

# *Friction Mechanisms: Atomic to Macroscopic*

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Sponsored by the National Science Foundation

## Questions:

Where do surfaces contact?

How is friction produced in contacts?

How do static and kinetic friction differ and age?

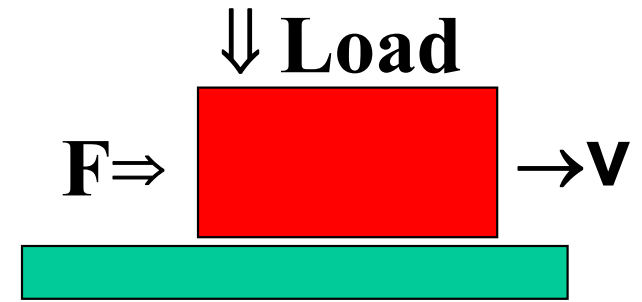
How does concept of contact depend on scale?

Do similar mechanisms of frictional locking,  
stick-slip, fracture, ... operate at different scales?

Can studies of mechanisms at small scales provide  
essential input for modeling larger scales?

Can large scale experiments test small scale models?

## Typical measurement of friction →



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  $\propto$  load → constant  $\mu = F/\text{Load}$ .
- Friction force independent of the  
apparent contact area  $A_{\text{app}}$ .

But: Amontons coated all surfaces with pork fat

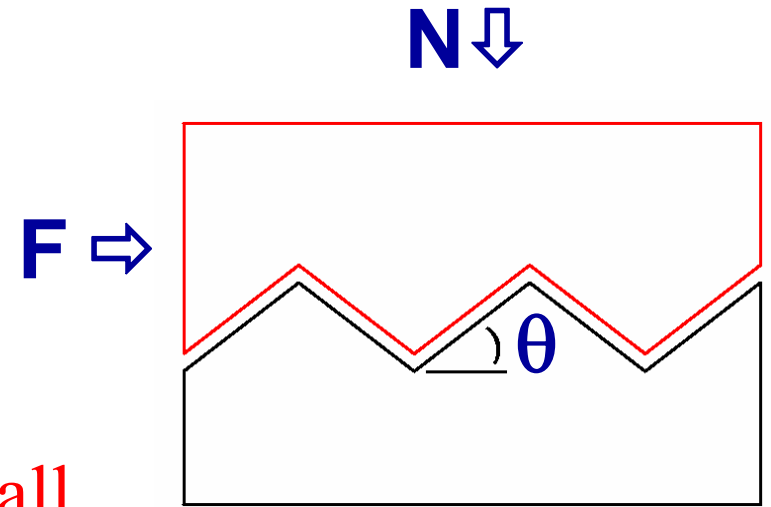
Friction at zero and negative loads  $\propto A_{\text{app}}$

Friction depends on history

# Why Friction $\propto$ Load, Independent of Apparent Area?

Geometric explanation (Amontons, Parents, Euler, Coulomb)

- Surfaces are rough
- Friction = force to lift up ramp formed by bottom surface
- $F = N \tan \theta \Rightarrow \mu = \tan \theta$



Problems:

- Most surfaces can't mesh,  $A/A_0$  small (Müser, Wenning, Robbins, PRL 86, 1295 (2001))
- Roughening can reduce  $\mu$  (hard disks)
- Monolayer of grease changes  $\mu$  not roughness
- Once over peak, load favors sliding  $\Rightarrow$  kinetic friction = 0

Static friction  $\Rightarrow$  Force to escape metastable state

*How can two surfaces always lock together?*

Kinetic friction  $\Rightarrow$  Energy dissipation as slide

*Why is this correlated to static friction?*

# *Surfaces Often Rough on Many Scales $\Rightarrow$ Self-Affine*

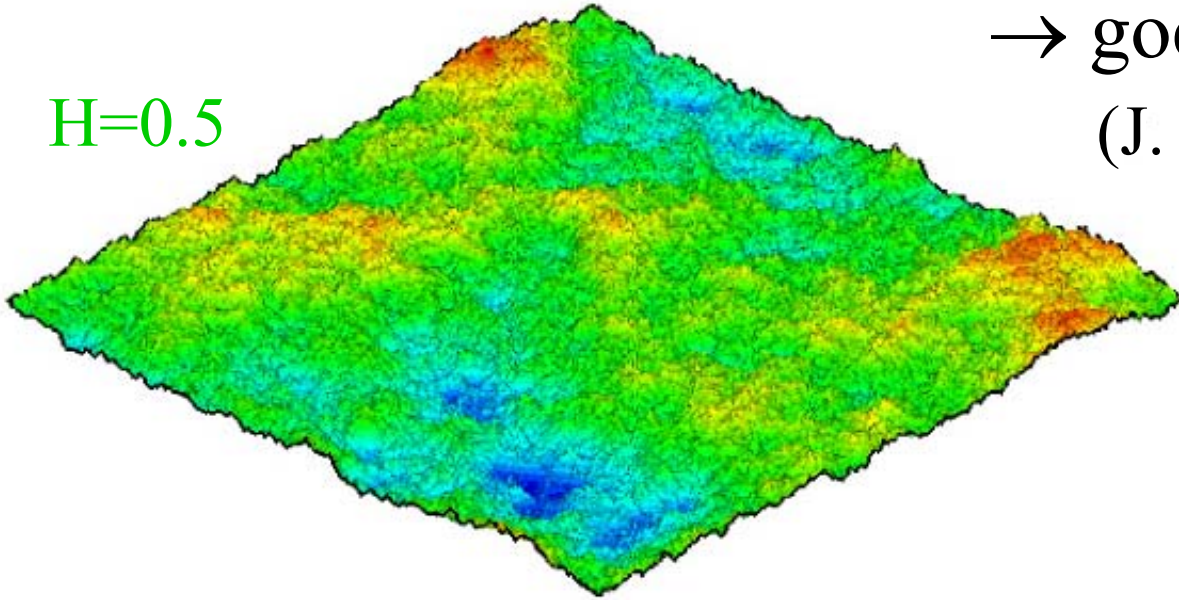
Height variation  $\Delta h$  over length  $\ell \rightarrow \Delta h \propto \ell^H \quad H < 1$

Average slope  $\Delta h / \ell \propto \ell^{H-1} \rightarrow$  diverges as scale  $\ell$  decreases

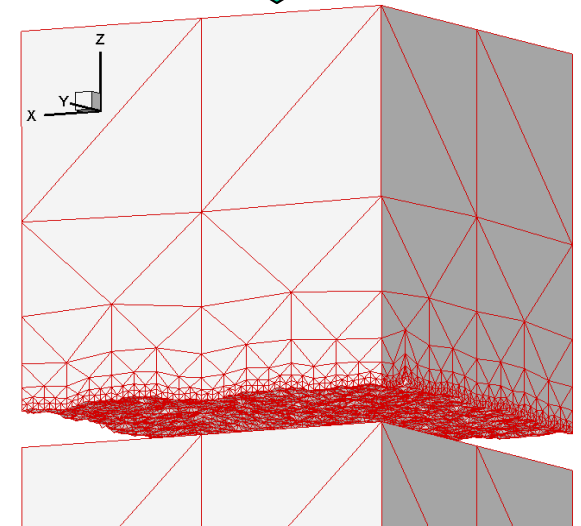
$\rightarrow$  goes to zero as  $\ell$  increases

(J. Greenwood)

$H=0.5$



Load



## **Finite-element calculation**

Rough surface on rigid flat (maps to 2 rough)

Elastic or J2 isotropic plastic constitutive law

Periodic boundary conditions,  $L=512$  nodes per edge

Full range of  $H$  and roughness amplitudes

# *Area $\propto$ load $N$ for nonadhesive contact*

Constant mean pressure in contact  $\langle p \rangle = N/A$  at low  $N$

Controlled by rms local slope,  $\Delta$ , not total roughness

Elastic:  $\langle p \rangle / E' = \Delta / \kappa$

$E' = E / (1 - \nu^2)$

=effective modulus

$$\Delta \equiv \sqrt{\langle |\nabla h|^2 \rangle}$$

=rms surface slope

$\kappa(H, \nu)$  from 1.8 to 2.2

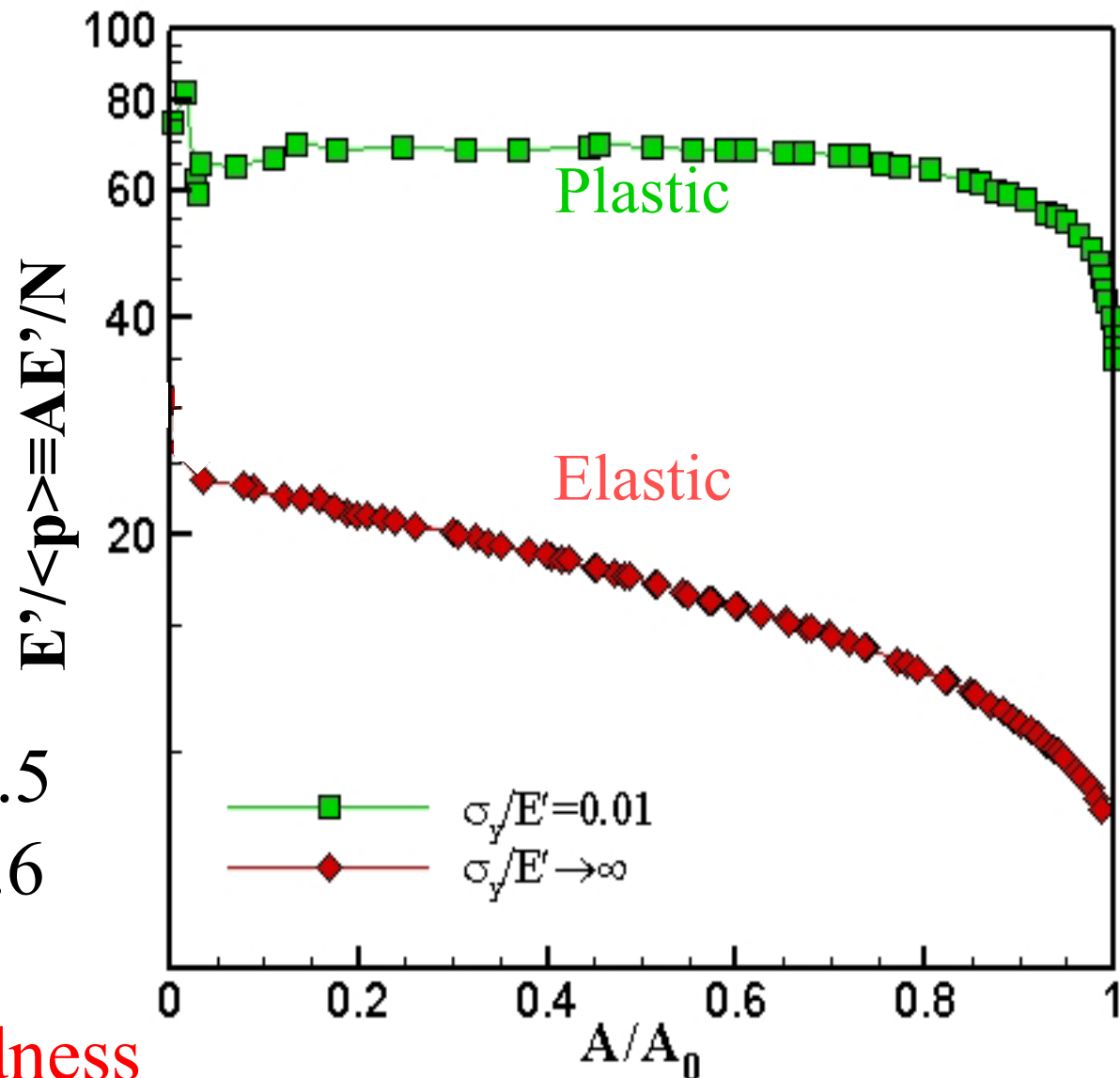
Analytic predictions:

Bush et al.,  $\kappa = (2\pi)^{1/2} \approx 2.5$

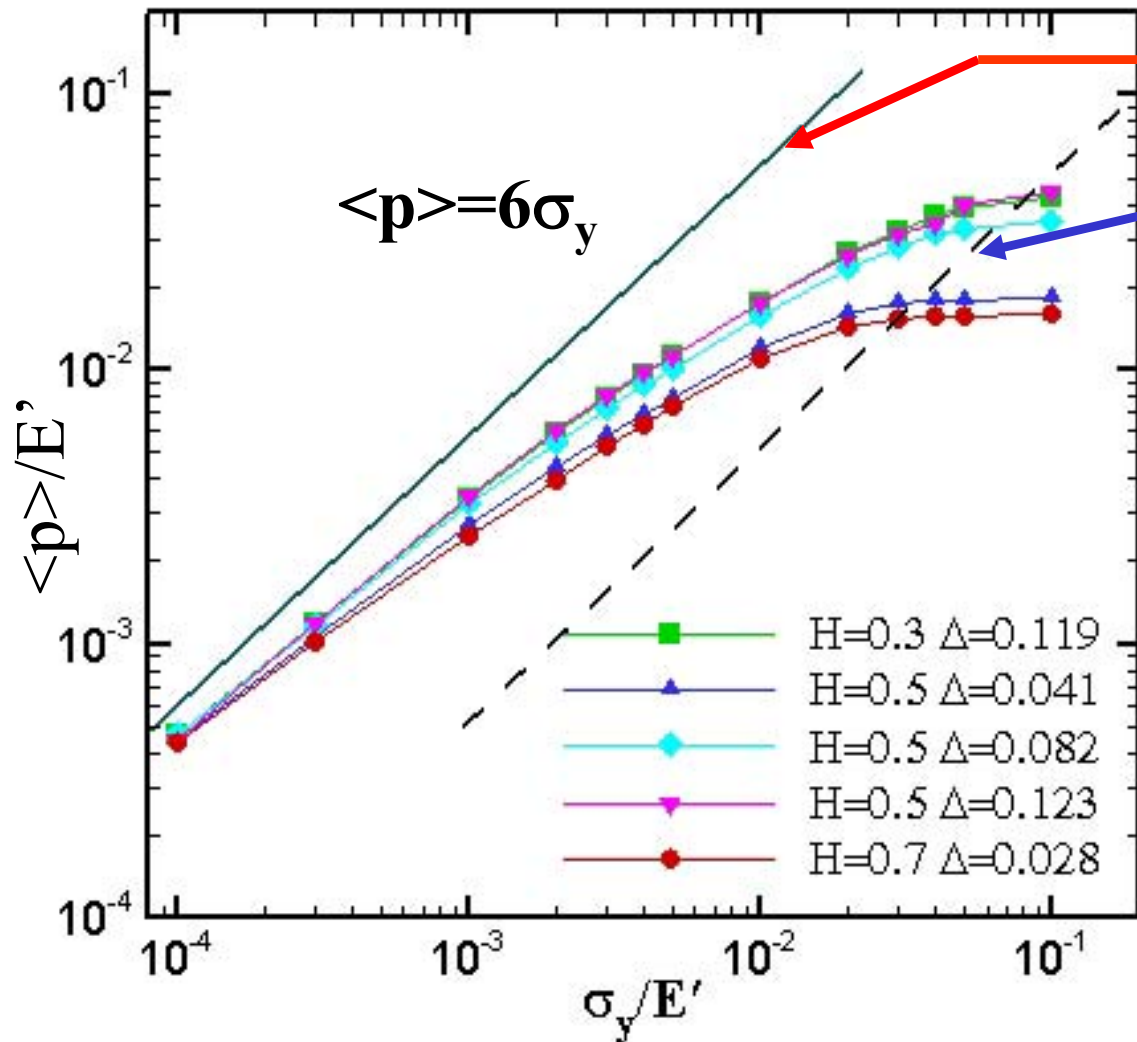
Persson  $\kappa = (8/\pi)^{1/2} \approx 1.6$

Plastic:  $\langle p \rangle \neq 3\sigma_y$

$3\sigma_y$  = single-asperity hardness



# Unexpected Dependence of $\langle p \rangle$ on Yield Stress $\sigma_y$



Only elastic for  $\langle p \rangle < \sigma_y/2$   
 $\langle p \rangle/E' \sim \Delta/\kappa$

Bowden and Tabor:

$\langle p \rangle \approx 3\sigma_y$   
 = single-asperity hardness

For small  $\sigma_y/E'$ ,  $\langle p \rangle$  is about twice this value. (Gao & Bower)

Power law regime  $\langle p \rangle \propto \sigma_y^x$ ,  
 $x \approx 2/3$  for typical  $\sigma_y/E'$ .

High strength steel  $6 \times 10^{-3}$

Titanium  $9 \times 10^{-3}$

Bone  $7 \times 10^{-3}$

Silicon  $3 \times 10^{-2}$

Amorphous metal  $2-5 \times 10^{-2}$

# *Complex Morphology Varies with Constitutive Law*

Power law distribution of connected areas  $a_c$ :  $P(a_c) \propto a_c^{-\tau}$

Connected regions are fractal  $a_c \propto r^{D_f}$

Ideal Elastic

$$\tau > 2, D_f = 1.6$$

Spread evenly

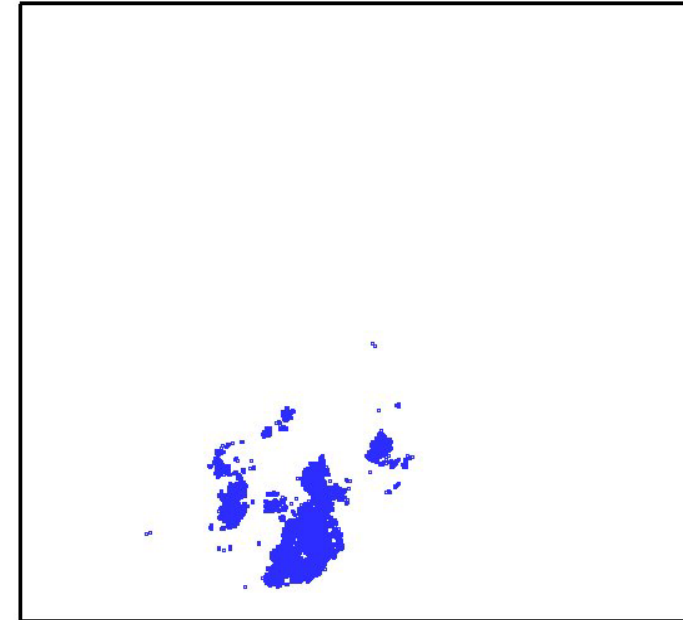
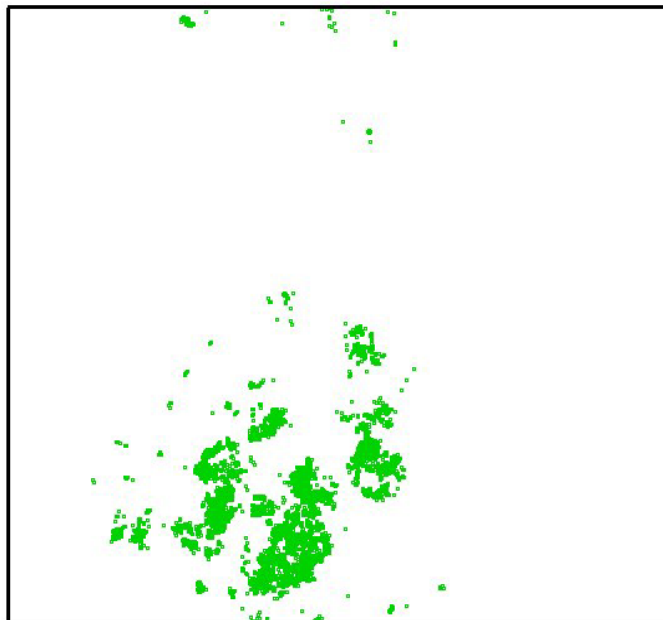
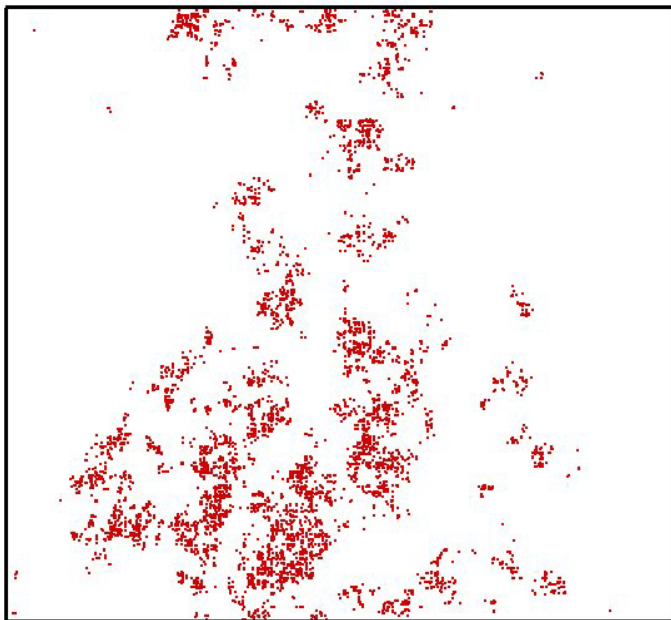
Perfectly Plastic

$$\tau \approx 2, D_f = 1.8$$

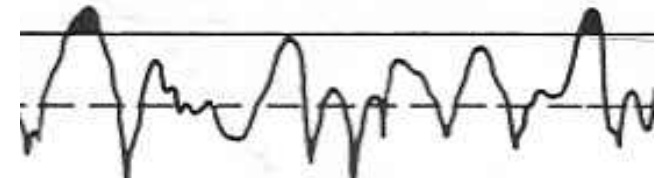
Overlap Model

$$\tau = (2 - H/2), D_f = 2$$

Near highest peak



All results for same surface,  
0.015% in contact.



# *Conclusions of Continuum Studies of Non-Adhesive Contact*

- Area proportional to load  $\rightarrow \langle p \rangle = \text{constant}$   
Elastic:  $\langle p \rangle / E' = \Delta / \kappa$    Plastic:  $\langle p \rangle \propto \sigma_y^{2/3}$
- Constitutive law changes:
  - Power law distribution of contact sizes
  - Fractal dimension of contact areas
- Ignoring interactions between asperities gives qualitatively wrong spatial distribution of contacts
- Most contacts at smallest scale
  - $\rightarrow$  results dominated by small scale cutoff
  - $\rightarrow$  continuum mechanics may fail even though total area is very large
  - $\rightarrow$  reason  $kT$  remains important at macroscale?



# *What are limits of Continuum Theory?*

Continuum theories: Hertz, Johnson-Kendall-Roberts

Assume: 1) continuous displacements, bulk elastic const.

2) smooth surface (often spherical) at small scales

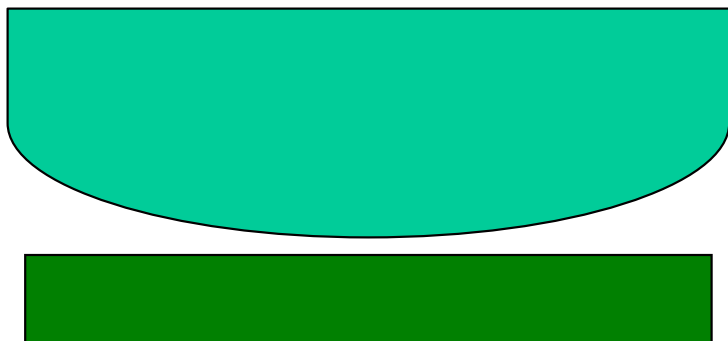
Only tested for atomically flat mica bent into cylinders

and elastomers with liquid behavior on small scales

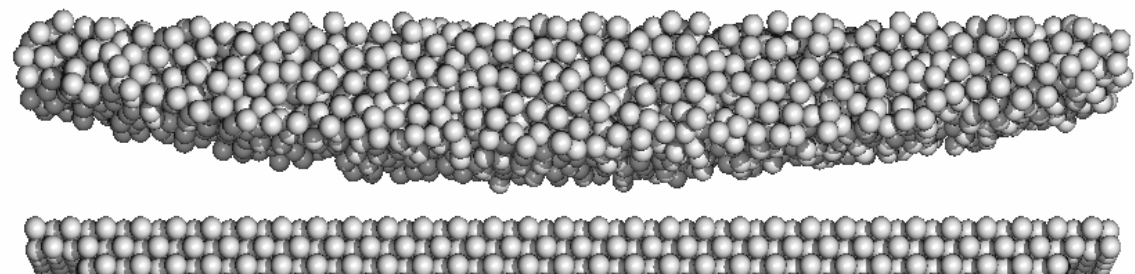
Find (1) valid down to a few atomic diameters, but atomic scale roughness causes failure of continuum theories.

