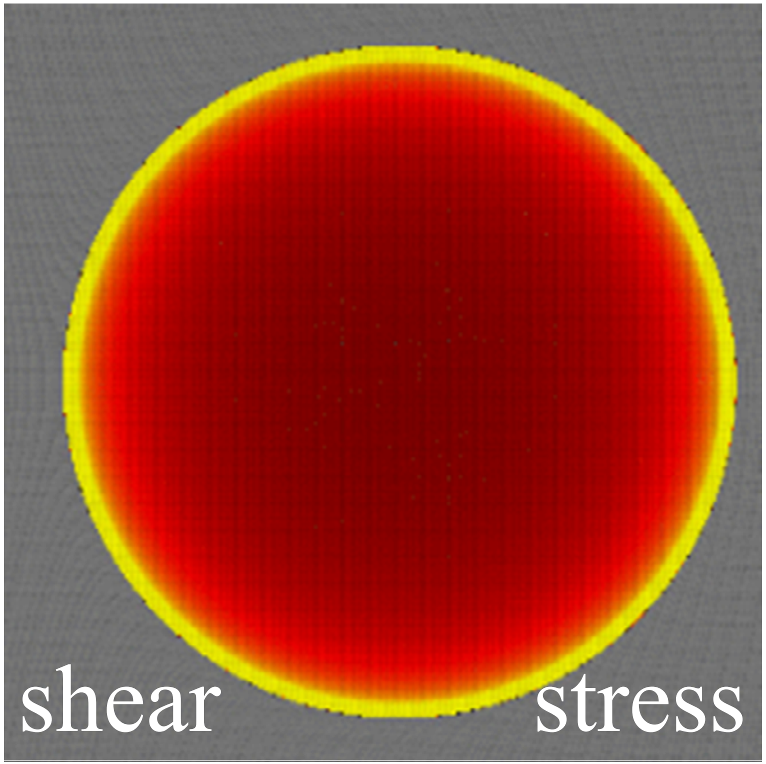
# *Contact of Rough Surfaces*

Mark O. Robbins, Johns Hopkins University

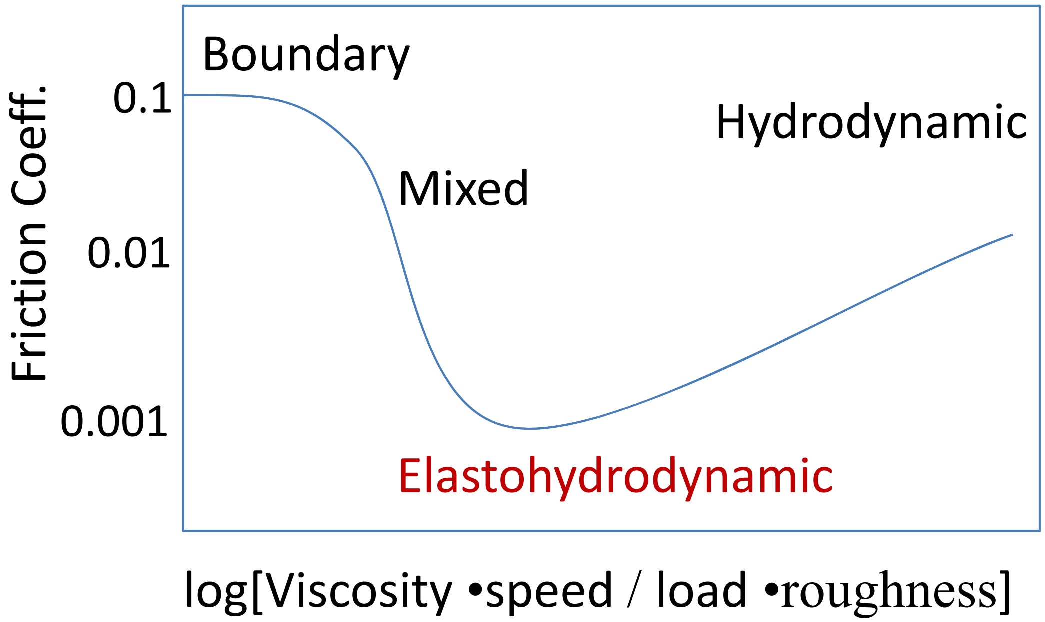
KITP, Univ. of California, Santa Barbara, Jan. 20, 2018

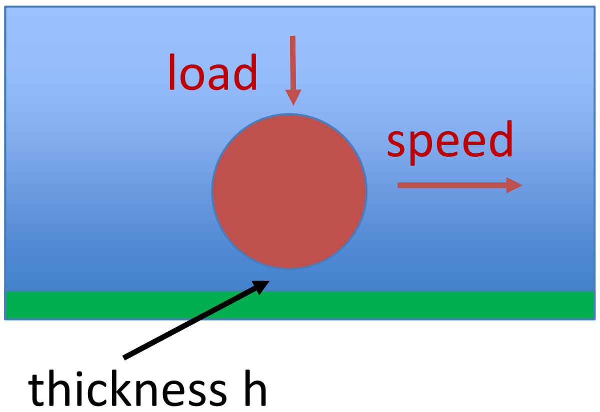
With: L. Pastewka, T. Sharp, J. Monti, S. Akarapu, S. Cheng,
G. He, S. Hyun, B. Luan, J. F. Molinari, M. H. Muser, L. Pei


**Supported by NSF, AFOSR, European Commission**

# *Lubrication Regimes ⇨ Stribeck Curve*



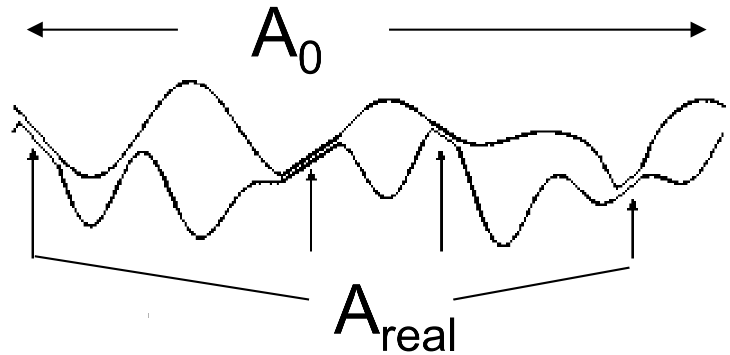




Related to h/roughness

Key regimes of lubrication as increase sliding speed, thickness h

- Boundary lubrication – bulk lubricant squeezed out
- Mixed lubrication – lubricant film h ~ roughness, partial contact
- Hydrodynamic lubrication – thick lubricant film h >> roughness
  Simple Newtonian fluid – constant viscosity
- Elastohydrodynamic lubrication – high pressure, thin film
  → elastic deformation of solid, change in viscosity of film, shear thinning

# *Is Friction Proportional to Load or 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 $\tau_{shear}$

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

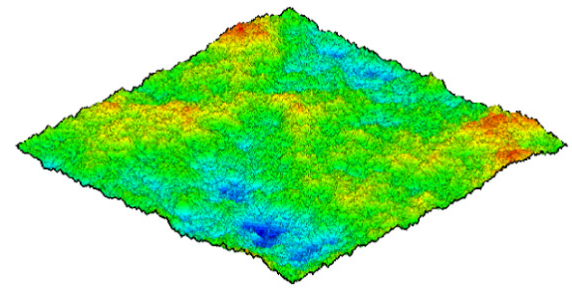
Bowden & Tabor – hard sphere on polymer

# *Surfaces Often Rough on Many Scales ⇒ Self-Affine*

Artificial landscape – computer generated self-affine fractal

http://thornyissues2.blogspot.com/2014/06/beauty-in-nature-fractals_21.html

# *Height Correlation Function*



Height change over r $\langle |h(x+r)-h(x)|^2 \rangle \sim r^{2H}$

Fourier transform of correlation function:

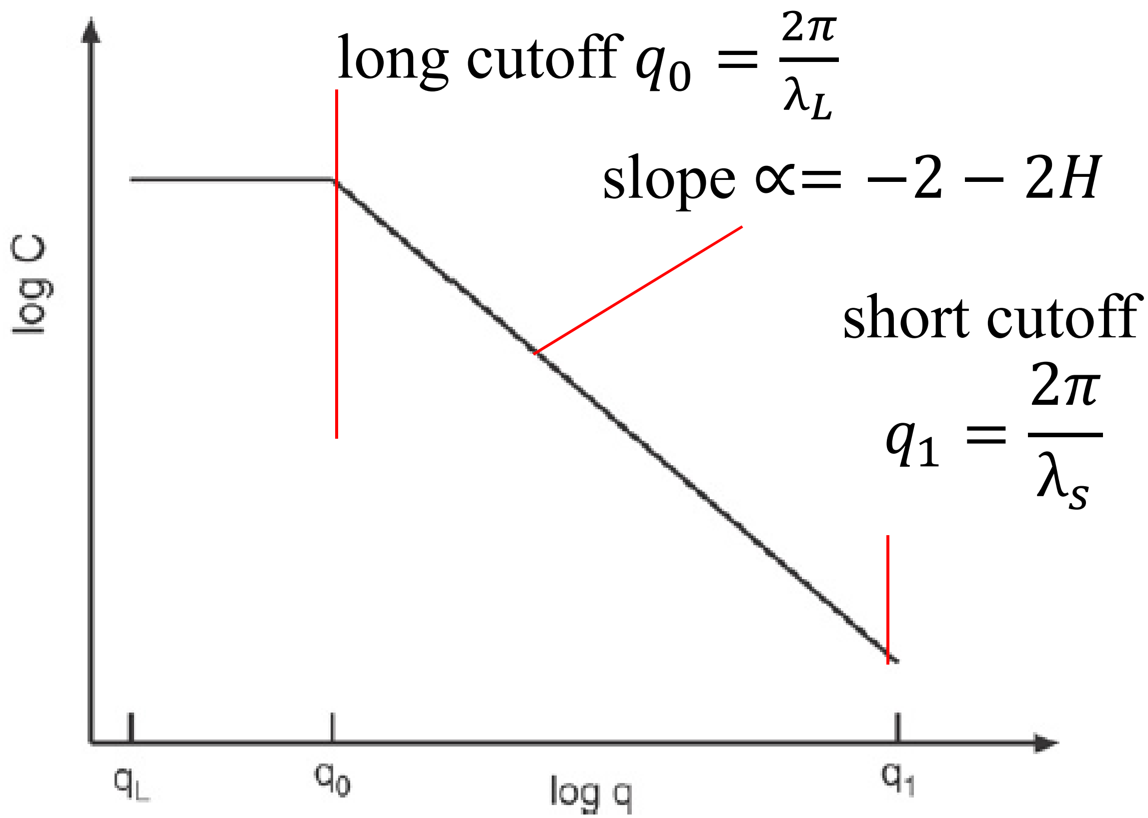
$C(q)=|h(q)|^2 \sim q^{-2(1+H)}$ for $2\pi/\lambda_L < q < 2\pi/\lambda_s$

