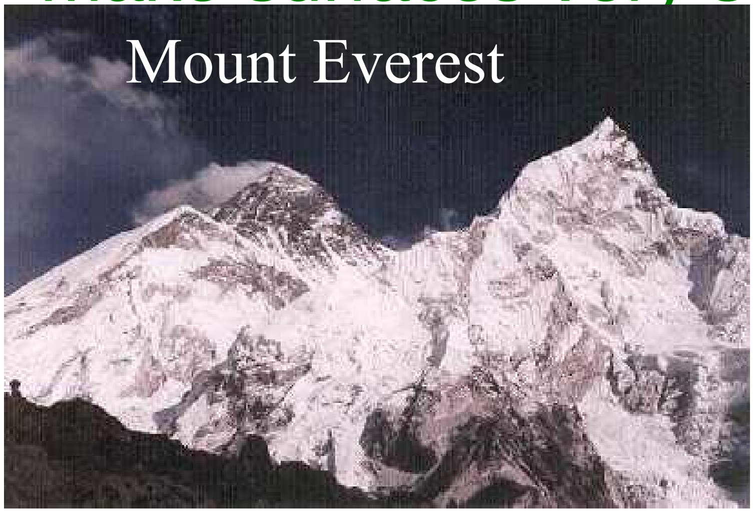
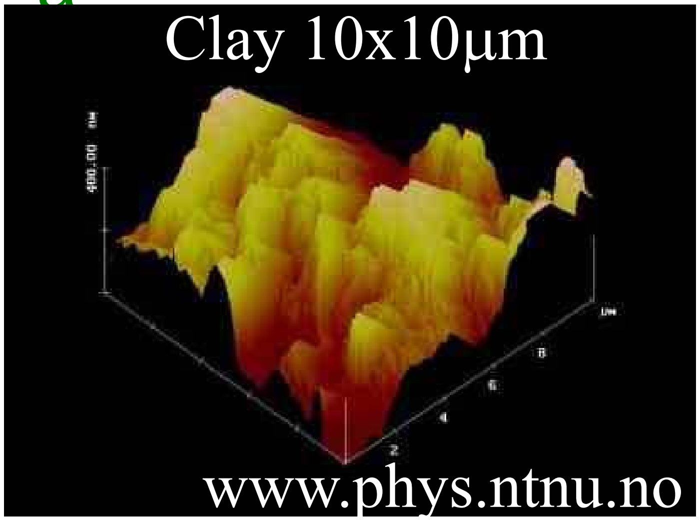
Hertz – $p_H = \frac{N^{1/3}}{\pi}\left[\frac{4E'}{3R}\right]^{2/3}$

Surfaces sticky only if break link between E' and w
– make surfaces very soft < 1MPa



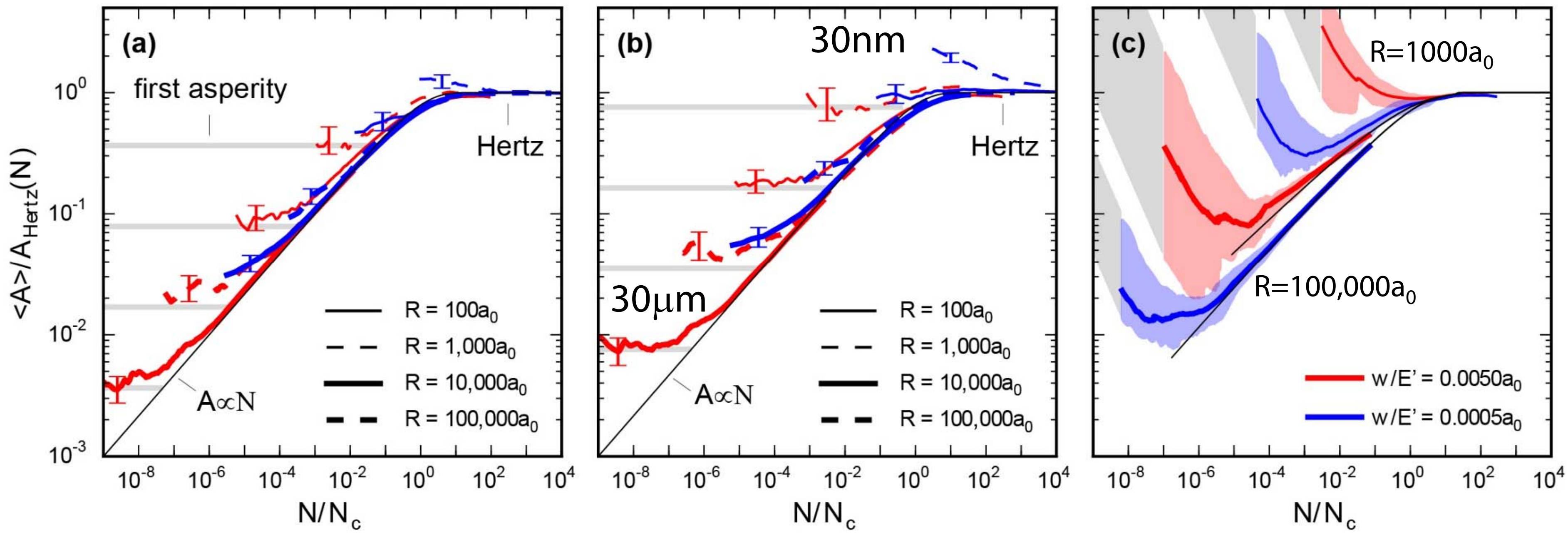
Examples with H=0.8



Area Divided By Hertz Prediction

Transition from $A \propto N$ to $A \propto N^{2/3}$ at $N_c = E' R^2 (9/16)(\pi h'_{rms}/\kappa)^3$