Important for small contacts between rough surfaces and ideal single asperities: scanning probe or nanoindenter

Macro View



Molecular View



Luan & Robbins, Nature 435, 929 (2005)

# *Pressure distribution for sphere on flat*

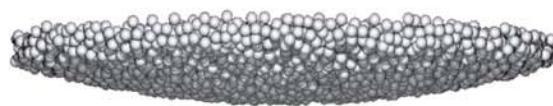
Atomic scale roughness qualitatively changes pressure, yield  
Bent crystal agrees with Hertz/JKR, more realistic tips do not

$R=100\sigma$   
 $\sim 30\text{nm}$

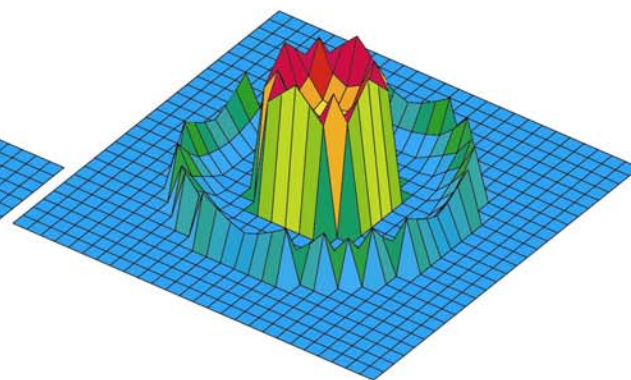
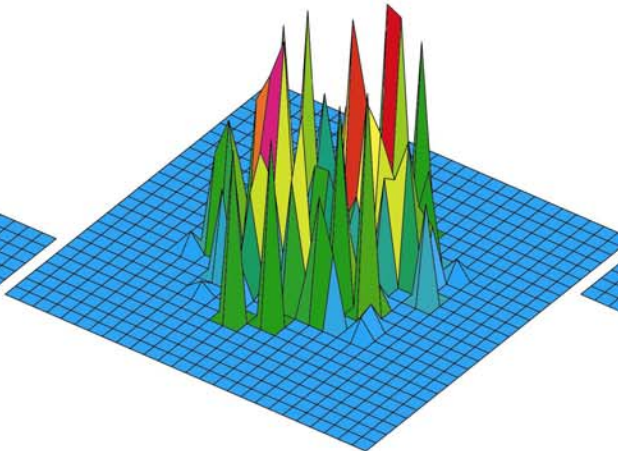
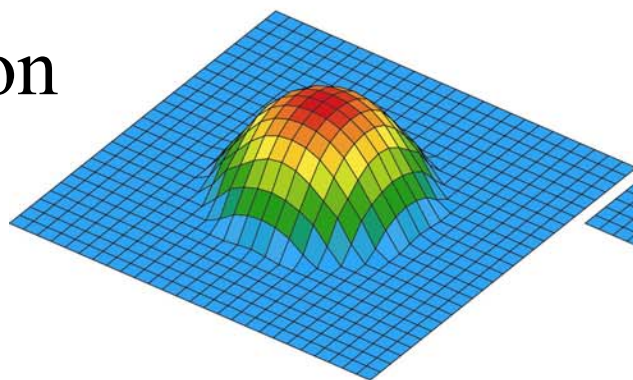
Bent crystal

Amorphous

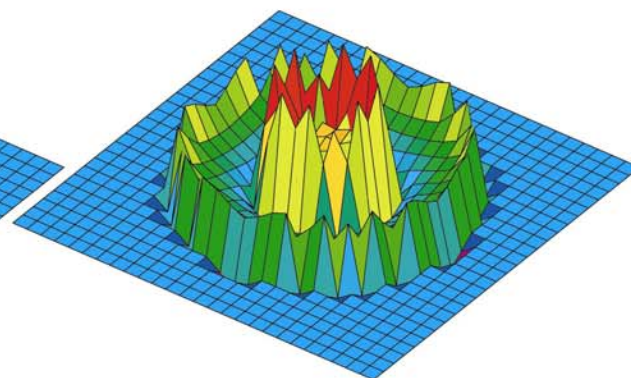
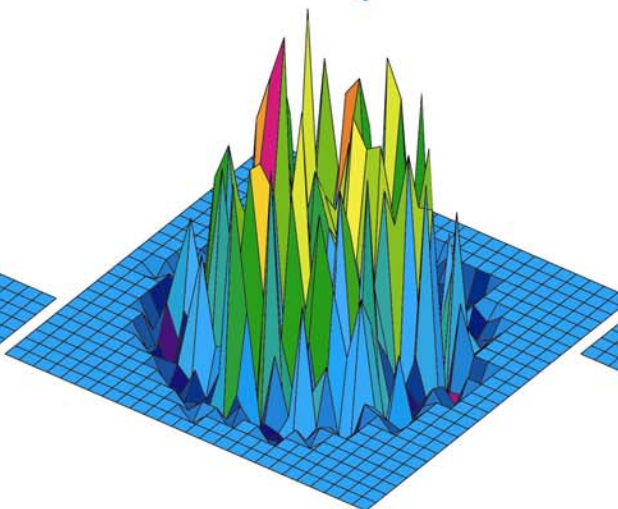
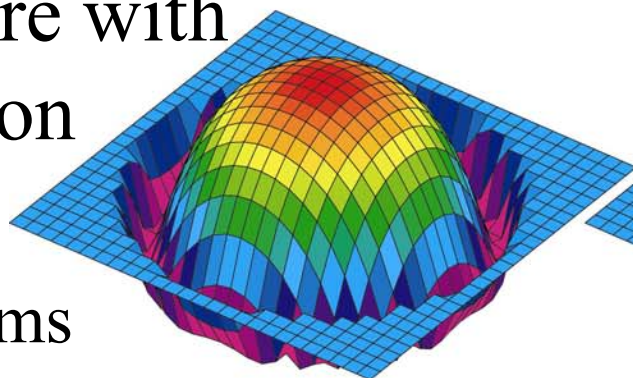
Stepped Crystal



Pressure without  
adhesion

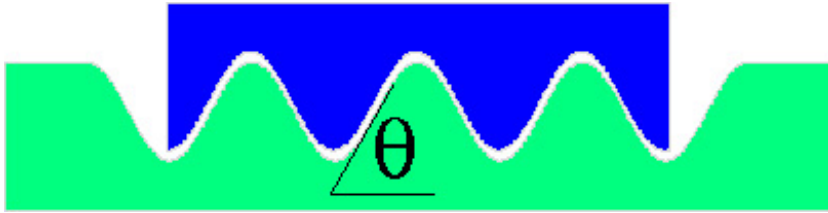


Pressure with  
adhesion

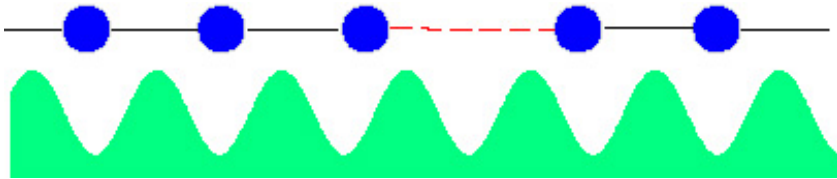


$\sim 10^7$  atoms

# *Friction Mechanisms in Contacts*



Geometrical Interlocking:  $F=N \tan \theta$   
Unlikely to mesh,  $F$  goes up as smooth  
Kinetic friction vanishes



Elastic Metastability:



Mixing or Cold-Welding



Plastic Deformation (plowing)



Mobile third bodies – hydrocarbons,  
wear debris, gouge, ...

# Simple Models of Friction

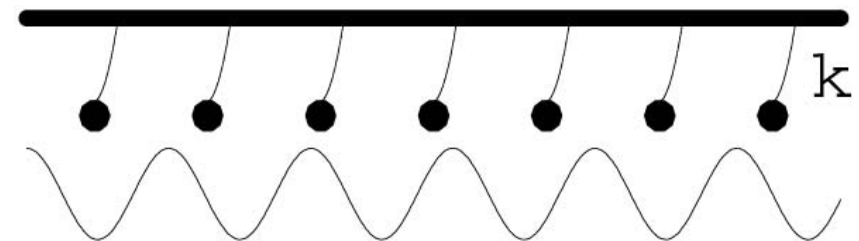
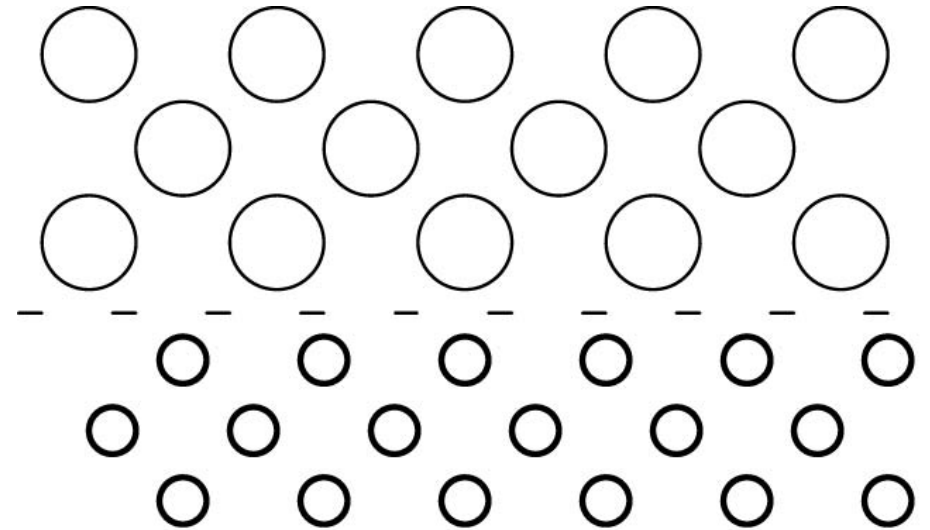
Two flat crystalline surfaces  
generally have different periods  
⇒ incommensurate

⇒ Elastic metastability gives  
non-zero  $F_s$  when interfacial  
interactions strong compared  
to internal stiffness

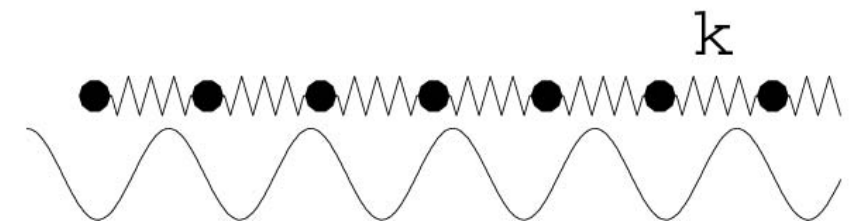
⇒ Dissipate energy in pops  
between metastable states that  
remain rapid even as mean  
velocity goes to zero:  $F_k \approx F_s$

**Problem: Metastability unlikely**  
⇒ **Expect  $\tau_s=0$  almost always**

Müser, Urbakh, Robbins, Adv. Chem. Phys.  
126, 187 (2003)



Prandtl-Tomlinson



Frenkel-Kontorova

# Quartz Crystal Microbalance – Krim et al.

Fluid or incommensurate layers on substrate → no static friction

$$F = -v M/t_s$$

$v$ =velocity relative to substrate

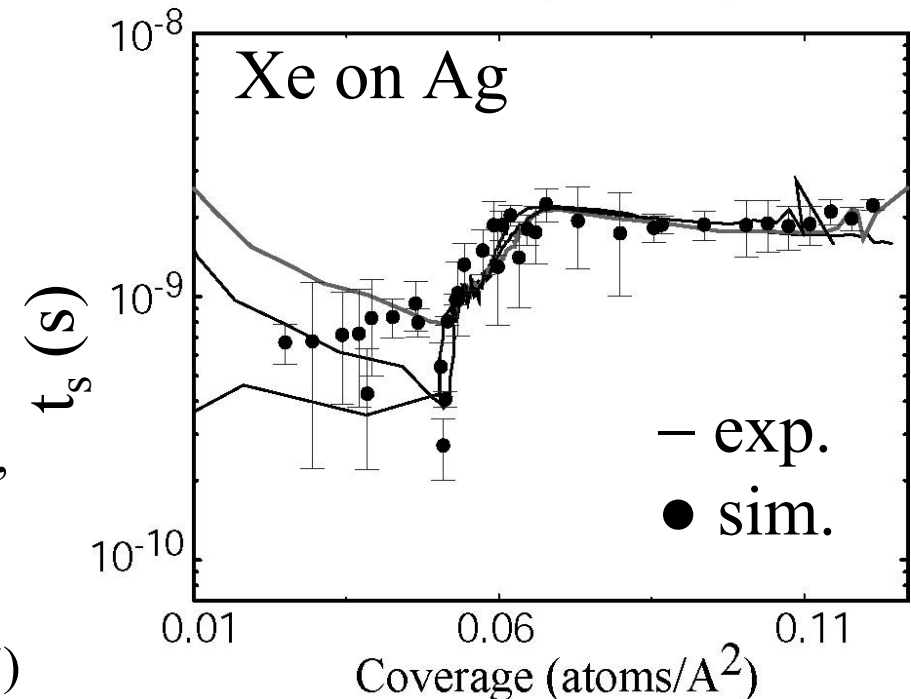
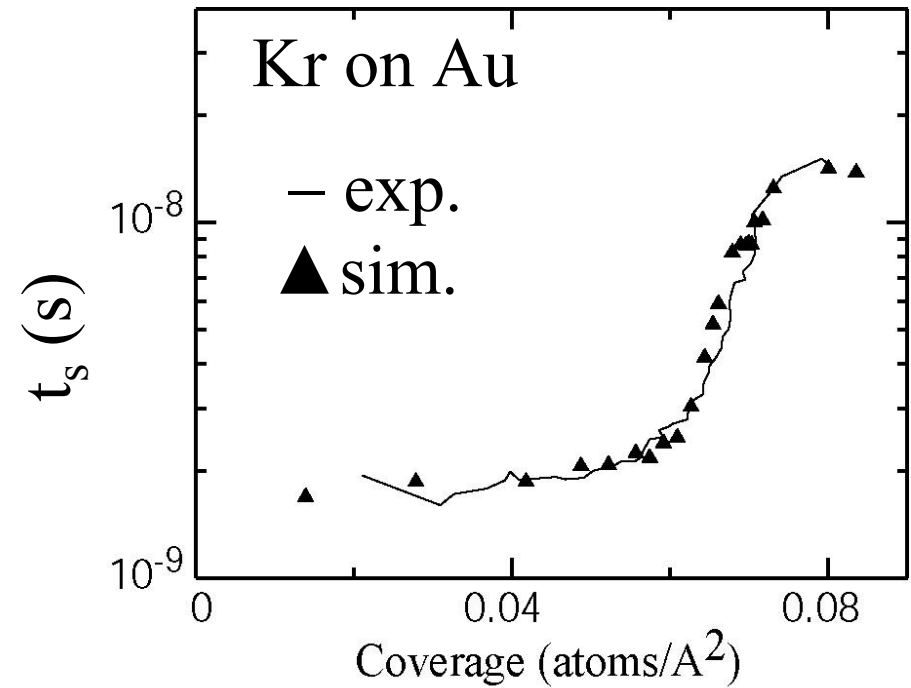
Increase coverage → film solidifies  
 $t_s$  increases → friction goes down!