Large scale cutoff → $h_{rms}$

$$h_{rms}^2 = 2\pi \int_{q_0}^{q_1} dq\, q\, C(q) \sim q_0^{-2H}$$

Small scale cutoff → $h'_{rms}$

$$h'^{\,2}_{rms} = \int_{q_0}^{q_1} \frac{dq}{2\pi} q^3 C(q) \sim q_1^{2-2H}$$



# *Surfaces Often Rough on Many Scales ⇒ Self-Affine*

Height variation $\delta h$ over length $\ell \rightarrow \delta h \propto \ell^{H}$ $\quad 0<H<1$

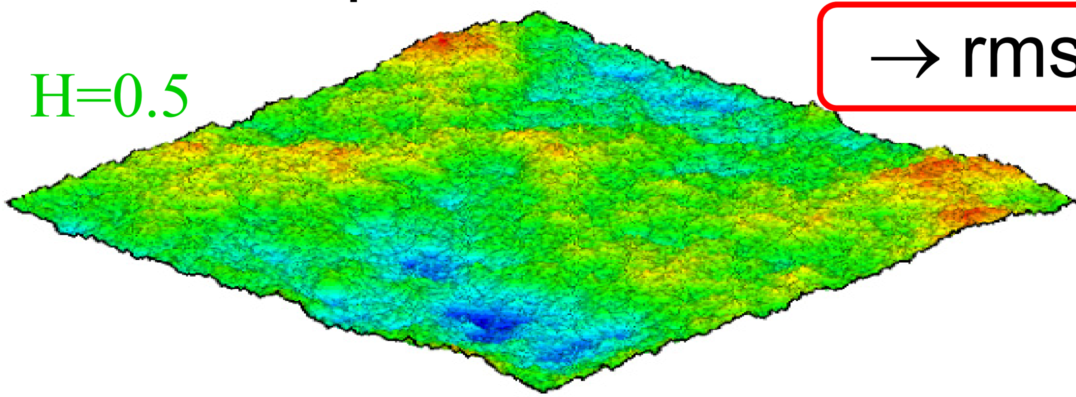
for wavelengths $\lambda_s < \ell < \lambda_L$ - range can matter

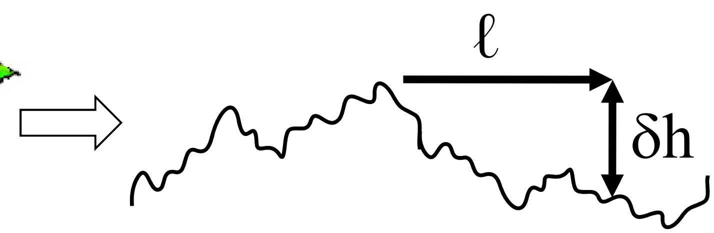
Total rms height variation: $h_{rms} \sim \lambda_L^{H}$

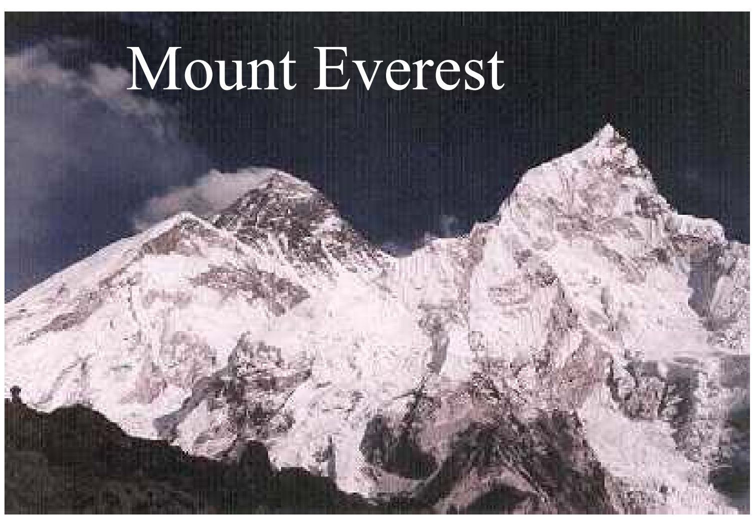
RMS slope $\delta h/\ell \propto \ell^{-(1-H)} \rightarrow 0$ as $\ell$ increases

$\rightarrow$ rms slope $h'_{rms} \sim \lambda_s^{-(1-H)}$

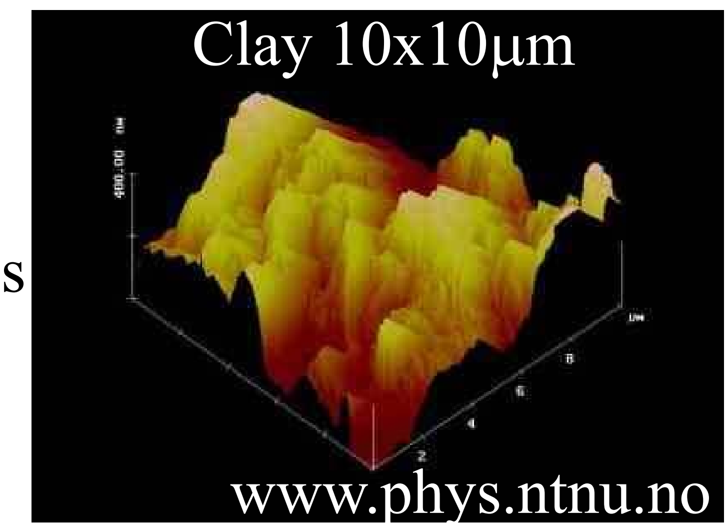
H=0.5






Examples with H=0.8



## *Surfaces Often Rough on Many Scales ⇒ Self-Affine*

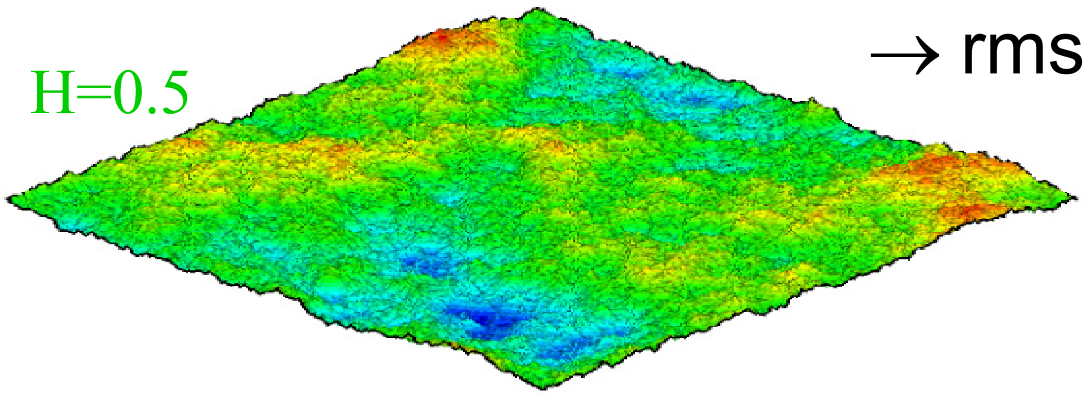
Height variation $\delta h$ over length $\ell \rightarrow \delta h \propto \ell^{H}$ $\quad 0<H<1$

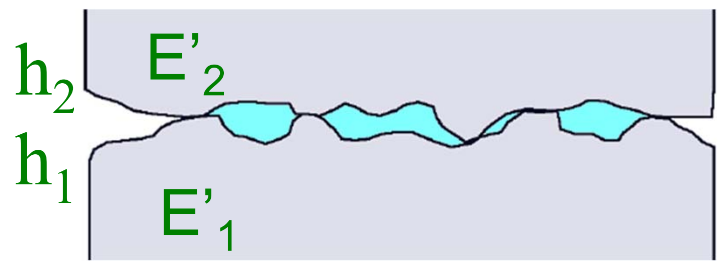
for wavelengths $\lambda_s < \ell < \lambda_L$ - range can matter

Total rms height variation: $h_{rms} \sim \lambda_L^{H}$

RMS slope $\delta h/\ell \propto \ell^{-(1-H)} \rightarrow$ 0 as $\ell$ increases

$\rightarrow$ rms slope $h'_{rms} \sim \lambda_s^{-(1-H)}$




Continuum theory (contact not friction):

2 rough elastic solids ⇒ rough rigid and elastic flat

heights $h_1$, $h_2$ ⇒ $h=h_2-h_1$

Moduli $E'_1$, $E'_2$ ⇒ $E'=1/(1/E'_1+1/E'_2)$

$E'=E/(1-\nu^2)$; E=Young's modulus, $\nu$=Poisson ratio

# *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

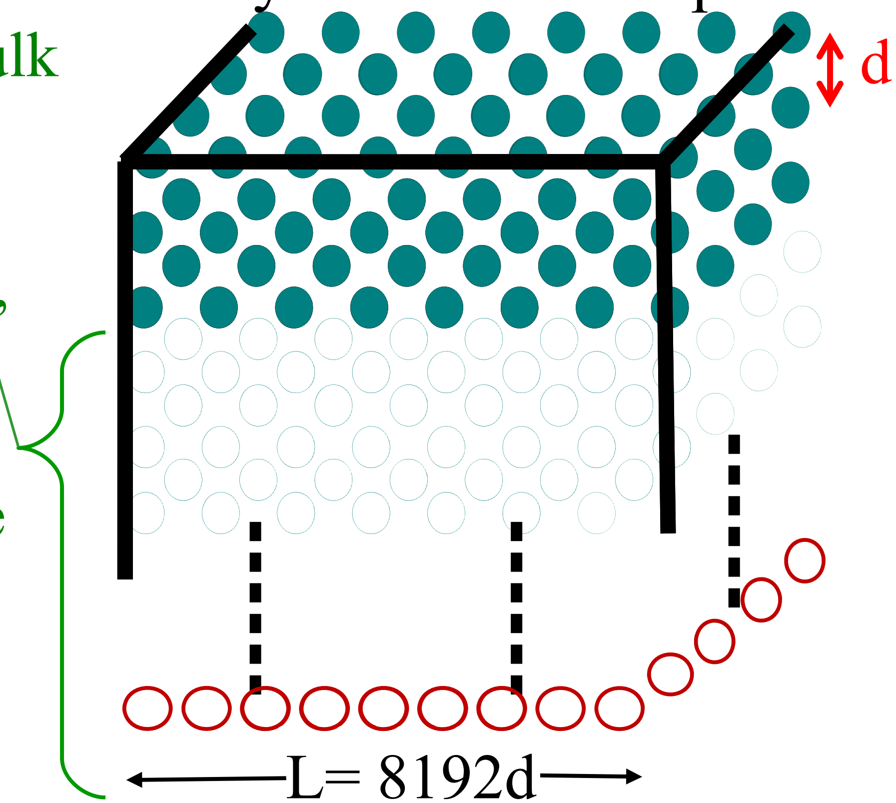
Similar to Campana & Muser

Extended to long range interactions,

analytic GF, multibody potentials

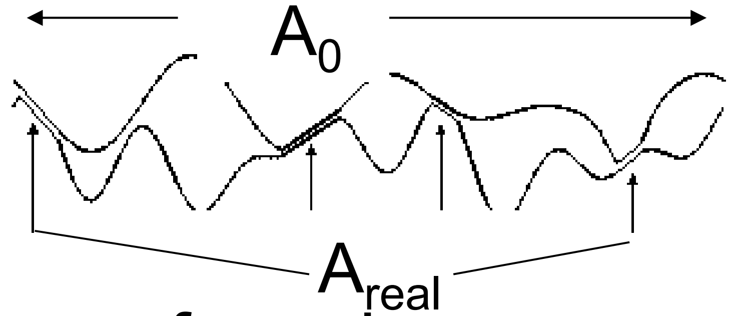
EAM, Stillinger-Weber, …

Periodic boundaries or semi-infinite




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

# *Area ∝ Load ⇒ Dimensional Analysis*




No adhesion ⇒ contact modulus
$E' = E/(1-\nu^2)$ only material prop.