Hard wall   Soft wall   Adhesive



Black- analytic, Red $h'_{rms}=0.1$, Blue $h'_{rms}=0.01$, $a_0 \sim 0.3$nm

Parameter free analytic interpolation captures statistical behavior

Deviation at small loads – just a few asperities

Consistent with friction$\propto N^{2/3}$ for metal sphere on polymer, etc.

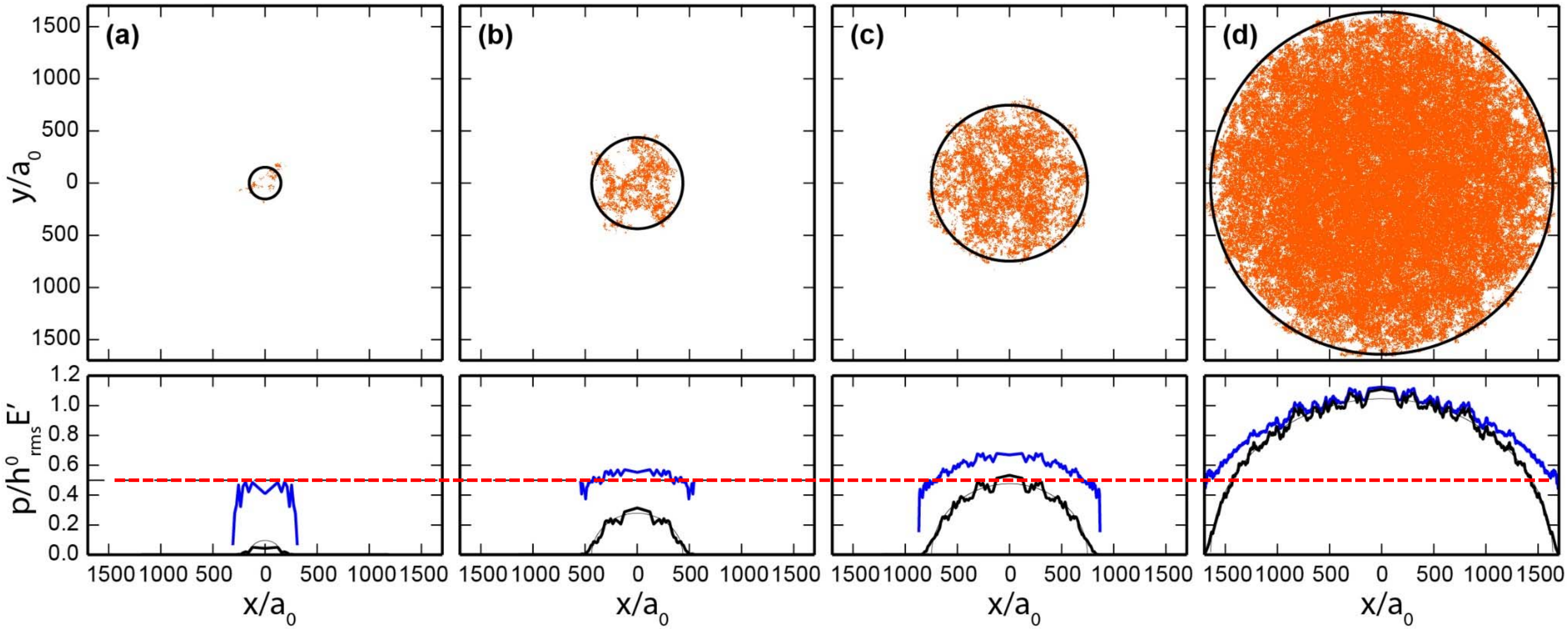
Small spheres act like smooth – first asperity ~ sphere.

Sphere on Flat

Parallel plates are hard to align ⟹ experiments use sphere-on-flat

Like parallel at small loads, Hertz at large loads

Top – contact in orange, solid=Hertz radius,



Bottom – black=mean pressure at a given radius

blue= mean pressure in contacting regions

red= flat surface prediction for p_{rep}

[Pastewka and Robbins, Applied Physics Letters**108**, 221601 (2016)]

Conclusions

- Have analytic understanding of relation between contact area and load: $p_{rep}=N/A=E'/\kappa_{rep}h'$ *⇐please measure*
- Parameter-free theory for onset of adhesion
  Adhesion rare, typical $w/E' \equiv l_a$ << atomic spacing
- Parameter-free theory for sphere on flat contact
- Proportionality between area and load is not enough to explain Amontons' laws even in nonadhesive case
  → Unless h' is a material parameter?
  → Clean surfaces - friction exponentially weak
  → Plowing, wear, … geometry changes τ
  → Welding may give constant τ for polymers?
- Third bodies give $\tau_s=\tau_0+\alpha p$, material property of body
  $\alpha \Rightarrow \mu$ independent of uncontrolled exp. parameters
  gives rate state behavior with right energy scale