Misaligned mica, MoS<sub>2</sub>, graphite also show ~no static friction

(Hirano et al. PRL 67, 2642 (1991); Martin et al., Dienwiebel et al. PRL 2004)

Kr on Au: Cieplak, Smith, Robbins, Science **265**, 1209 (1994)

Xe on Ag: Tomassone, Sokoloff, Widom, Krim, PRL **79**, 4798 (1997)



# Friction Only for Commensurate (100) Tips (Sørensen, Jacobsen & Stoltz, Phys. Rev. B 1996)

Copper tip aligned with substrate

⇒ geometrical interlocking and friction

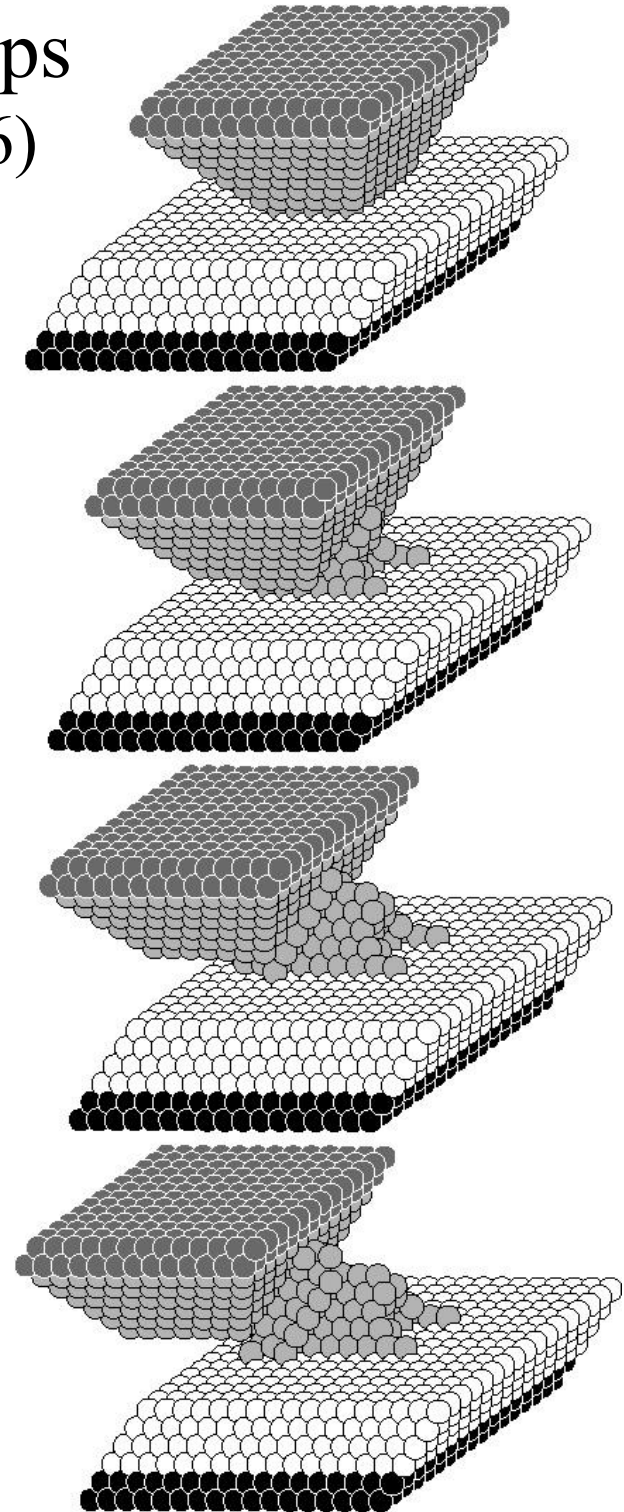
⇒ wear for (100) surfaces not for (111)

Rotate copper tip so incommensurate

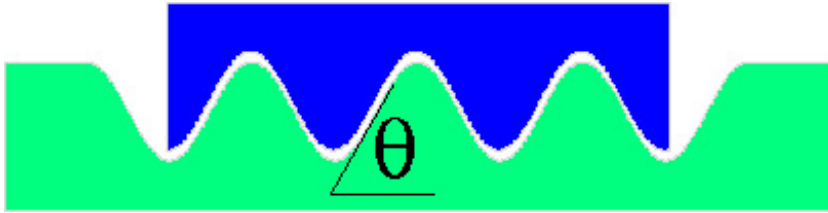
⇒ no interlocking, friction, or wear

*unless* tip is very small (5x5 atoms)

Copper (100) tip on Copper (100)  
surface slid in (011) direction.

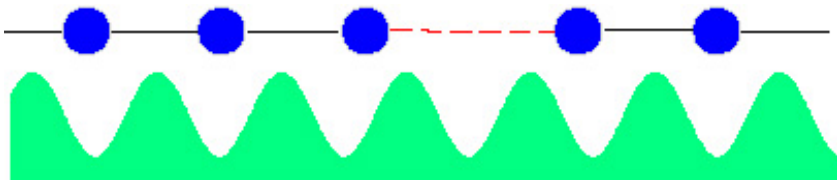


# *Friction Mechanisms in Contacts*



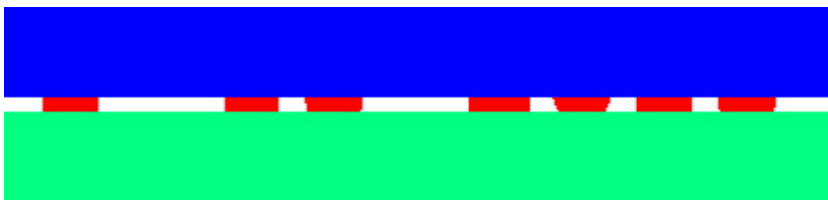
Geometrical Interlocking:  $F=N \tan \theta$

Unlikely to mesh,  $F$  goes up as smooth  
Kinetic friction vanishes



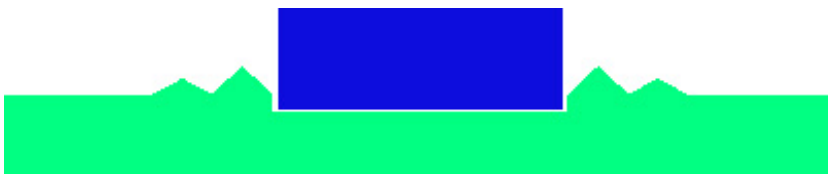
Elastic Metastability:

Intersurface interaction too weak



Mixing or Cold-Welding

Hard to observe in sims. even with  
clean, unpassivated surfaces in vacuum



Plastic Deformation (plowing)

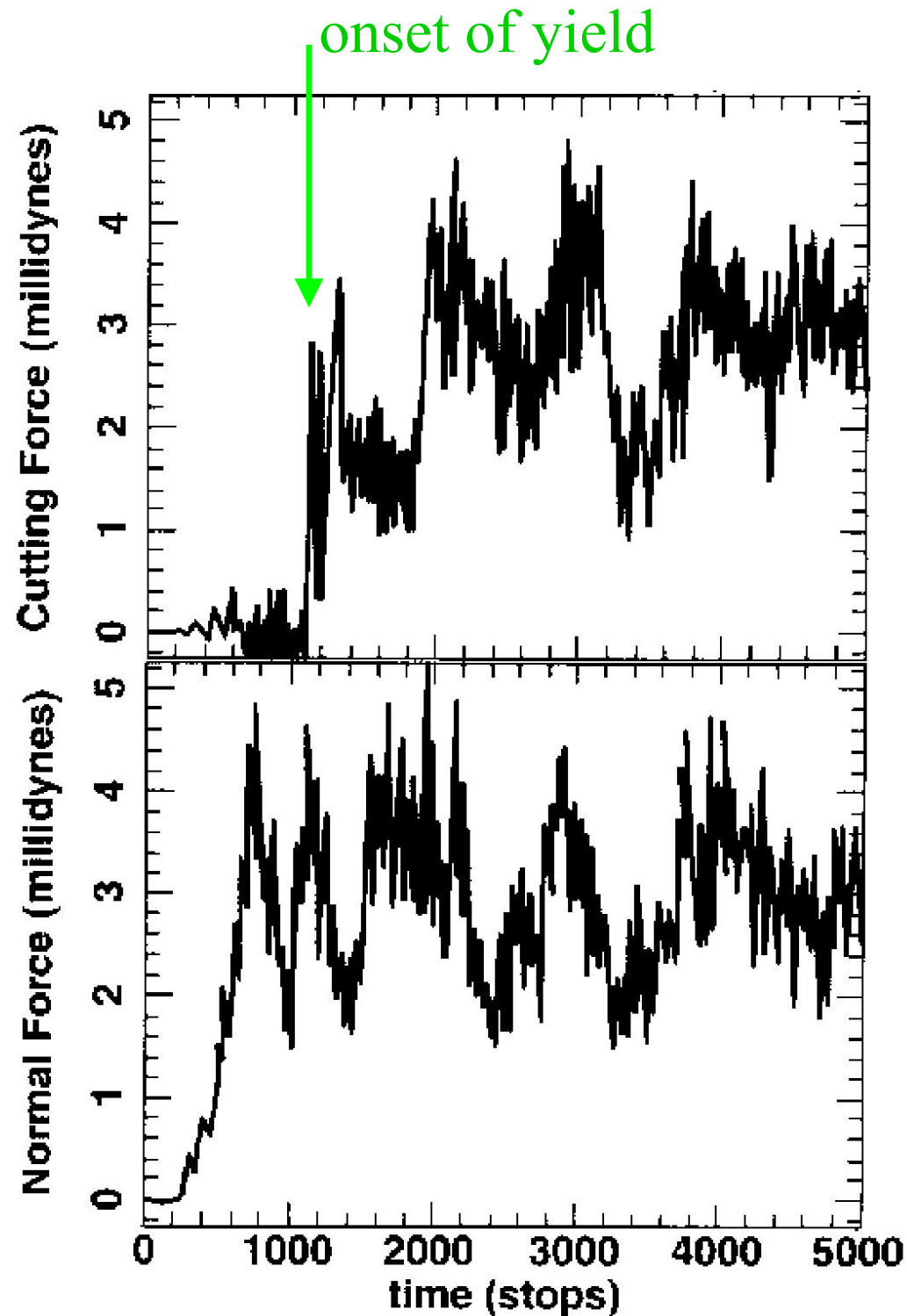
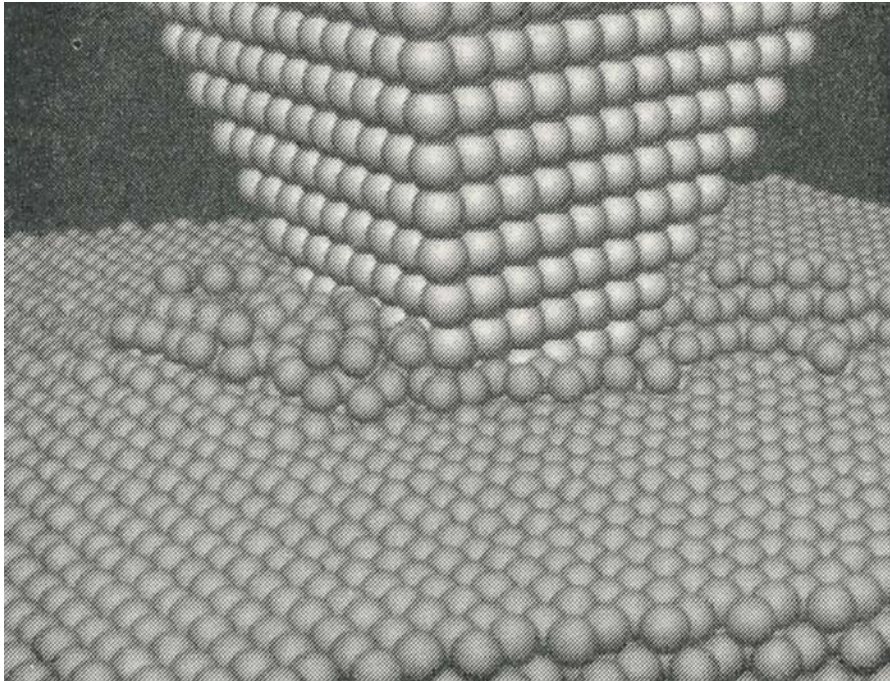
Load and roughness dependent  
 $\Rightarrow$ High loads, sharp tips



Mobile third bodies – hydrocarbons,  
wear debris, gouge, ...