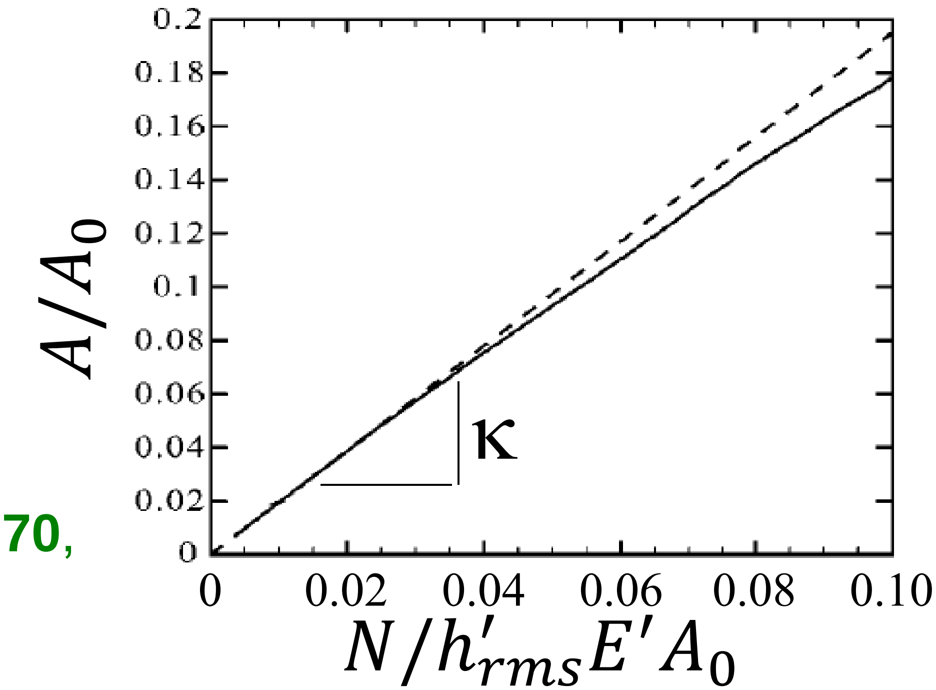
E' & Load/$A_{real}$ have same units

Slope $h'_{rms}$ – dimensionless measure of roughness

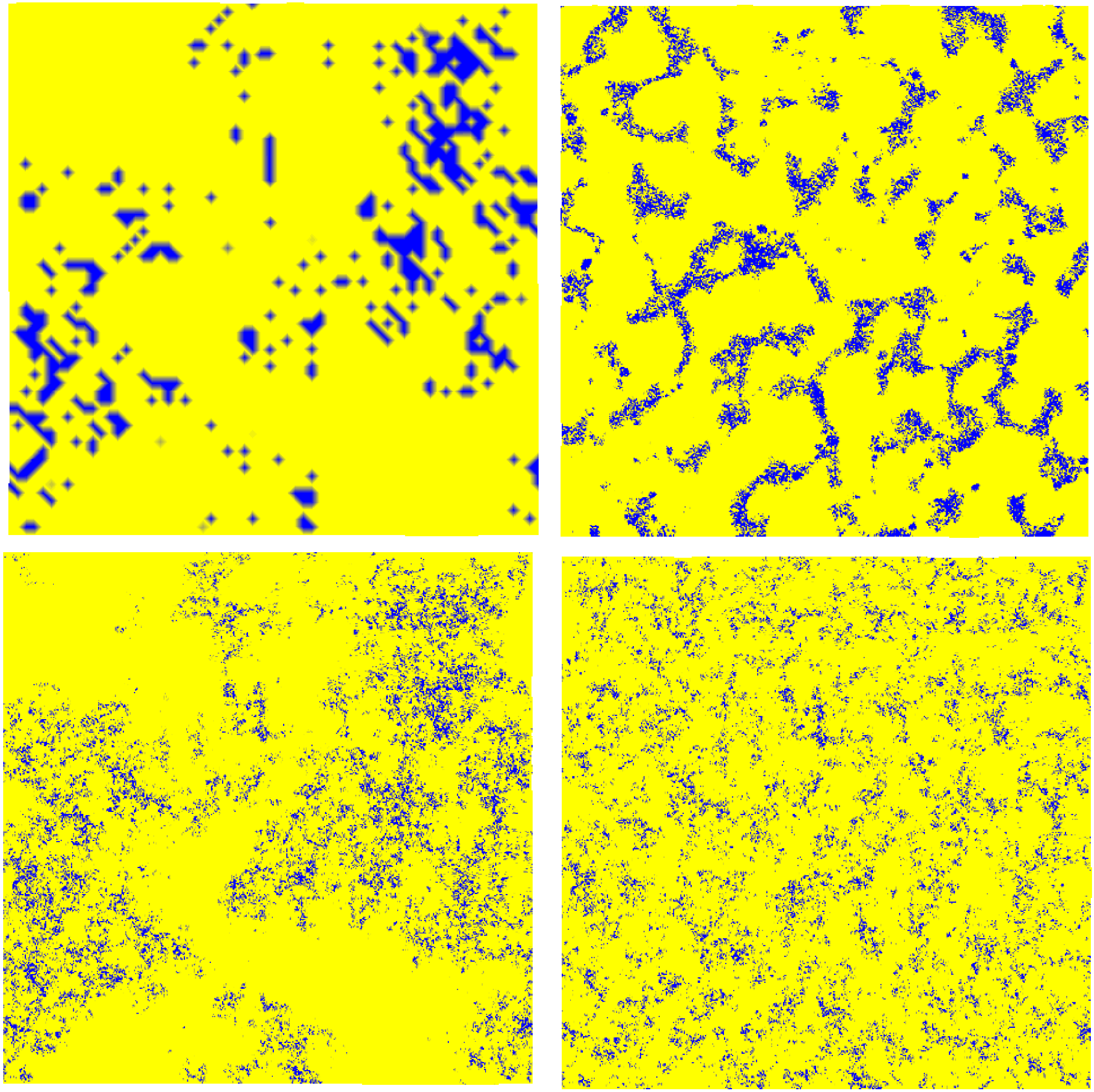
⇒$A_{real} = \kappa$ Load/ E' $h'_{rms}$ - steeper → less area
→ independent of $\lambda_L$, $h_{rms}$, system size

Numerical solution:
$\kappa \sim 2$ for all H, $h'_{rms}$ , $\nu$, …

Fixed pressure in contact
$p_{rep} = E' h'_{rms}/\kappa$



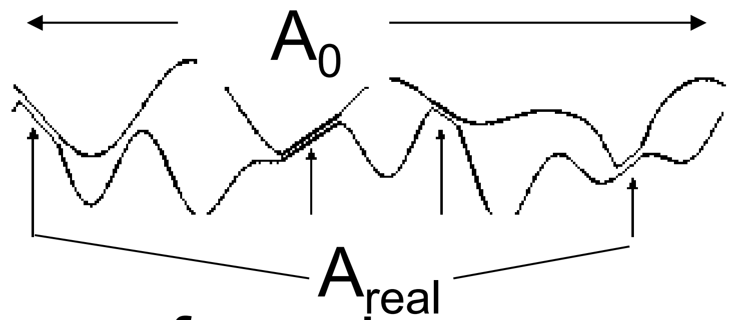

Hyun, Pei, Molinari, & Robbins, PRE **70**, 026117, '04; JMPS **53**, 2385, '05; Trib Int. **40**, 1413, '07



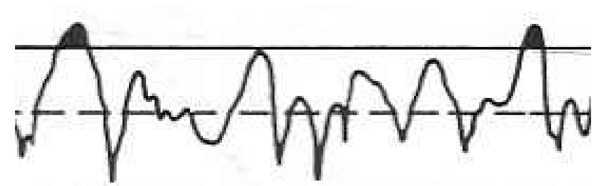
Very different surface roughness profiles give same $\kappa$=2.0