# Rigid Tip on Clean Cu Surface (Belak and Stowers, Fundamentals of Friction, 1992)

No sliding friction (cutting force)  
until plastic deformation occurs



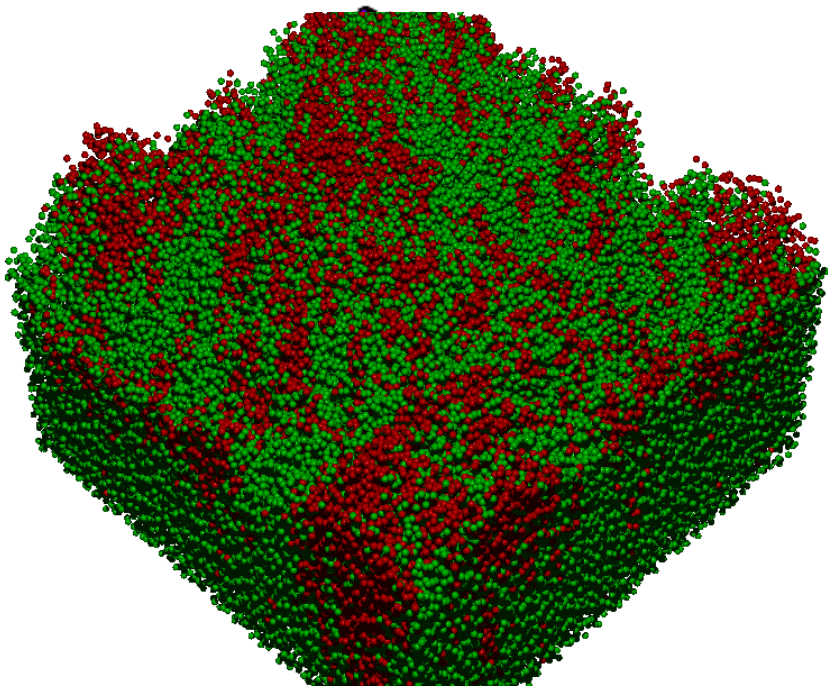


# Friction Between Self-Affine Surfaces

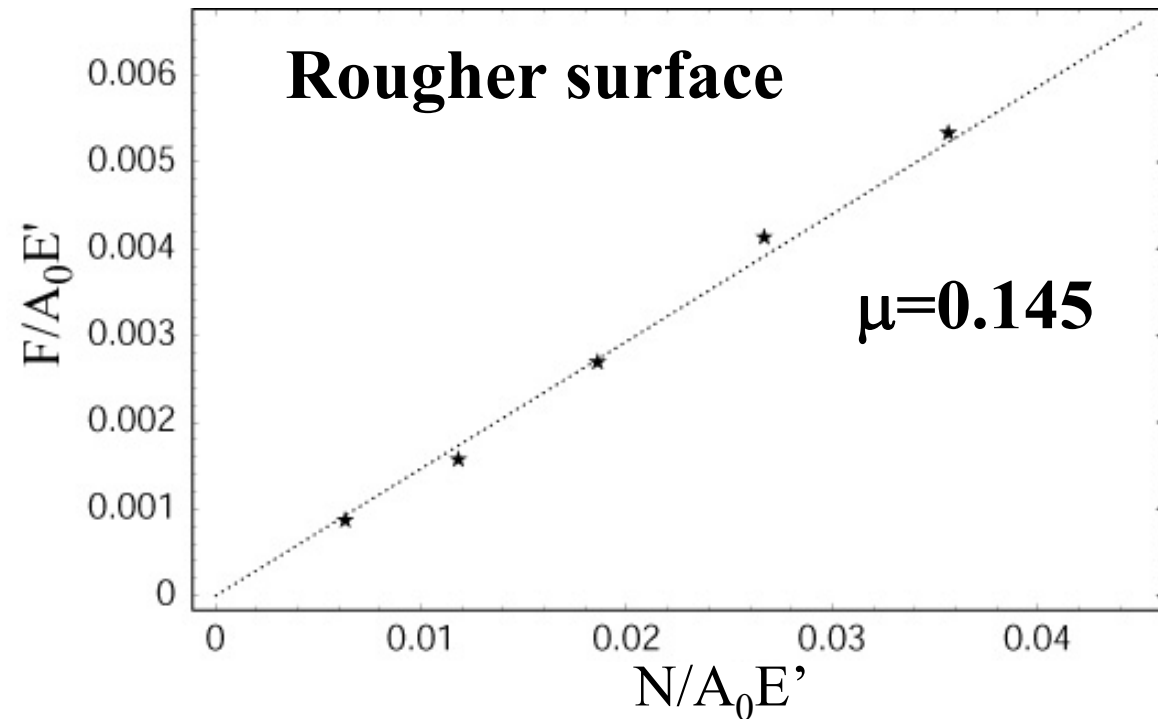
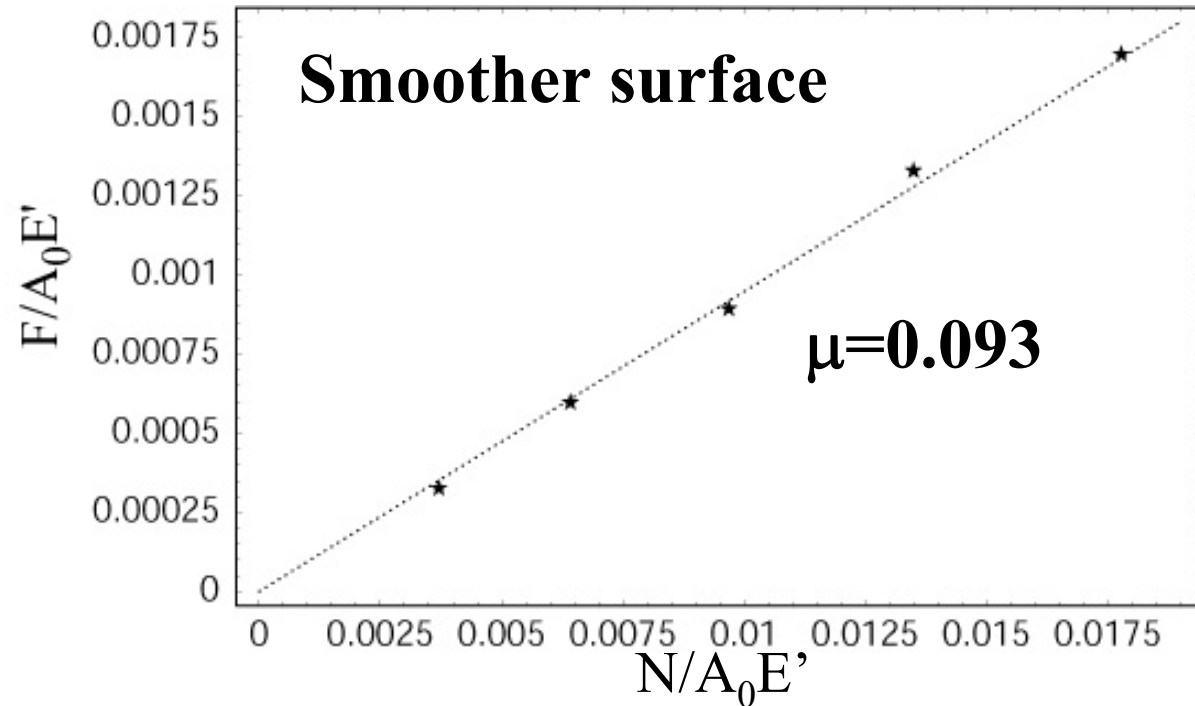
$$F = \mu N \quad (N = \text{Load})$$

$\propto$  rate of plasticity

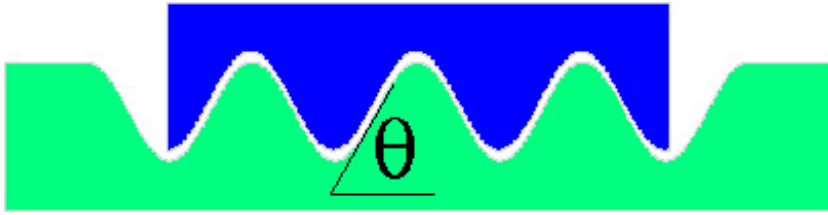
$\mu \propto$  rms roughness



**Red atoms: neighbor  
bond changed > 20%**

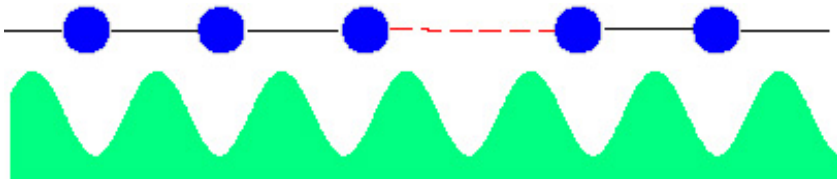


# Friction Mechanisms in Contacts



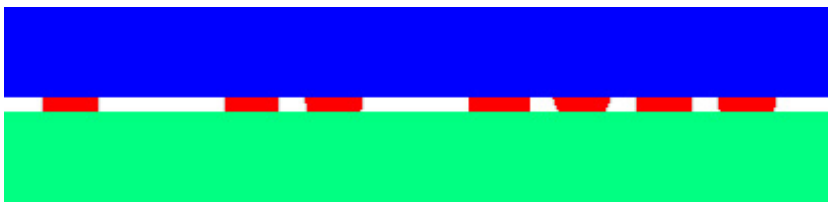
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Elastic Metastability:

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Plastic Deformation (plowing)

Load and roughness dependent  
 $\Rightarrow$ High loads, sharp tips



Mobile third bodies  $\rightarrow$  “glassy state”  
hydrocarbons, wear debris, gouge, ...

Glass seen in Surface Force Apparatus,  
Robust friction, Mech. on many scales

# Why is friction often proportional to load?

- Not just  $A_{\text{real}} \propto \text{Load}$  and  $F \propto A_{\text{real}}$  since  $A_{\text{real}}$  varies with parameters like  $\Delta$  that have weaker effect on  $\mu$
  - Friction between clean surfaces very sensitive to local structure, surface orientation, ... but measured  $\mu$  is not
- Assume friction from yield stress  $\tau_s$  of molecular contacts

Glassy systems:  $\tau_s$  rises linearly with pressure  $p$

If:  $F_s = A_{\text{real}} \tau_s(p)$  with  $\tau_s = \tau_0 + \alpha p$  (Briscoe)

Then:  $F_s = A_{\text{real}} \tau_0 + \alpha \text{Load}$

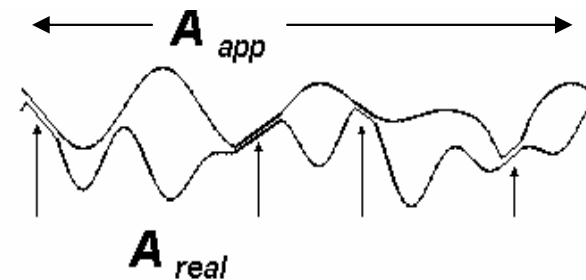
$$\mu_s = F_s / \text{Load} = \alpha + \tau_0 / \langle p \rangle$$

→ Constant  $\mu$  if  $\langle p \rangle = \text{Load} / A_{\text{real}} = \text{const.}$

or  $\tau_0 \ll \langle p \rangle$  (Independent of distribution of pressure)

→ Friction at zero or negative load with adhesion, as observed

⇒ Adsorbed layers give  $\tau_s = \tau_0 + \alpha P$  with small  $\tau_0$  and  $\alpha$  nearly independent of factors not controlled in experiment



# Model

- **N chains of n monomers → bead-spring model.**

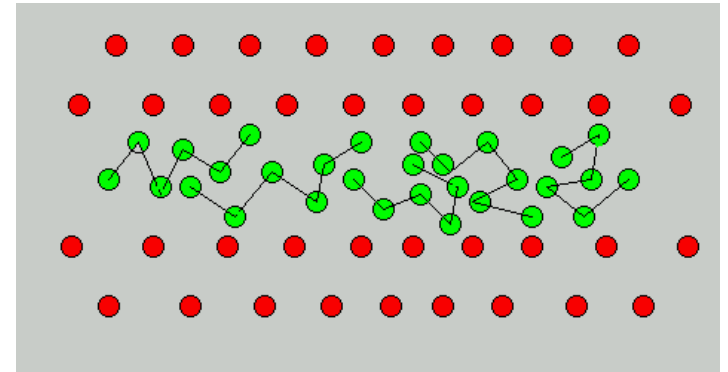
**Lennard-Jones interaction between monomers:**

$$V_{LJ} = 4\epsilon [(\sigma/r)^{12} - (\sigma/r)^6] \quad \text{for } r < r_c$$

**Neighbors on chain:**

$$V_{ch} = -\frac{1}{2} K_0 R^2 \ln[1 - r^2/R_0^2].$$

- **Wall atoms held to sites by springs  
(111) surface of fcc crystal here**



**Interact with monomers with  $V_{LJ}$ , but with  $\epsilon_w$  and  $\sigma_w$ .**

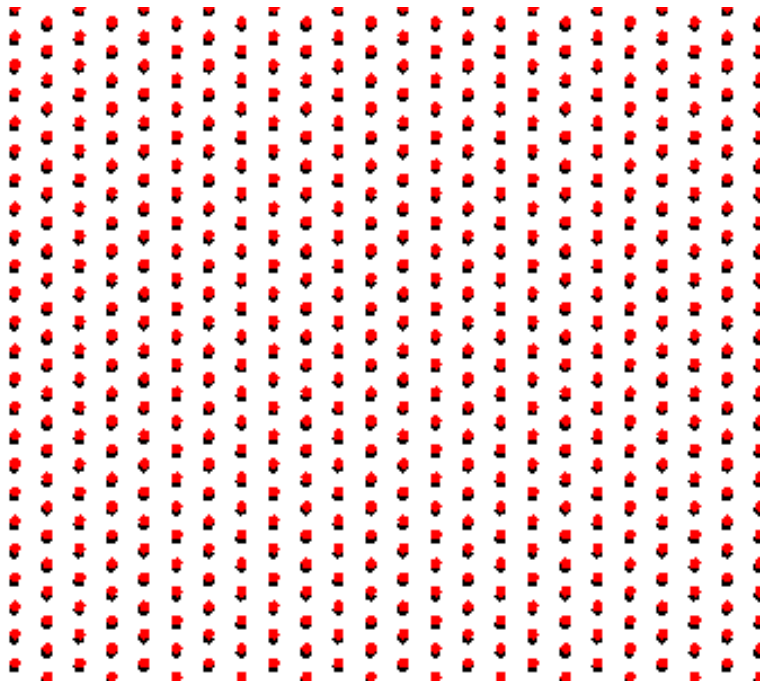
- **Increase force on top wall till slides to find  $\tau_s$  (static).  
Study diffusion of top wall to test if  $\tau_s > 0$   
Move wall at constant velocity  $v$  to find  $\tau_k$  (kinetic).**

- **Vary → Pressure P**

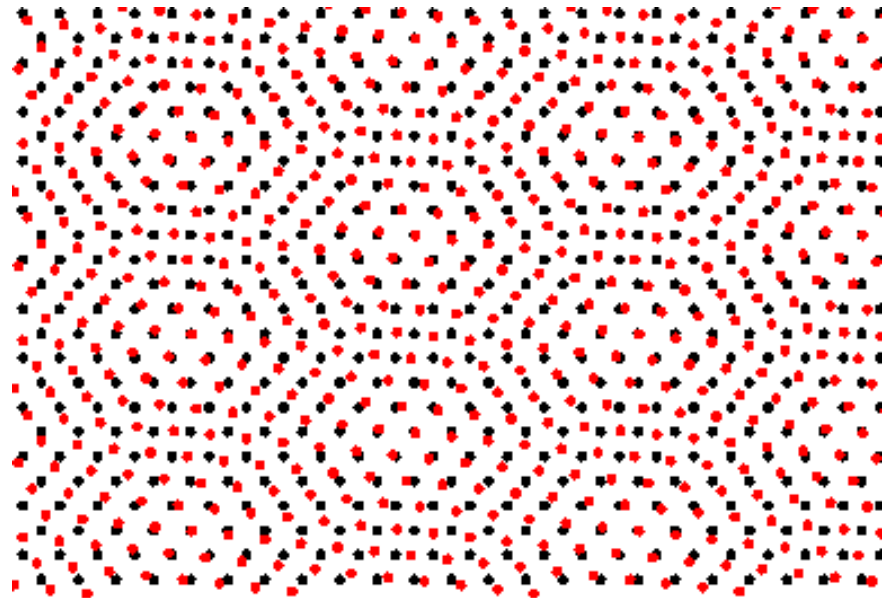
- **Relative orientation and lattice constants  $d$  of walls**
- **Direction and velocity of sliding**
- **Surface density (coverage) of monomers**
- **Chain length  $n$**
- **Strength  $\epsilon_w$ , length  $\sigma_w$ , and range  $r_c$  of potential.**