Results for different synthetic & experimental surfaces at $A/A_0$~0.1

# *Area ∝ Load ⇒ Dimensional Analysis*

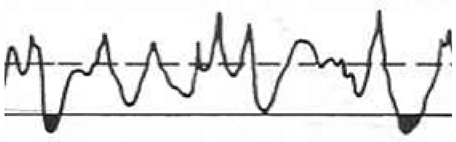


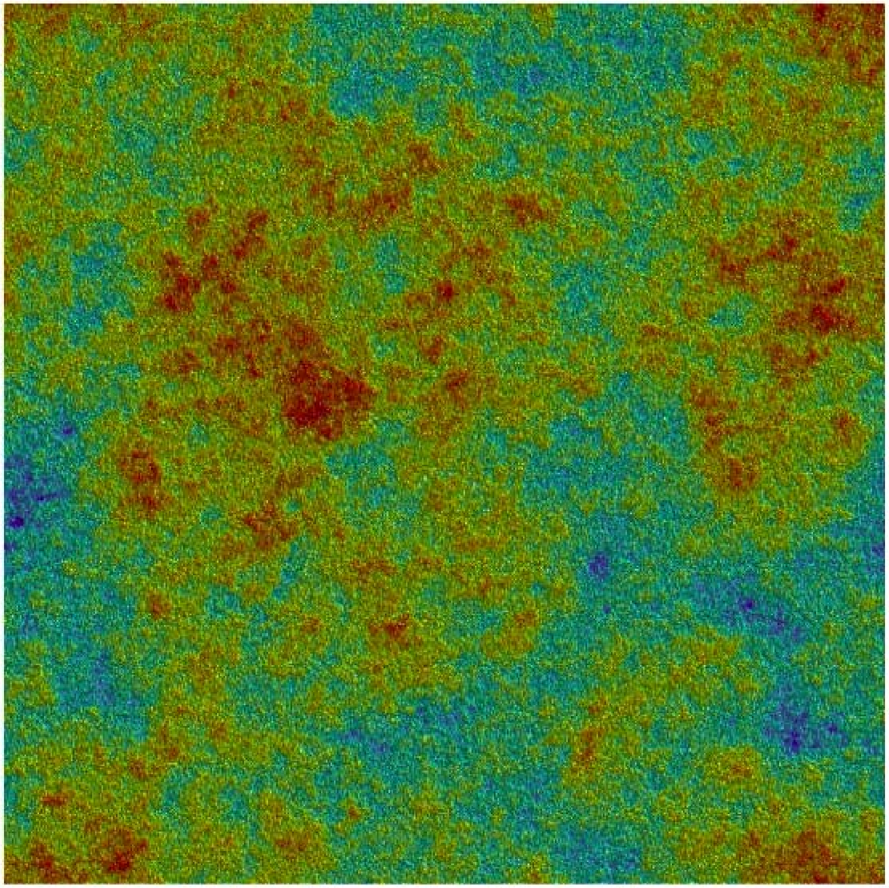

No adhesion ⇒ contact modulus
  $E' = E/(1-\nu^2)$ only material prop.
E' & Load/$A_{real}$ have same units
Slope $h'_{rms}$– dimensionless measure of roughness
⇒$A_{real} = \kappa$ Load/ $E' h'_{rms}$ - steeper → less area
  → independent of $\lambda_L$, $h_{rms}$, system size
Numerical solution: $\kappa \sim 2$ for all H, $h'_{rms}$, $\nu$, …
Very different analytic models→predict similar $\kappa$
  Bearing area – Greenwood-Williamson $\kappa=(2\pi)^{1/2}\approx 2.5$
  Persson's scaling theory $\kappa=(8/\pi)^{1/2}\approx 1.6$
Bearing area – contact where undeformed surfaces overlap⟶ no asperity interactions
    →wrong spatial structure



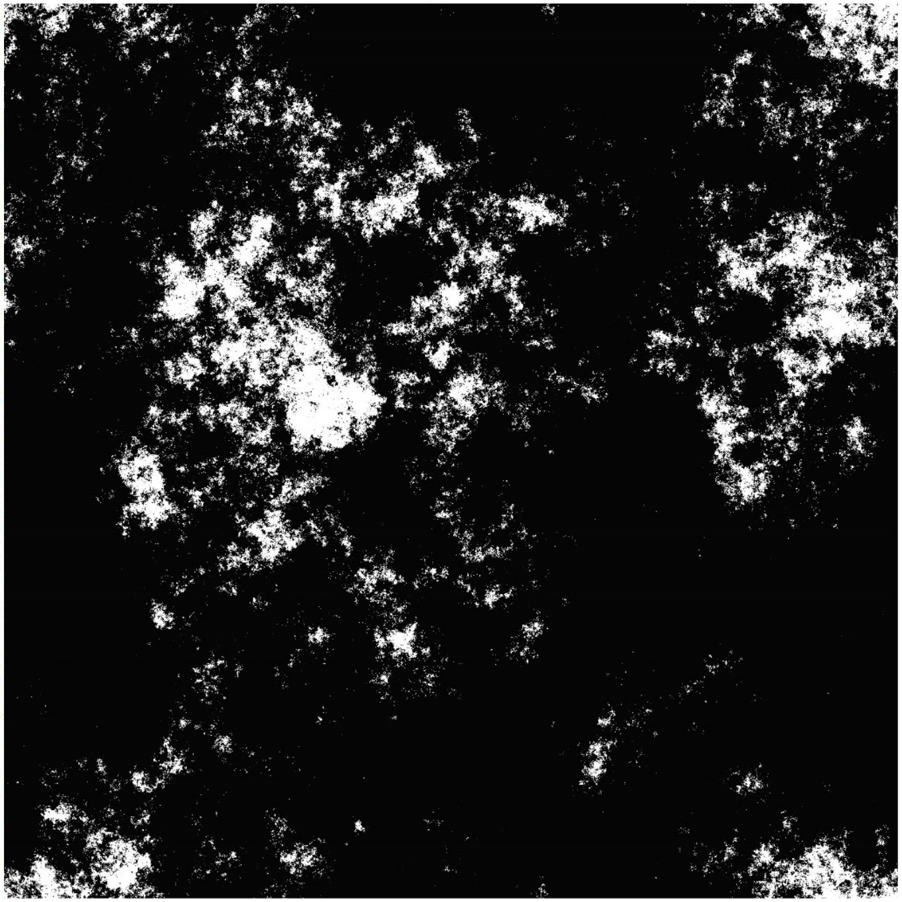
# *Models Predict Very Different Contact Geometry For Same Rough Surface and $A_{real}$*

Bearing area model ⟹ Contacts like lakes on fractal landscape – area ∝ diameter$^2$