# Wall Geometries

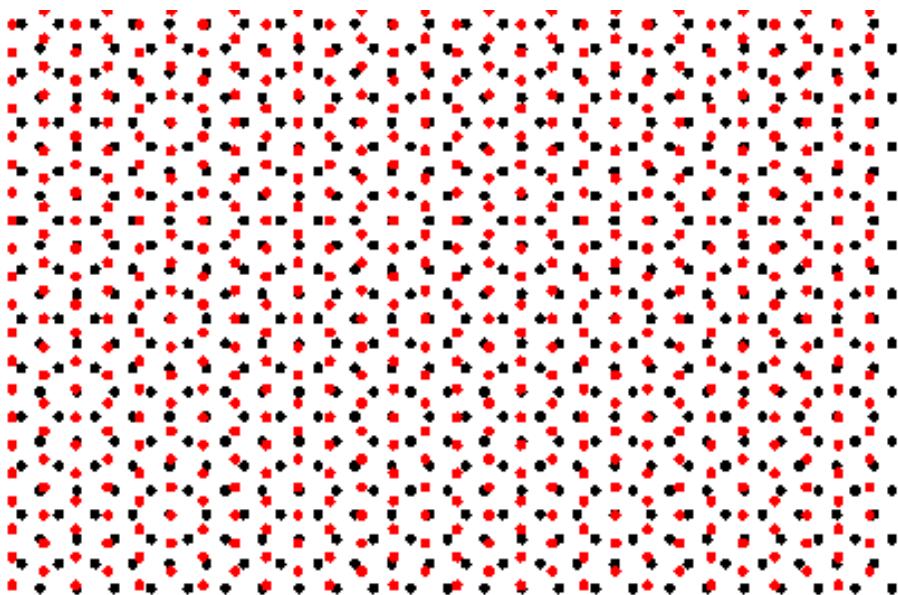
a)  $0^\circ$



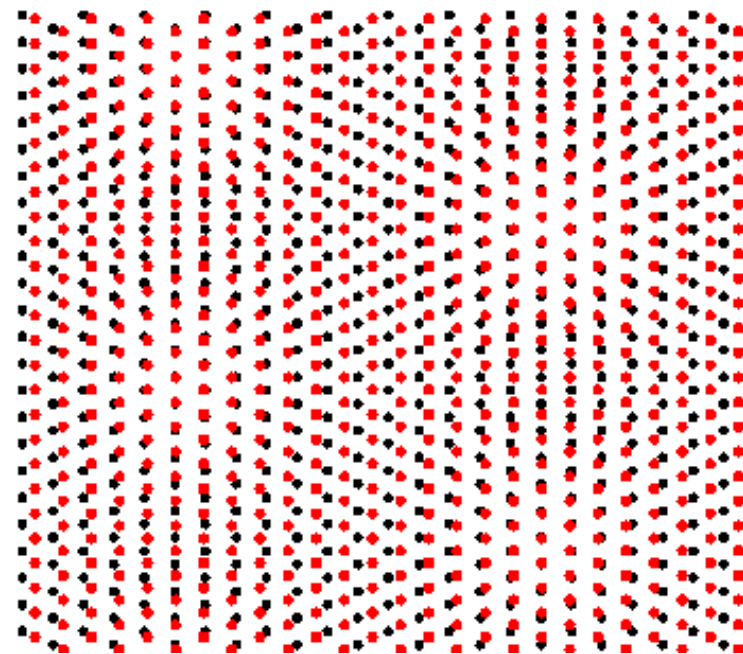
b)  $8.2^\circ$



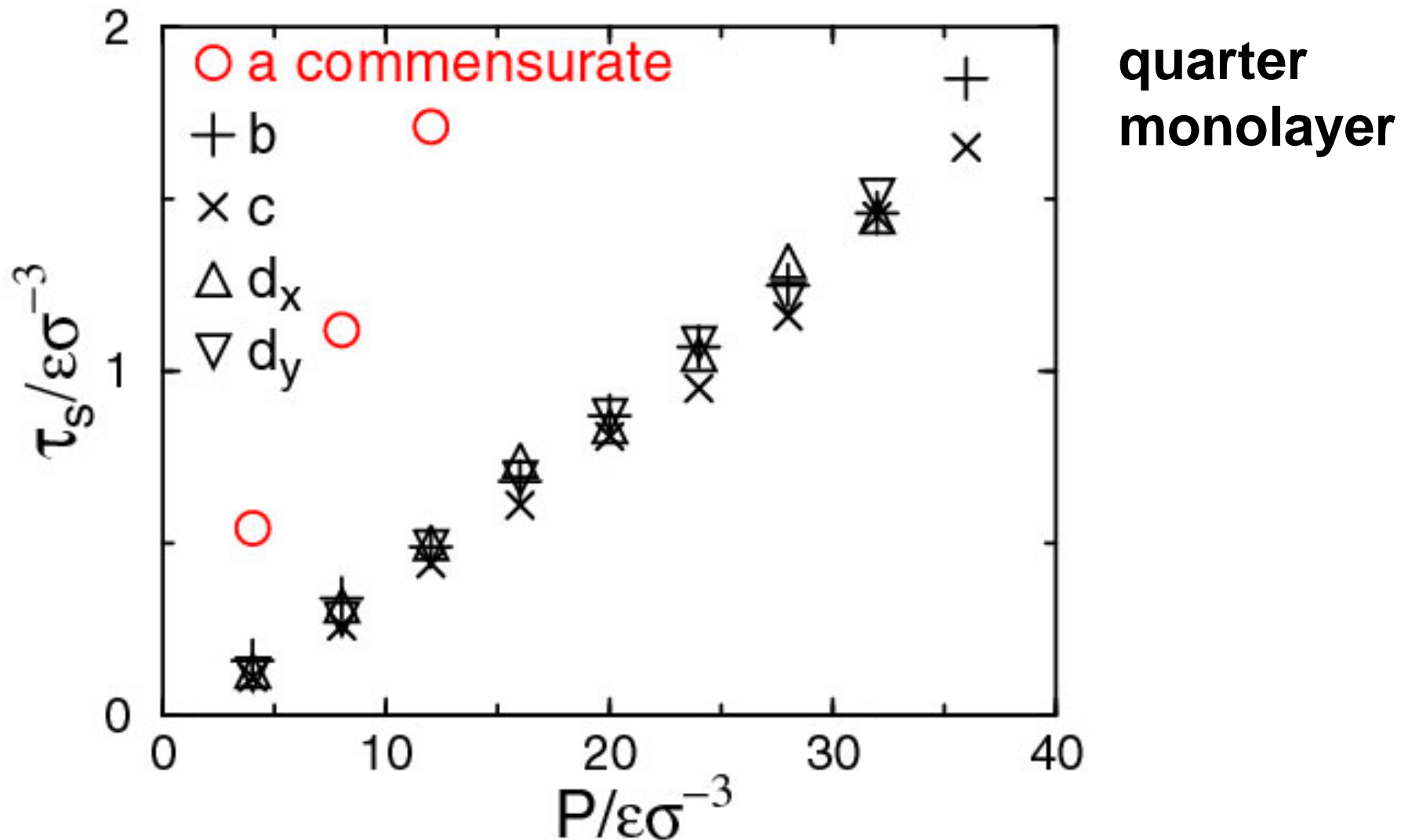
c)  $90^\circ$



d)  $d_{\text{top}}/d_{\text{bot}}=13/12$



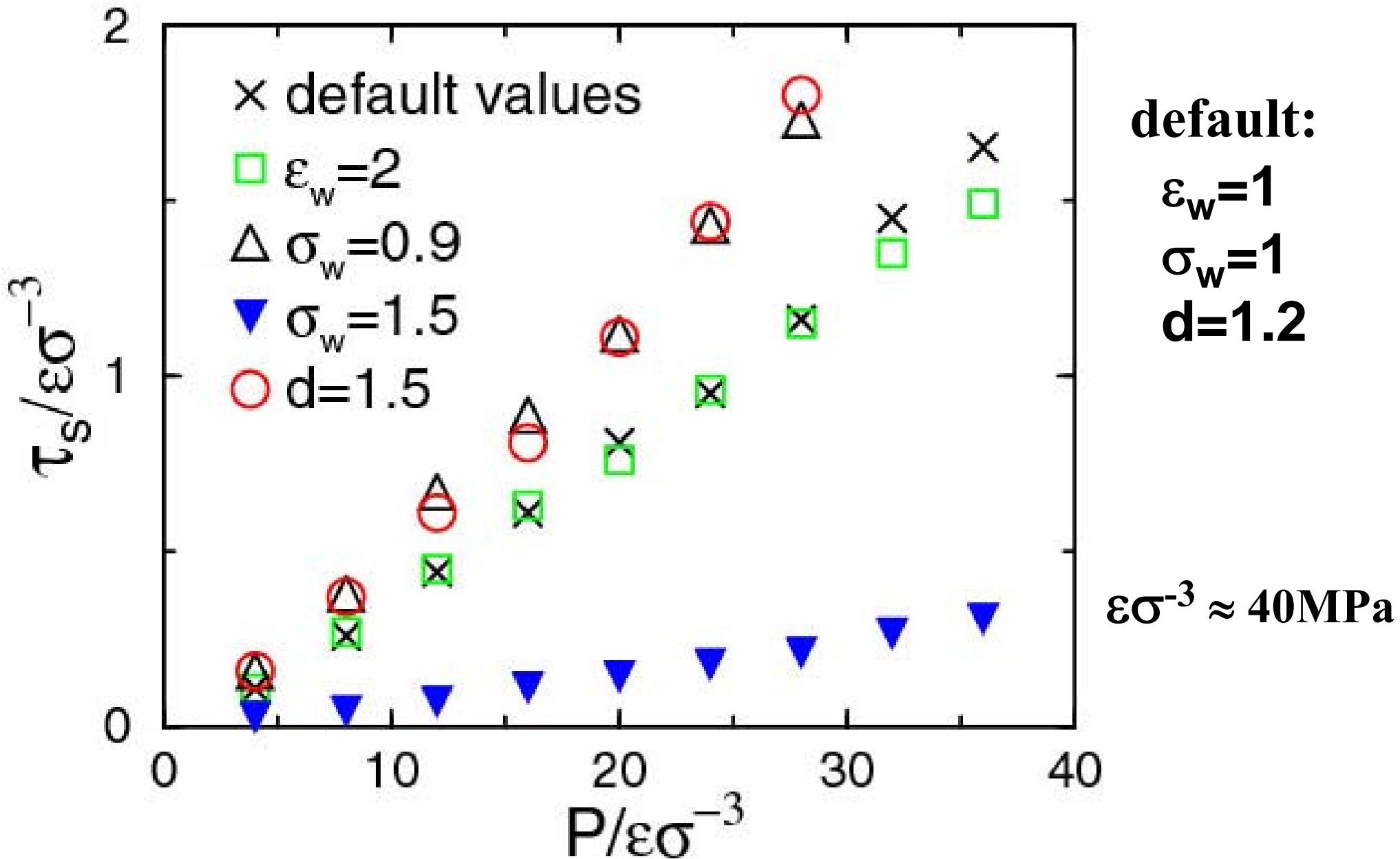
**Find:**  $\tau_s > 0$  for incommensurate walls **with** adsorbed film  
 All incommensurate walls (b-d) give same  $\tau_s$   
 $\tau_s$  independent of sliding direction: x, y, etc.  
 $\tau_s = \tau_0 + \alpha P$  up to  $P > 1\text{GPa}$  ( $\epsilon\sigma^{-3} \sim 40\text{MPa}$ )



# *Effect of Potential*

$\alpha$  independent of coverage, chain length ( $n \leq 6$ ),  $\epsilon_w$  or  $r_c$

$\alpha$  increases with  $d/\sigma_w \rightarrow$  “rougher” surface



# *Geometric Explanation*

If pressure high enough  $\rightarrow$  hard sphere limit

Repulsive force balances pressure

$$F \sim P/c \sim 48 (\epsilon_w / \sigma_w) (\sigma_w / r)^{13} \text{ where } c = \text{coverage}$$

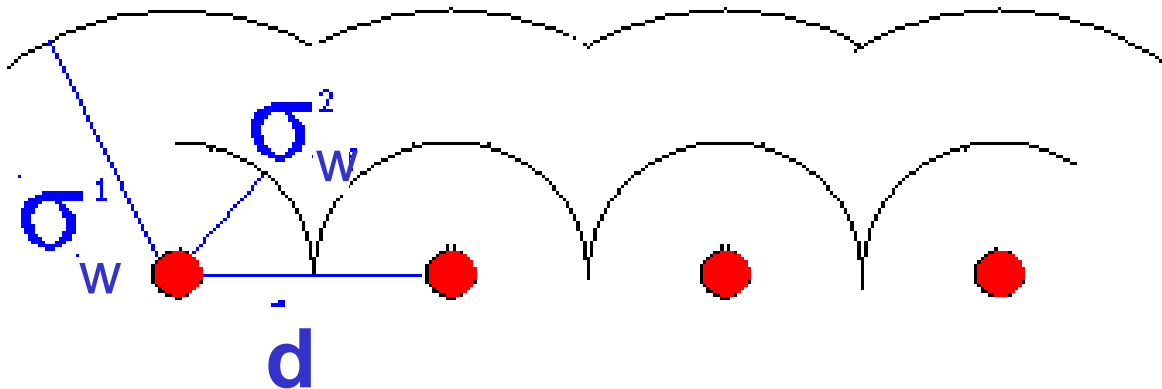
$$\Rightarrow r \sim \sigma_w (c \epsilon_w / P \sigma_w)^{1/13}$$

Effective hard-sphere radius: insensitive to  $c$ ,  $\epsilon_w$ ,  
 $P$  almost linear in  $\sigma_w$

Surface of closest approach depends on  $d / \sigma_w$

$\alpha \propto$  maximum slope, increases with  $d / \sigma_w$

Similar ideas explain rise in bulk yield stress with  $p$



Analytic theory: Muser, Wenning, Robbins PRL 86, 1295, '01

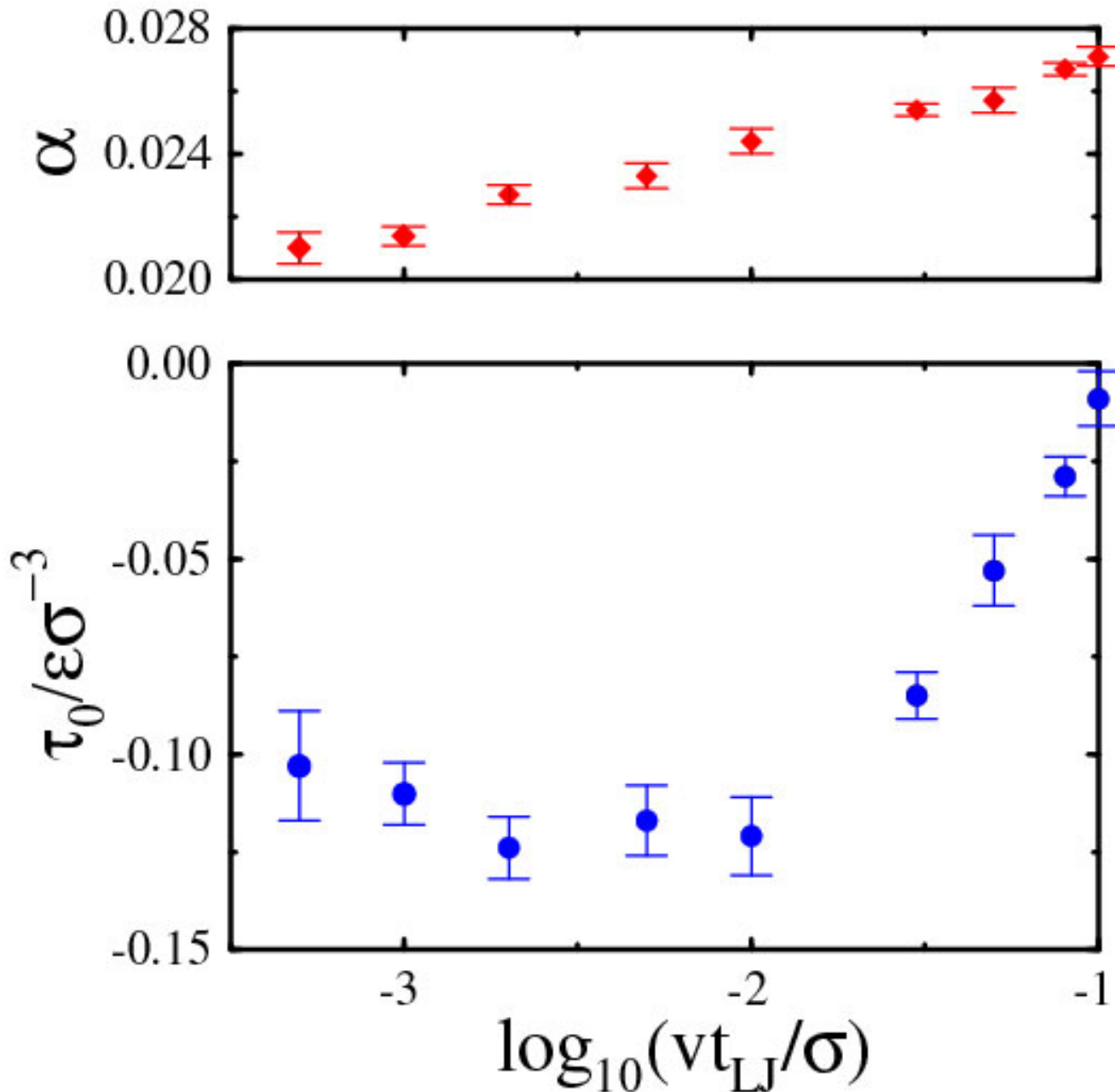


# *Airborne hydrocarbon films can explain Amontons' laws*

- ➔ Adsorbed layers (even diffusing) lock surfaces together producing a static friction consistent with macro experiments
- ✓  $\Rightarrow \tau_s = \tau_0 + \alpha P$  for  $P$  up to  $\sim 1 \text{ GPa}$
- ✓  $\Rightarrow \alpha$  of order 0.1 **crystal:  $\alpha \rightarrow 0.03$  to  $0.2$ , amorphous larger**
- ✓  $\Rightarrow \tau_0$  small compared to typical  $P$   $\tau_0 < 10 \text{ MPa}$
- ✓  $\Rightarrow \tau_s \approx$  independent of uncontrolled experimental parameters
  - ✓  $\rightarrow$  sliding direction
  - ✓  $\rightarrow$  wall orientation
  - ✓  $\rightarrow$  thickness of adsorbed film (coverage)
  - ✓  $\rightarrow$  chain length  **$n=1$  to  $6$  ( $\sim \text{C}_{20}\text{H}_{42}$  and smaller)**
- ➔  $\alpha$  primarily depends on relative size of wall atoms and adsorbed molecules in this simple model

G. He, M. H. Müser & M. O. Robbins, *Science* 284, 1650 (1999); *Phys. Rev. B* 64, 035413 (2001).

# Velocity Dependence of Kinetic Friction



**Still linear in P**

$$\tau_k = \tau_0 + \alpha P$$

$$\alpha = a + b \log(v)$$

**$\tau_0 = \text{const. for}$   
 $v \leq 10^{-2} \sigma/t_{LJ}$**

# *Connection to “Rate-State” Models*

For rocks, wood, metals,... (Dieterich, Ruina, Rice,...)

$$\mu = \mu_0 + A \ln(v/v_0) + B \ln(\Theta/\Theta_0) ; \quad d\Theta/dt = 1 - \Theta v/D_c$$

→ A represents change in shear stress with v

→ B change in area of contact with time

Our model has fixed area → only see A

Find:  $A \approx 0.001$  vs. 0.005 to 0.015 for rocks,

$A/\mu_0 \approx 0.05$  vs. 0.008 to 0.025 for rocks

$A \propto T$  as in experiments

$\mu \propto T \ln v$  follows from simple activation (Eyring) model

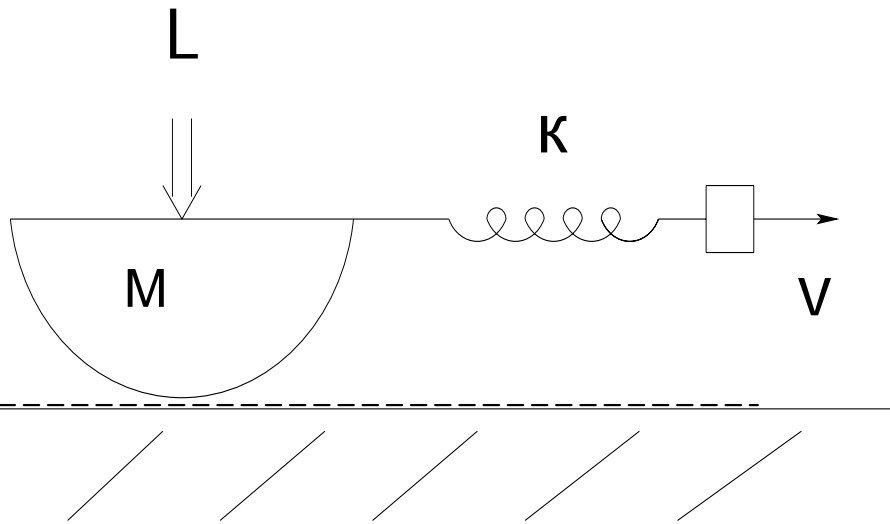
→ most molecules stable at any time

→ resist sliding just as for static friction

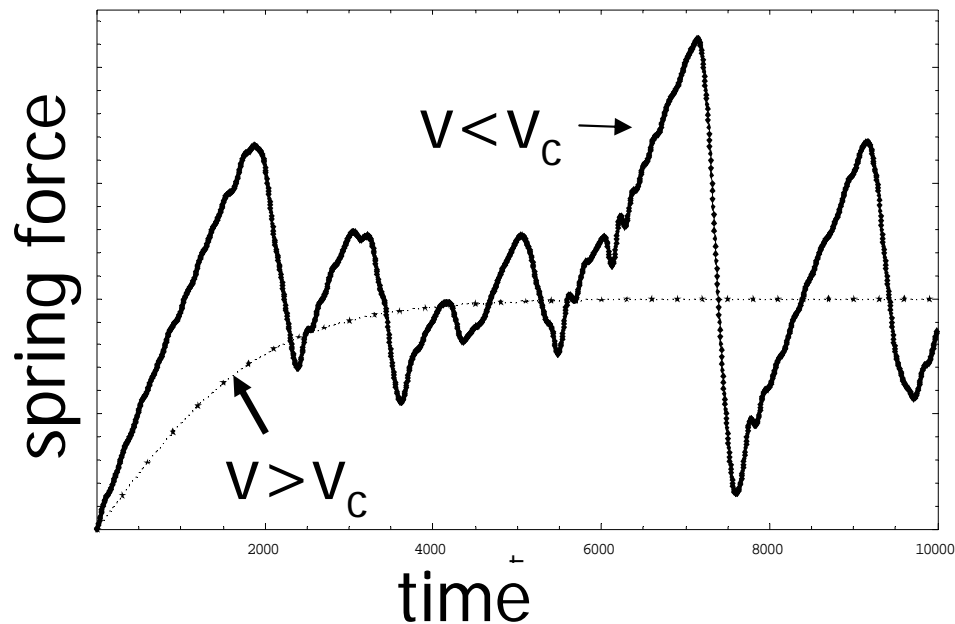
→ thermal activation over barrier reduces F