Red higher, blue lower

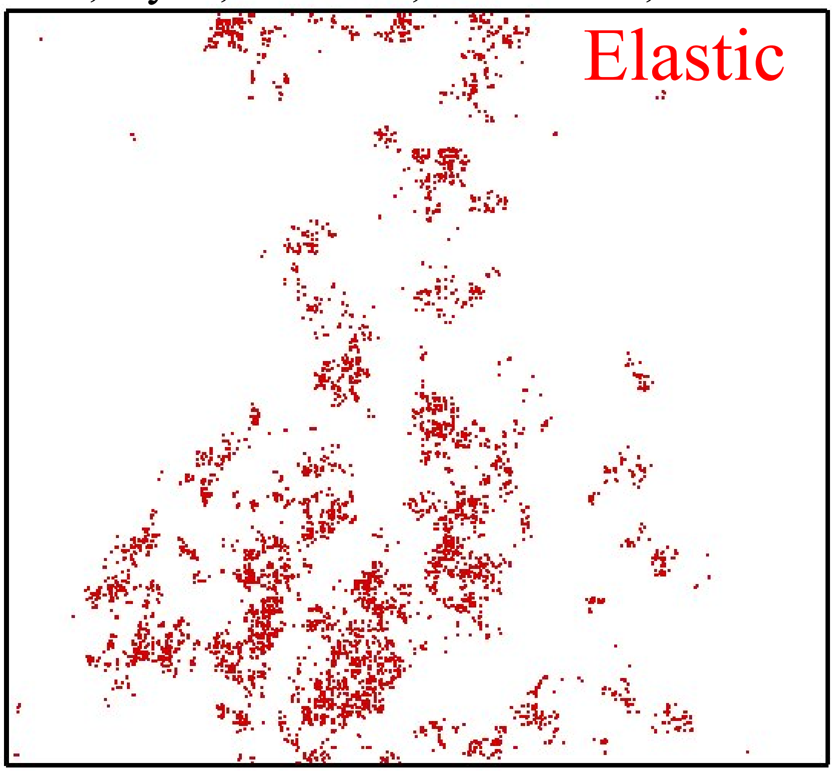


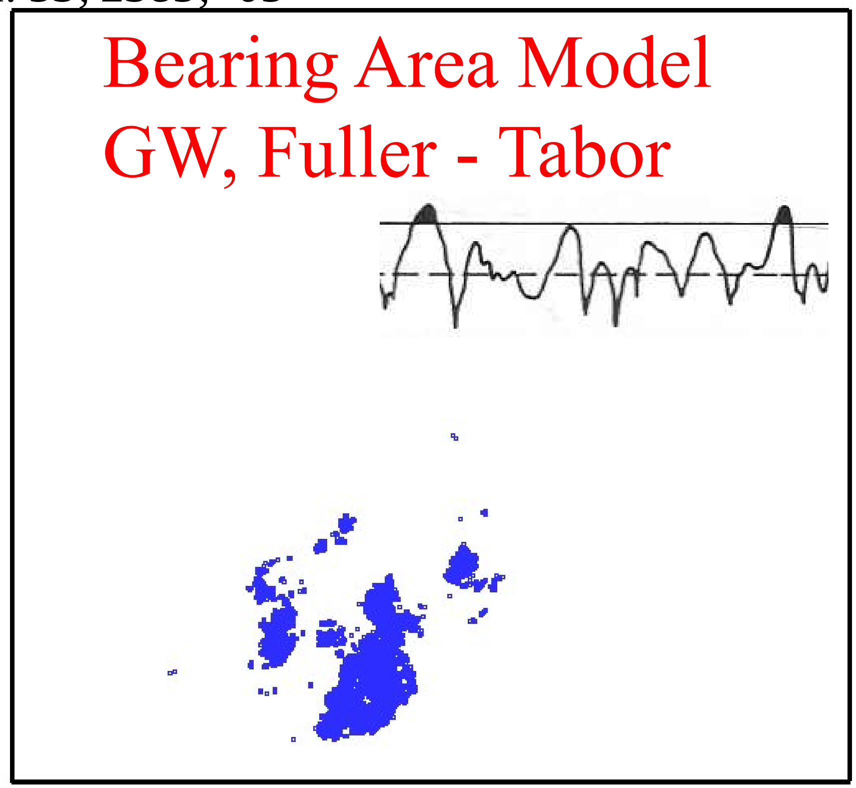
White regions contacts=lakes

# *Traditional Models ⇒ Very Different Contact Geometry For Same Rough Surface and $A_{real}$*

Ignore power law elastic interactions – change scaling

Pei, Hyun, Molinari, & Robbins, *J. Mech. Phys. Sol. 53, 2385, ’05*




Connected regions fractal — non-fractal

Area $a_c \propto r^{D_f}$ with $D_f \approx 1.6$ — $D_f = 2$

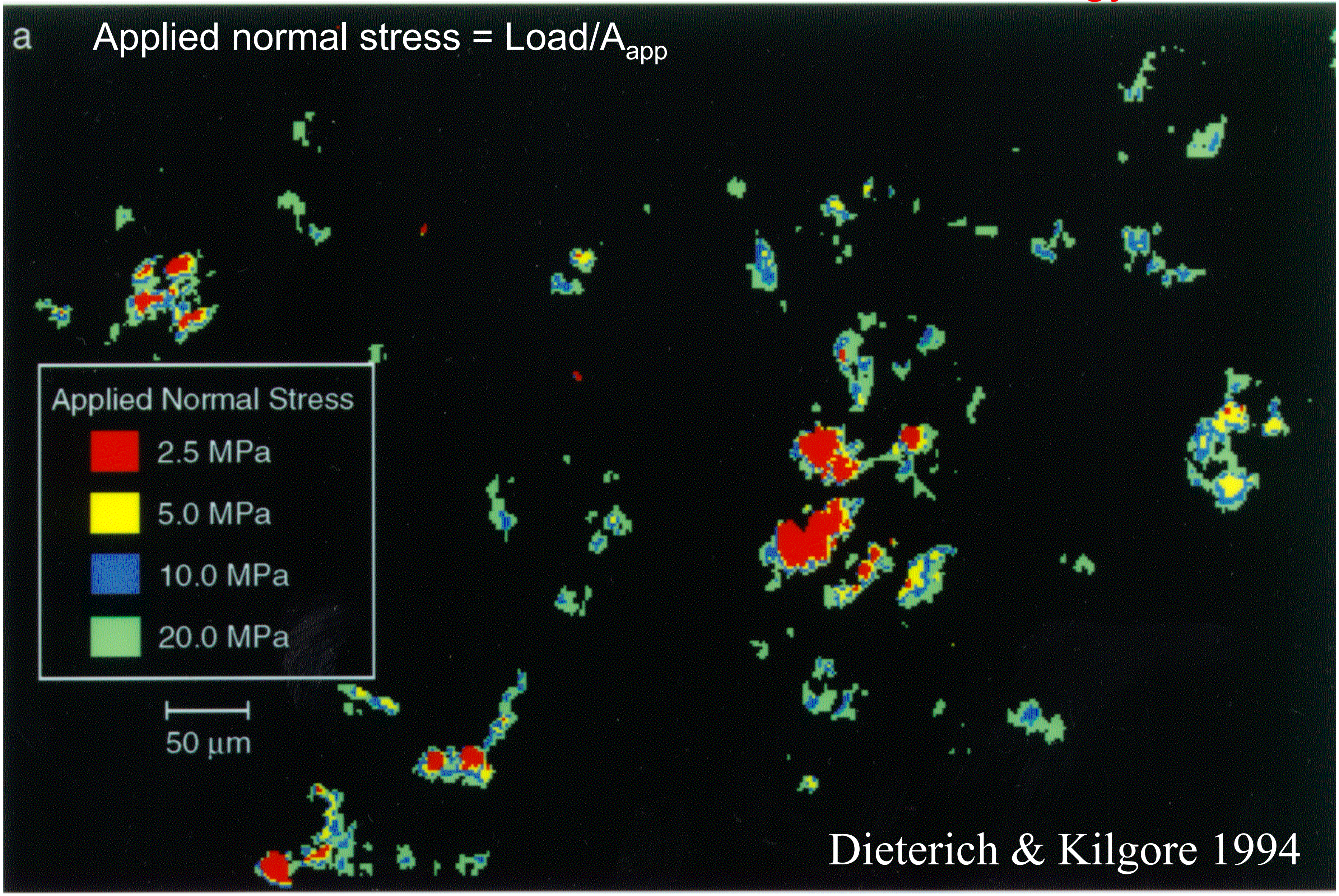
Dramatic change in conductance, stiffness, adhesion,…

***Contact area ∝ Load***

Two pieces of acrylic

***Even with Adhesion!***

→ Bulk fracture energy to slide



# *Why aren't all surfaces sticky?*

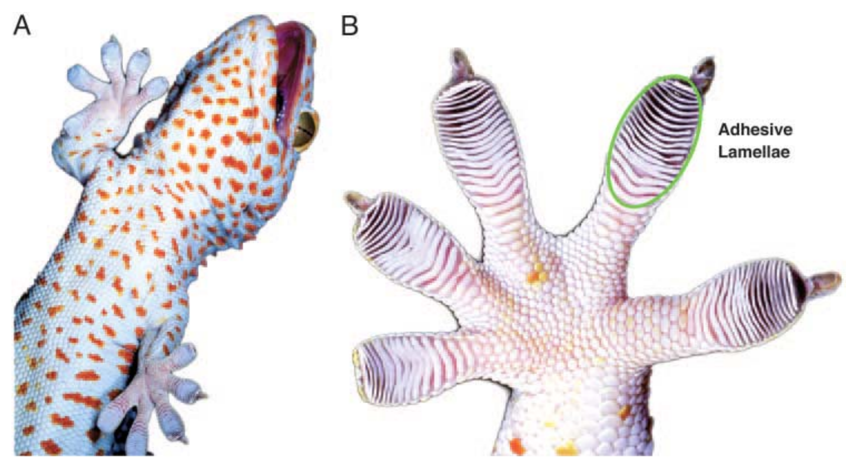
Adhesion Paradox (Kendall)

At atomic scales – surfaces feel van der Waals attraction

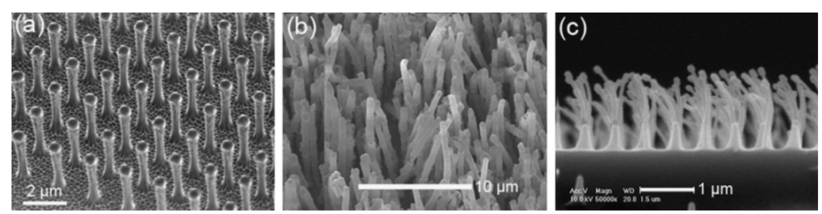
$\longrightarrow$ ~10MPa $\rightarrow$ 1cm$^2$ supports 100kg $\Rightarrow$ Spiderman!

At macroscopic scales – surfaces not sticky

$\longrightarrow$ no force to separate, contact theories ignore adhesion

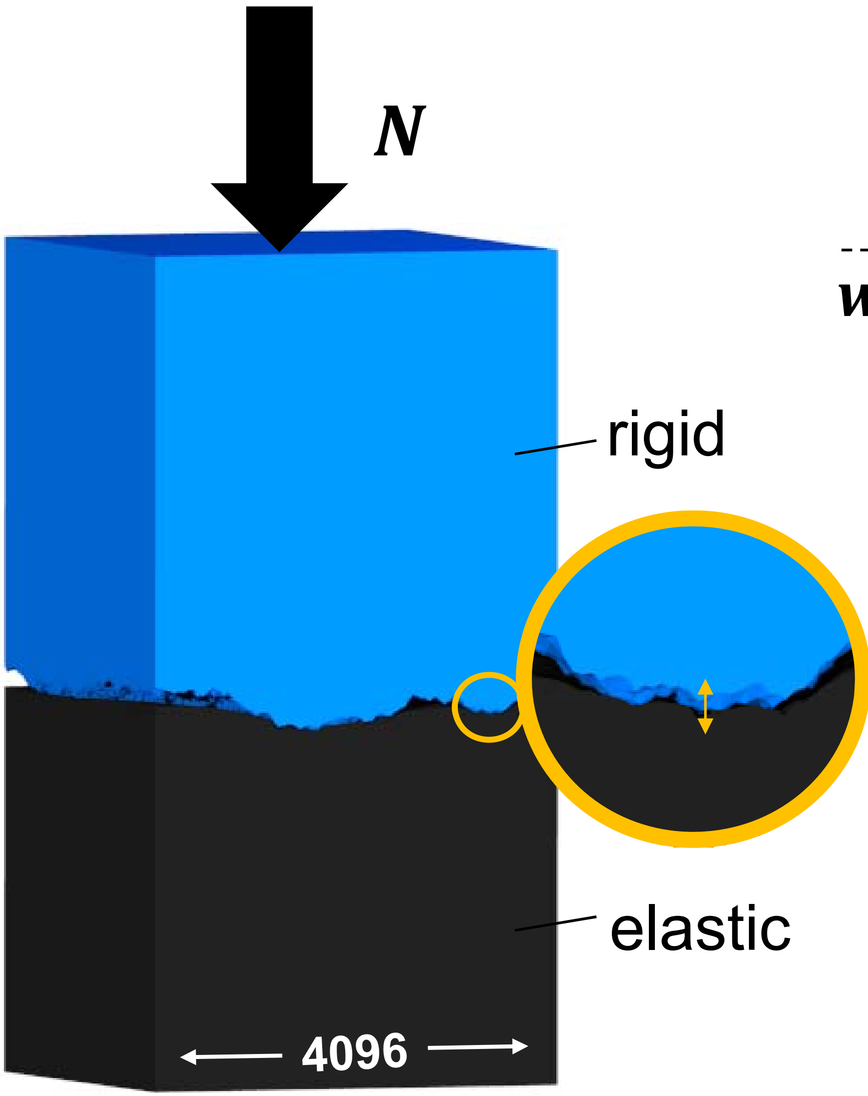




Hansen, Autumn, PNAS 102, 385 (2005)

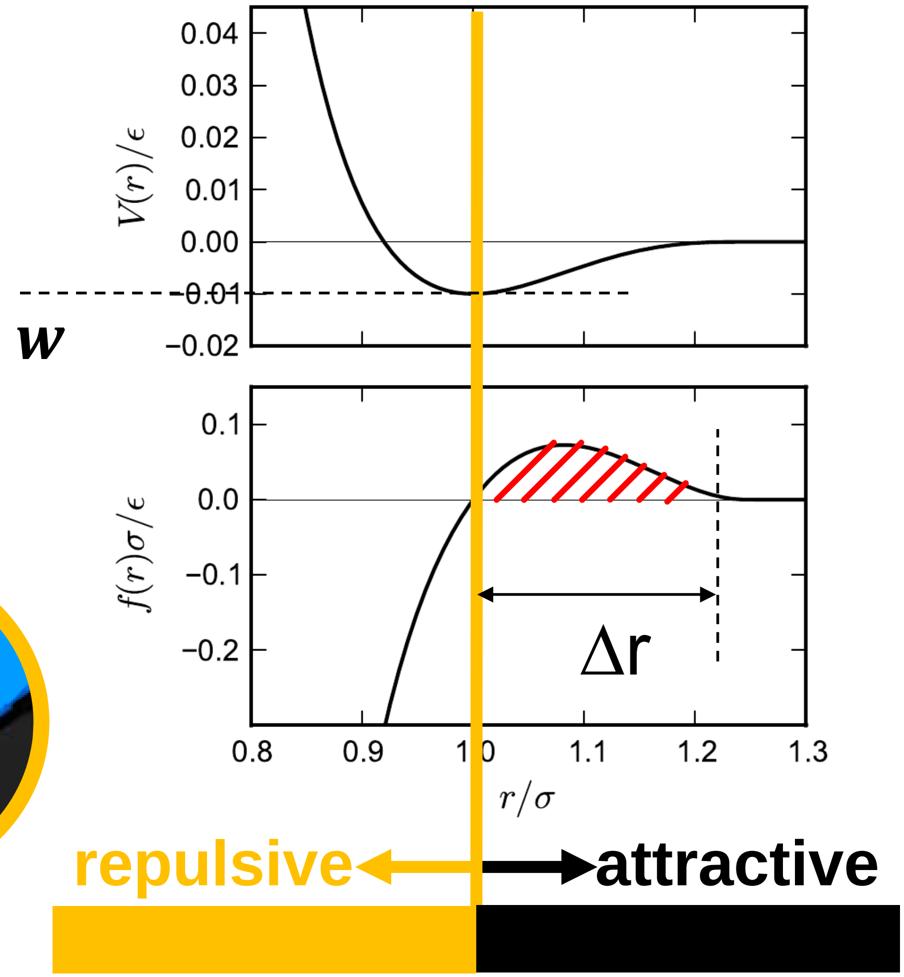



Jeong, Suh, Nano Today 4, 335 (2009)