⇒ lower v, more thermal excitation →  $F \propto \log v$

# *Dilation/Phase change in layer $\Rightarrow$ stick-slip*



Stick-Slip common in daily life:  
squeaky hinges, sound of violins  
Controlled by spring constant  $\kappa$ ,  
velocity  $v$



Stick-Slip usually observed  
below velocity  $v_c$ .

What determines  $V_c$  ?

# Models for $V_c$

- Experiments & simulations on confined films suggest stick-slip due to dynamic phase transitions between static solid and molten sliding states

(Gee et al., J. Chem. Phys. 93:1895, 1990; Thompson & Robbins, Science 250:792,1990)

- Critical velocity then determined by either

1) Time to change phase (T&R 1990, Yoshizawa & Israelachvili, J. Chem. Phys. 97:11300, 1993, Persson & Volokitin, Surf. Sci. 457, 345, 2000)

2) Ability to absorb kinetic energy into potential energy

(Robbins & Thompson, Science 253:916,1991)

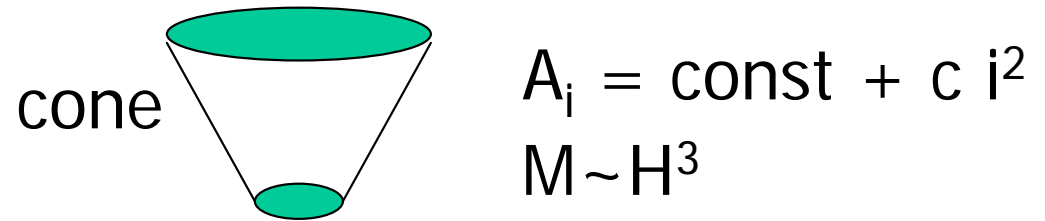
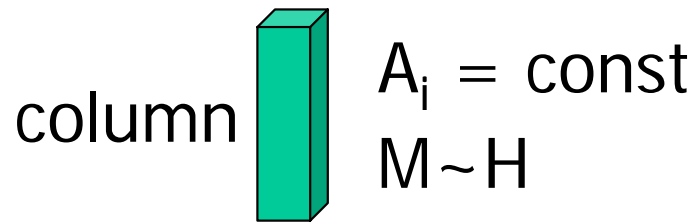
$$\frac{1}{2}Mv_c^2 \sim F_s \sigma \Rightarrow v_c \propto M^{-1/2} = \text{slider mass}$$

BUT above neglects elasticity of slider,

Persson and Braun argue that  $V_c$  stays large.

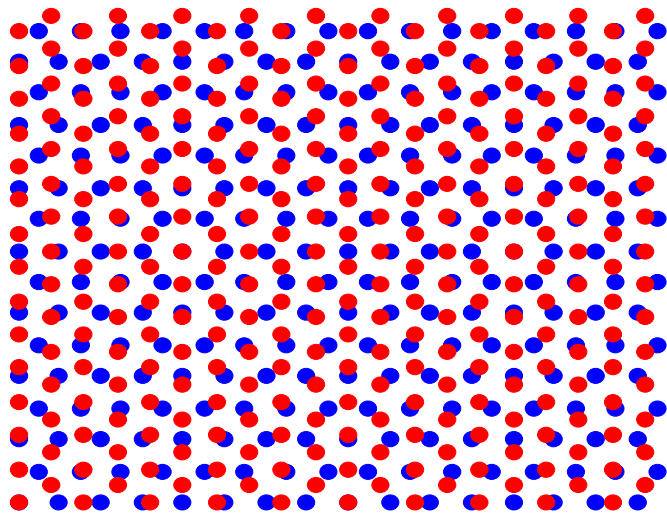
**Find role of elasticity depends on geometry of slider**

# Two Slider Geometries

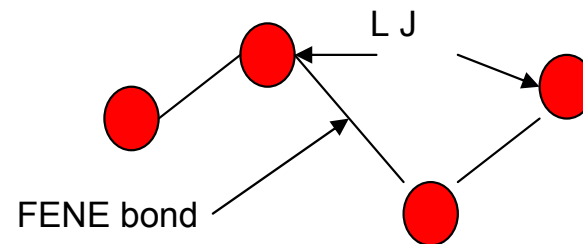


Divide slider into  $L$  layers,  $i^{\text{th}}$  coupled by springs to  $(i \pm 1)^{\text{th}}$   
 Mass  $M_i$  and coupling spring  $k_i$  proportional to layer area  $A_i$ .  
 Shear velocity  $V_s \sim (k_i/M_i)^{1/2} d \sim 10-20$ ,  $d = \text{lattice constant}$

At interface  $\rightarrow$  Thin film between two incommensurate walls



Temperature:  $T \sim 0.7$

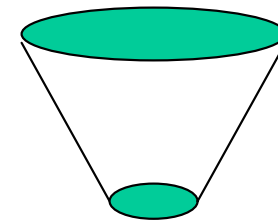


Film  $\rightarrow$  bead-spring chain molecules  
 Repulsive Lennard-Jones interaction  
 between wall and chain molecules.  
 All quantities in LJ units

# Results for $V_c$

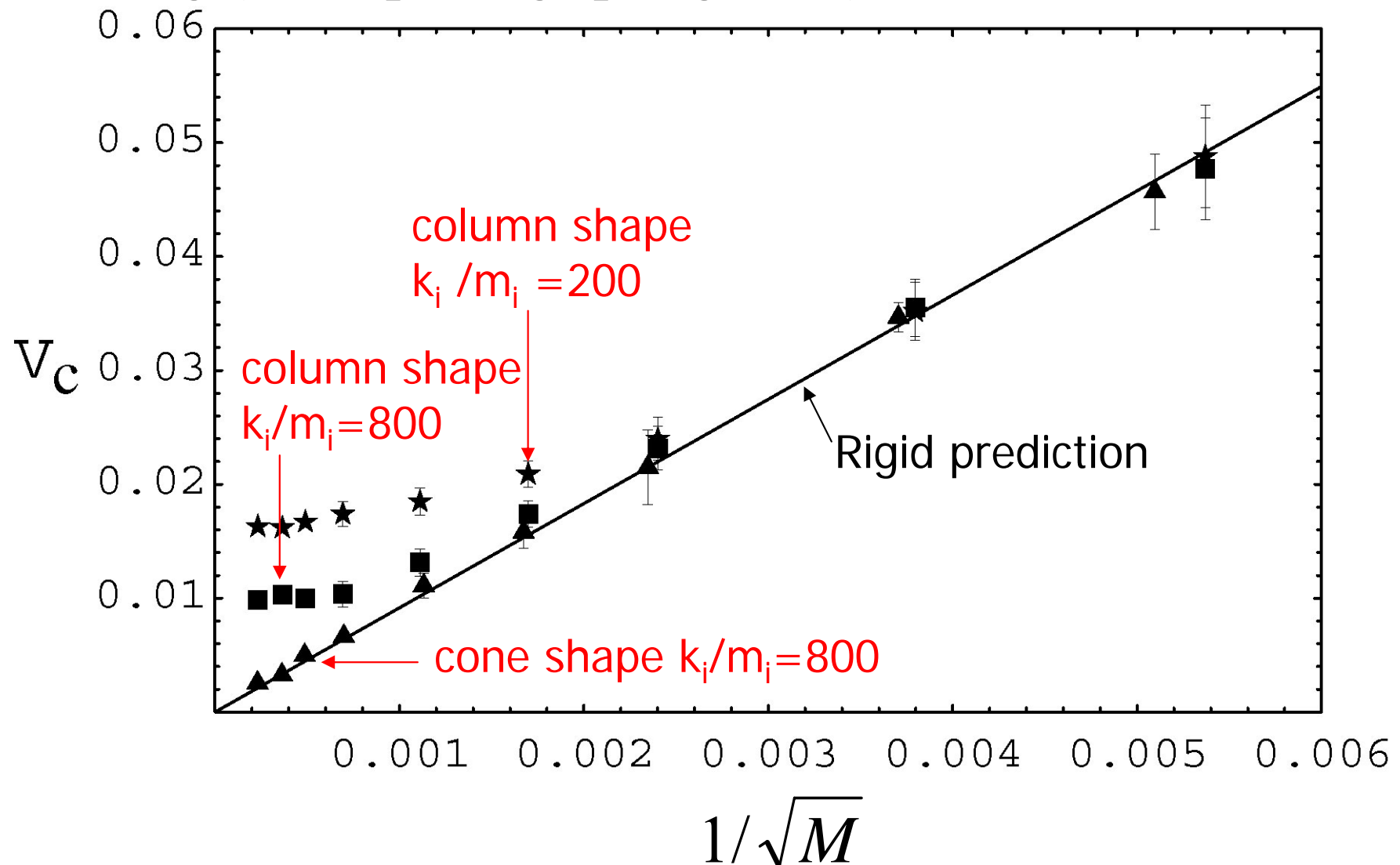


Column  
 $M \sim H$



Cone  
 $M \sim H^3$

Find  $V_c$  from minimum constant force where slider keeps sliding (weak pulling spring limit)



# Theoretical explanation

Two key time scales:

1. Time for slider to stop:  $t_d \sim d/V_c$
2. Time for elastic wave to propagate over the height  $H$  of slider:  $t_s = H/V_s$

Slider acts like rigid object when  $t_s \ll t_d \rightarrow V_c \sim M^{-1/2}$

Check scaling of times with  $H$  assuming  $V_c \sim M^{-1/2}$

Column shape:  $M \sim H \rightarrow t_d \sim H^{1/2} \rightarrow t_d \ll t_s$ , if  $H$  large

Cone shape:  $M \sim H^3 \rightarrow t_d \sim H^{3/2} \rightarrow t_d \gg t_s$ , if  $H$  large

$\Rightarrow$  As  $H \rightarrow \infty$ , cone is rigid but column is not

$\Rightarrow$  Surface force apparatus like cone, but earthquake more like column?



# *Adsorbed layers explain many experiments*

→ **Lock surfaces together** (even when diffusing)

⇒  $\tau_s = \tau_0 + \alpha P$  for  $P$  up to  $\sim 1$  GPa

⇒  $\tau_s \approx$  independent of uncontrolled experimental parameters

$\alpha$  primarily depends on relative atomic sizes in our model

→ **Kinetic friction also linear:**  $\tau_k = \tau_0 + \alpha P$

⇒  $\alpha, \tau_0$  follow same trends as for  $\tau_s$

→ At low  $v$ ,  $\alpha$  is 10 to 20% smaller than for static case

→  $\alpha$  shows  $k_B T \log v$  dependence seen in experiment

→ Most molecules stable at any time, resist sliding just as for static friction, each pops and dissipates separately

**Biggest contribution to friction from those close to popping**

⇒ **As  $v$  decreases, more thermal excitation,  $F \propto \log v$**

Pedagogical intro. to friction mechanisms and illustrating simulations

J. Ringlein and M. O. Robbins, Am. J. Phys. 72, 884-891 (2004)

# *Friction Mechanisms: Atomic to Macroscopic*

## Questions:

Where do surfaces contact?

How is friction produced in contacts?

How do static and kinetic friction differ and age?

How does concept of contact depend on scale?

Do similar mechanisms of frictional locking, stick-slip, fracture, ... operate at different scales?

Can studies of mechanisms at small scales provide essential input for modeling larger scales?

Can large scale experiments test small scale models?

Pedagogical intro. to friction mechanisms and illustrating simulations

J. Ringlein and M. O. Robbins, *Am. J. Phys.* 72, 884-891 (2004)