# *Calculation Methods*




Volume $(4096a_0)^3$

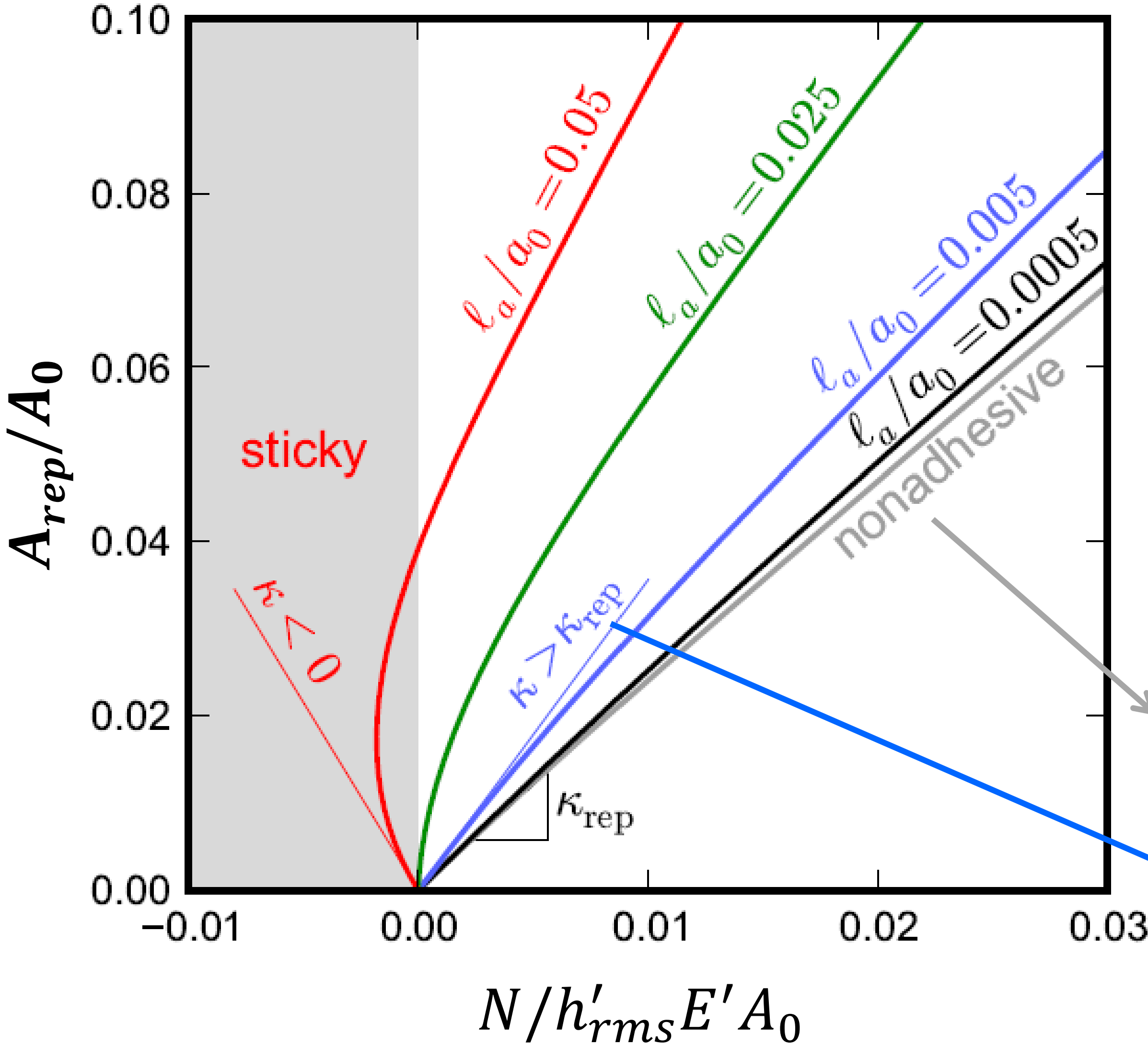


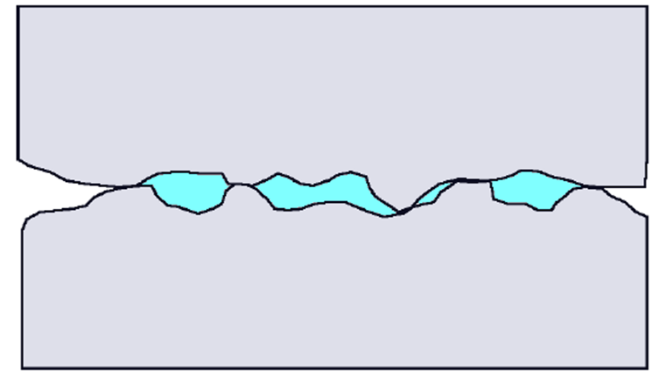

average attractive stress $\frac{w}{\Delta r}$

adhesion length $\ell_a = \frac{w}{E'}$

Contact area = $A_{rep}$ where atoms repel

# *Add Adhesion - First κ changes, then sticks*



$h'_{rms}$ - rms slope

$E'$ - contact modulus

$\ell_a = w/E'$

$a_0$=atomic spacing

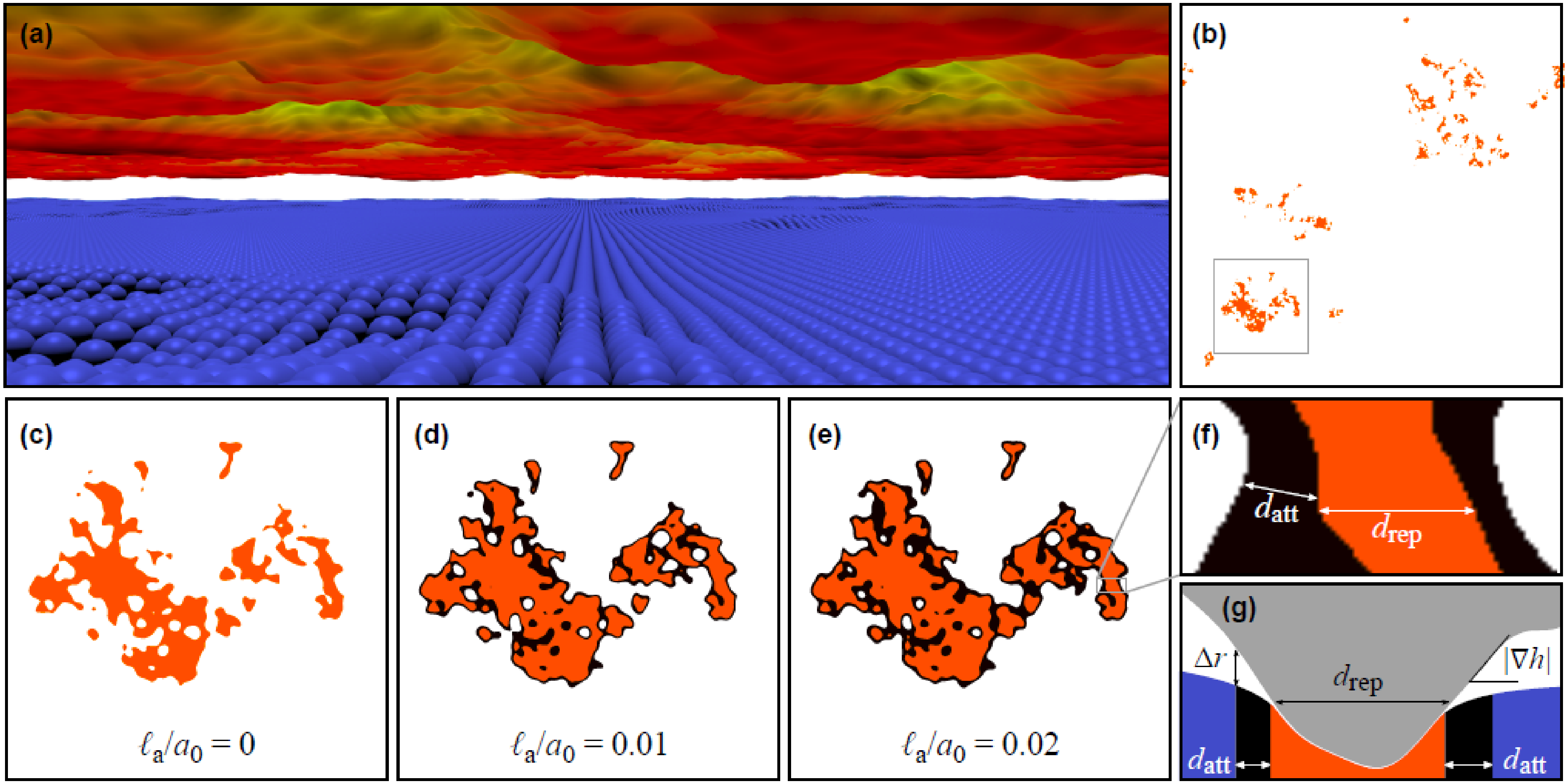
$$\kappa_{rep} = \frac{h'_{rms}E'A}{N} \approx 2$$

$$1/\kappa = 1/\kappa_{rep} - 1/\kappa_{att}$$

$\kappa < 0 \longrightarrow$ sticky

κ also describes changes in stiffness and conductance

# *Geometry $\longrightarrow$ Analytic prediction for $\kappa$*



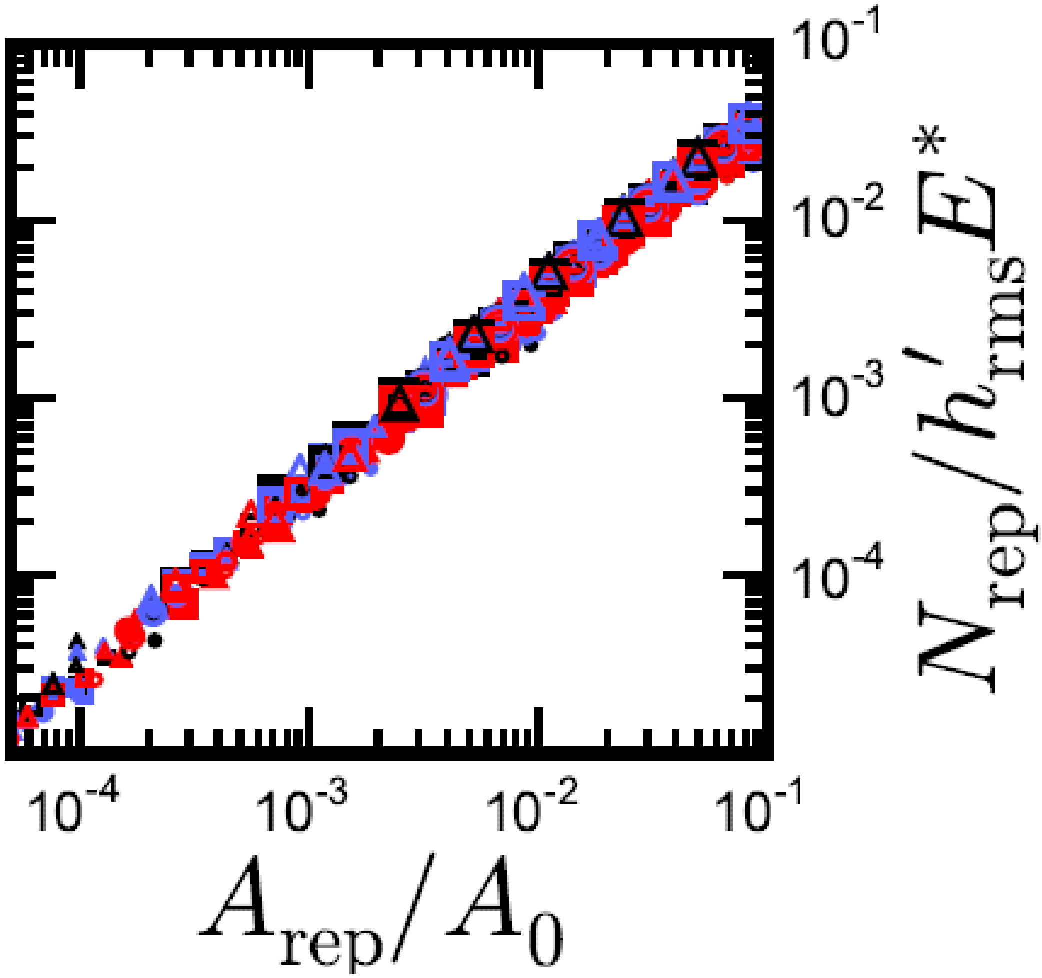

Adhesion doesn't change geometry just adds attraction – DMT limit

$\Rightarrow$ $N_{rep}=A_{rep}\, p_{rep}$ , $p_{rep} = E'\, h'_{rms}/\kappa_{rep}$

$\Rightarrow$ Attractive area $A_{att}$ (black) spreads around perimeter of $A_{rep}$

$N_{att}=A_{att}\, p_{att}$, $p_{att} = w/\Delta r$ and $A_{att} \propto A_{rep}$ *because fractal*

# *Same Area vs. Load in Repulsive Regions*

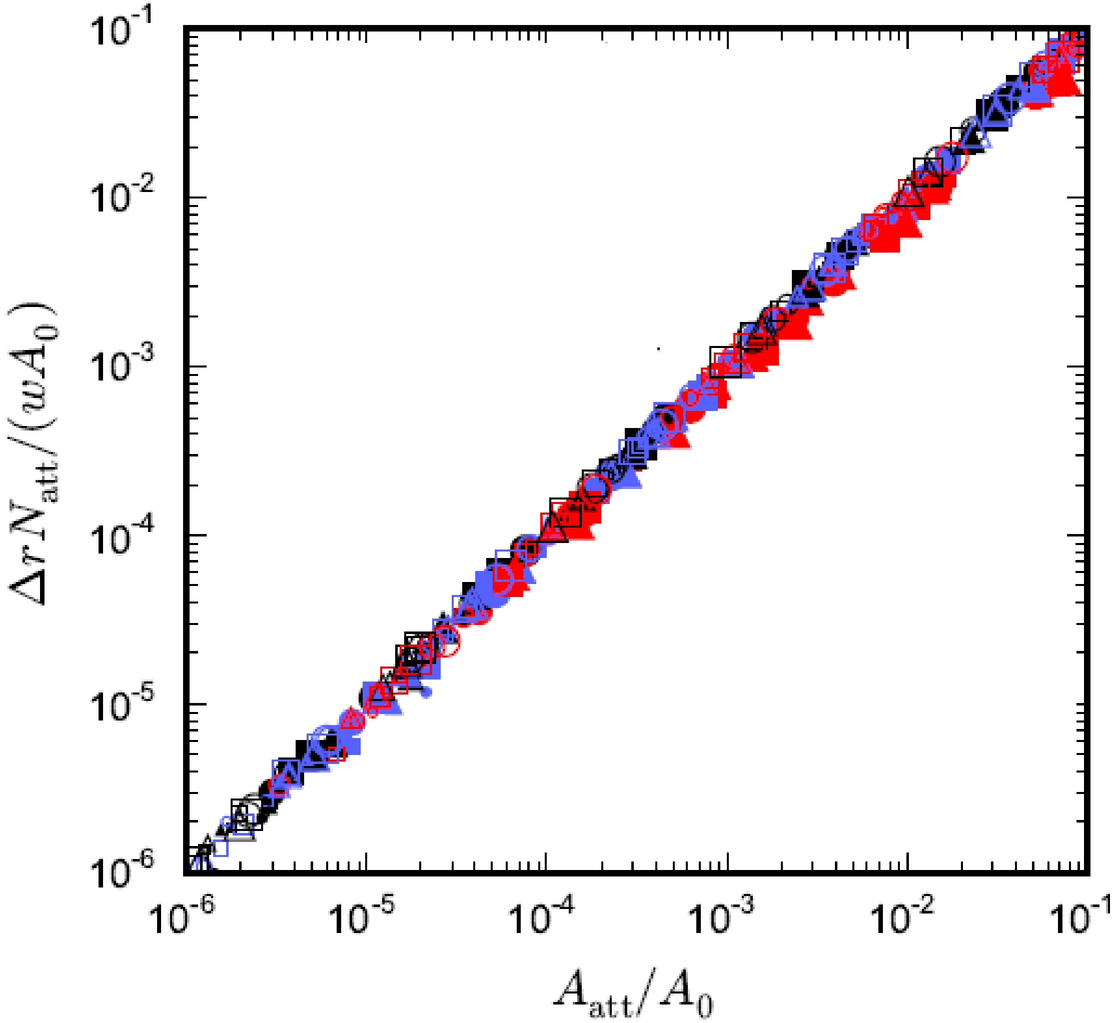



$\ell_a/a_0$=0.0005
$\ell_a/a_0$=0.005
$\ell_a/a_0$=0.05
H=0.3 ▲
H=0.5 ■
H=0.8 •
$\lambda_s/a_0$=4, 8, 16, 32, 64 increases with symbol size
$h'_{rms}$=0.3 □
$h'_{rms}$=0.1 ■

Results for all systems show that even with adhesion $N_{rep}$ and $A_{rep}$ are still related by $\kappa_{rep}$~2

Pastewka and Robbins, PNAS, 111(9), 3298-3303 (2014).

# *Connecting Attractive Area and Load $N_{att}$*




$\ell_a/a_0$=0.0005

$\ell_a/a_0$=0.005

$\ell_a/a_0$=0.05

H=0.3 ▲

H=0.5 ■

H=0.8 •

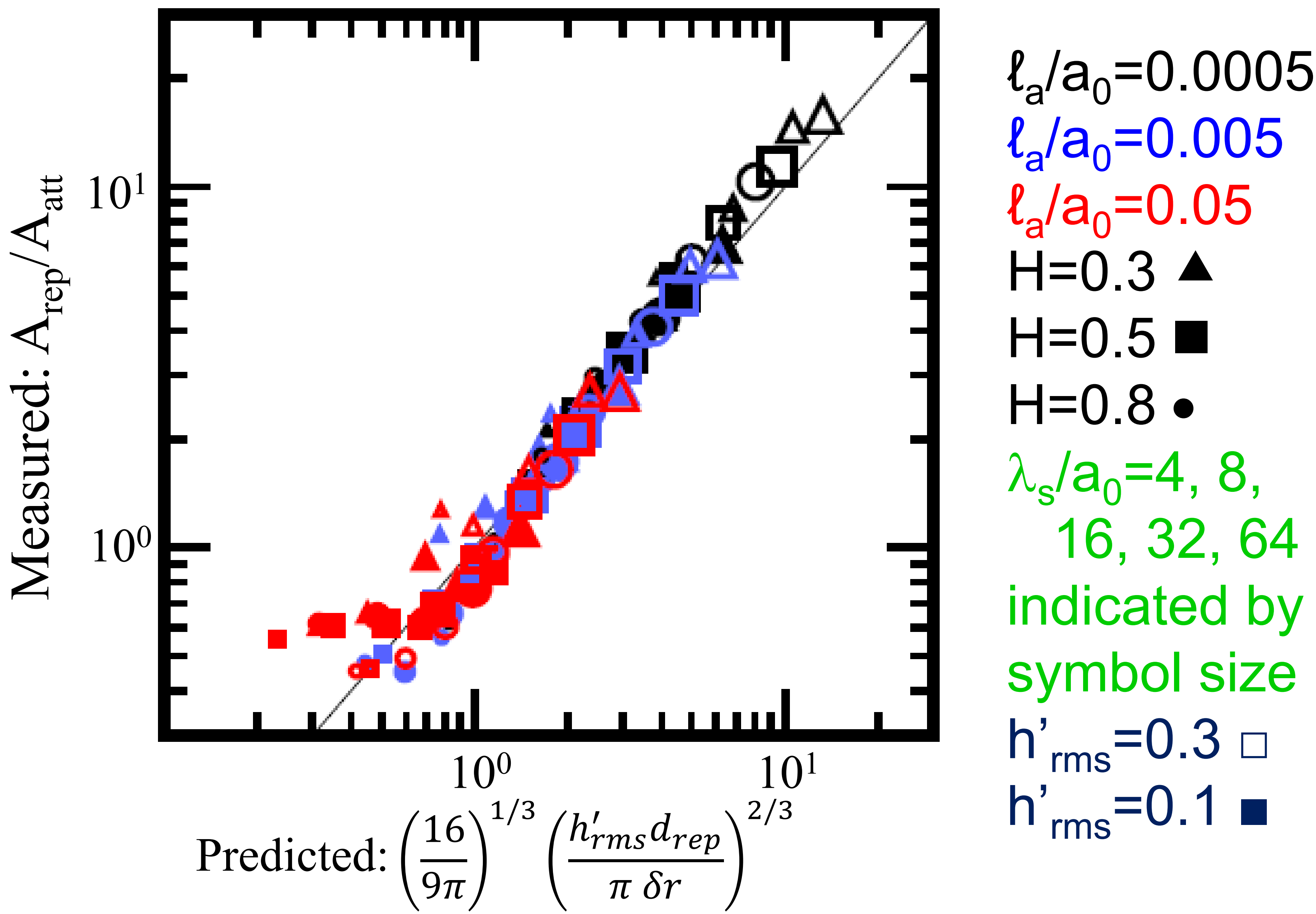
$\lambda_s/a_0$=4, 8, 16, 32, 64 indicated by symbol size

$h'_{rms}$=0.3 □

$h'_{rms}$=0.1 ■

Attractive load is just area times mean attractive pressure w/Δr

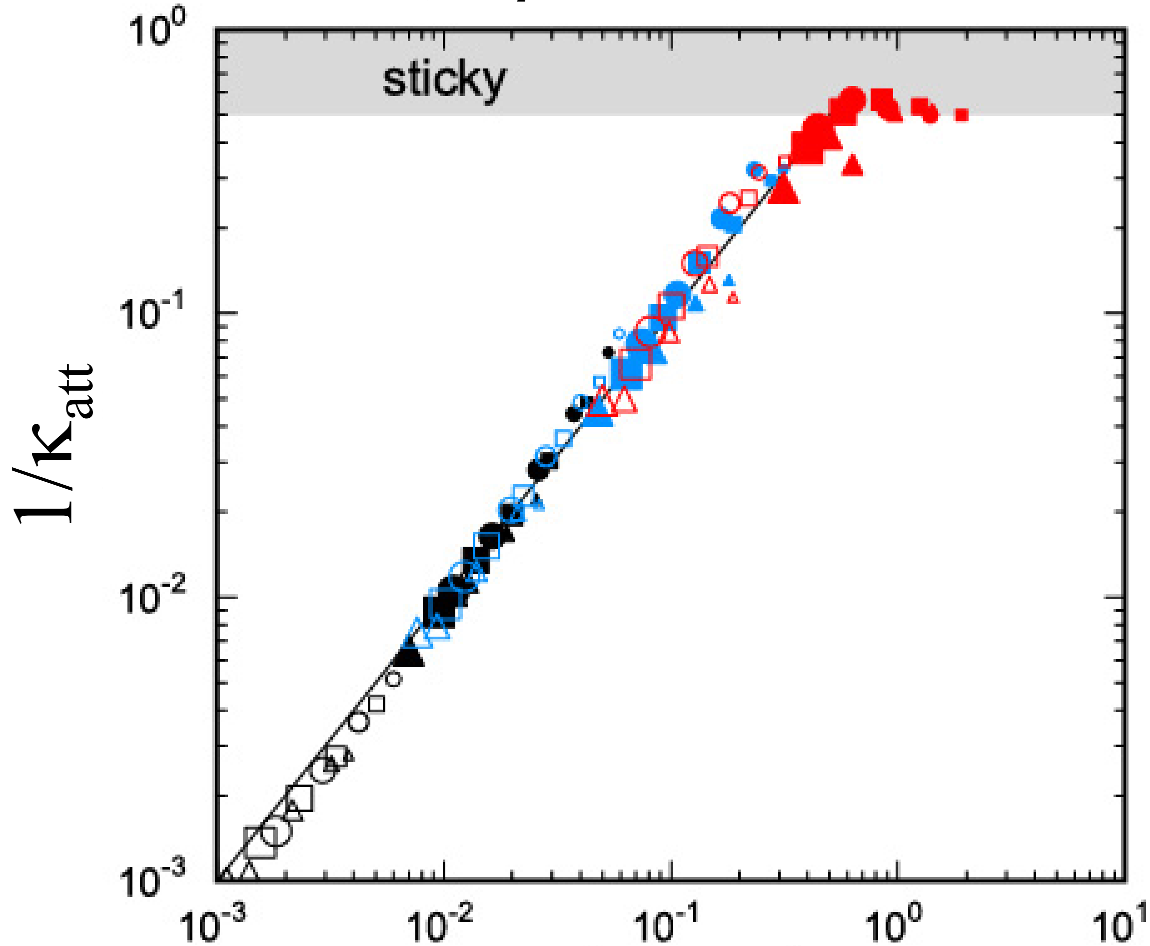
# *Predicted and Measured $A_{rep}/A_{att}$*




Pastewka and Robbins, PNAS, 111(9), 3298-3303 (2014).

# Predicted and Measured $\kappa_{att}$

$$N = N_{rep} - N_{\text{att}} = \left(\frac{1}{\kappa_{rep}} - \frac{1}{\kappa_{att}}\right) A_{rep} h'_{rms} \text{E}'$$




$\ell_a/a_0$=0.0005

$\ell_a/a_0$=0.005

$\ell_a/a_0$=0.05

H=0.3 ▲

H=0.5 ■

H=0.8 ●

$\lambda_s/a_0$=4, 8, 16, 32, 64 indicated by symbol size

$h'_{rms}$=0.3 □

$h'_{rms}$=0.1 ■

$$\text{Predict } 1/\kappa_{\text{att}} = \frac{\pi \ell_a}{2h'_{rms}}\left(\frac{2\Delta r}{h'_{rms} d_{rep}}\right)^{\frac{2}{3}}$$

Pastewka and Robbins, PNAS, 111(9), 3298-3303 (2014).

# *Why Are Sticky Surfaces Rare?*

*Necessary* condition for atomic surfaces

Ratio of adhesive to repulsive pressure $$\frac{w/\Delta r}{E' h'_{rms}/\kappa_{rep}} = \frac{\kappa_{rep}\ell_a}{\Delta r\ h'_{rms}} > 1$$

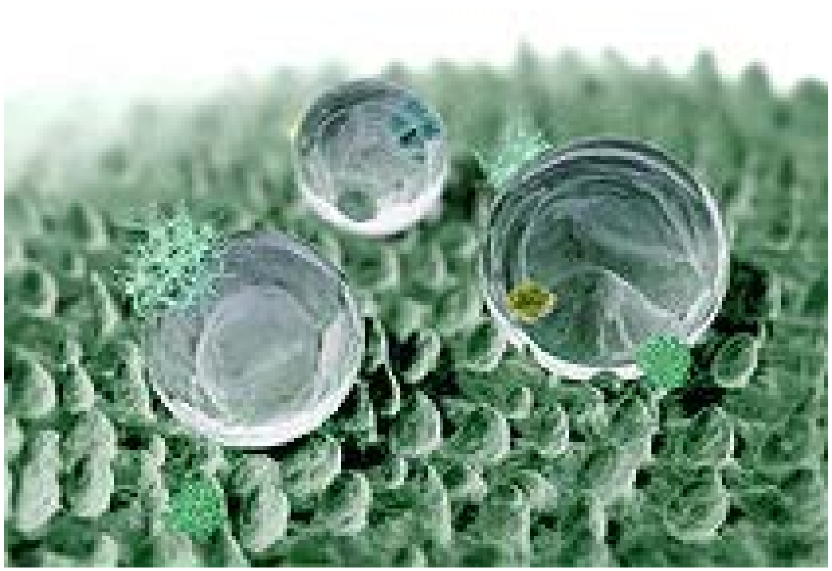
$\Delta r \sim a_0$ – atomic spacing⟶ w/(E'$a_0$)=$\ell_a/a_0$ >0.5 $h'_{rms}$

- Diamond/diamond bond $\ell_a/a_0$ =0.06, LJ $\ell_a/a_0$ =0.05
  Adhesion if $h'_{rms} < 0.1$
- Passivated surface – van der Waals at interface
  Reduce $\ell_a/a_0$ 100-fold
  ⟶Adhesion if $h'_{rms} < 0.001$ (wafer bonding)

Almost none of the surfaces around us show macroscopic adhesion even if nm scale attraction

# *Roughness and Superhydrophobicity*

Roughness also limits spreading of liquid on solid,
but need very high surface slope >1 to make nonwetting



http://en.wikipedia.org/wiki/Lotus_effect

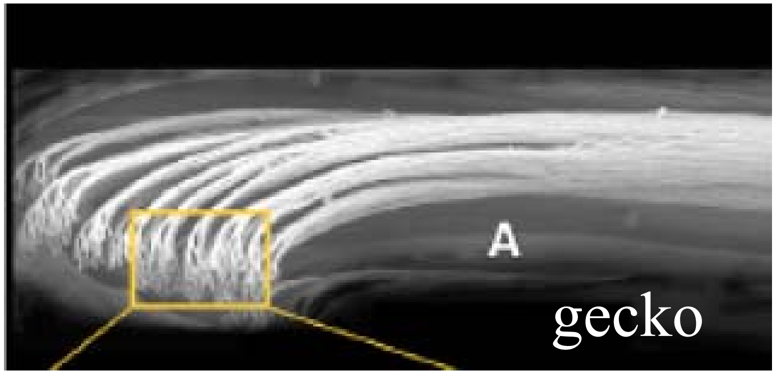
# *How Do We Make Things Sticky?*

*Necessary* condition for atomic surfaces

Ratio of adhesive to repulsive pressure
$$\frac{w/\Delta r}{E' h'_{rms}/\kappa_{rep}} = \frac{\kappa_{rep}\ell_a}{\Delta r\ h'_{rms}} > 1$$

$\Delta r \sim a_0$ – atomic spacing⟶ $w/(E'a_0)=\ell_a/a_0 > 0.5\ h'_{rms}$

- Animals lower E' in 2 ways
  – independent stalks
  or sparse network of beams
  in compliant shell



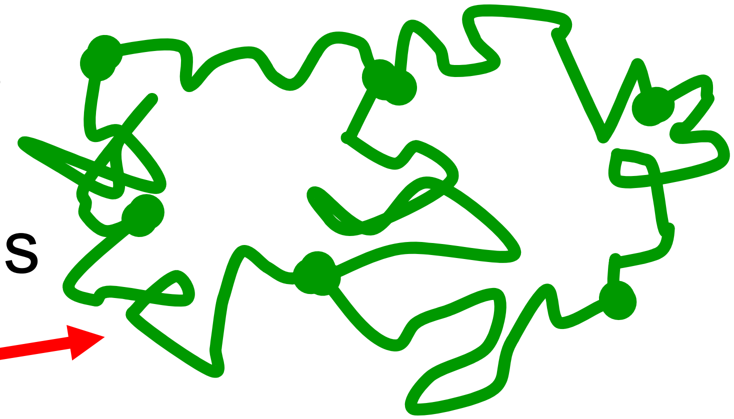
# *How Do We Make Things Sticky?*

*Necessary* condition for atomic surfaces

Ratio of adhesive to repulsive pressure $$\frac{w/\Delta r}{E' h'_{rms}/\kappa_{rep}} = \frac{\kappa_{rep}\ell_a}{\Delta r\ h'_{rms}} > 1$$

$\Delta r \sim a_0$ – atomic spacing$\longrightarrow$ $w/(E' a_0)=\ell_a/a_0 > 0.5\ h'_{rms}$

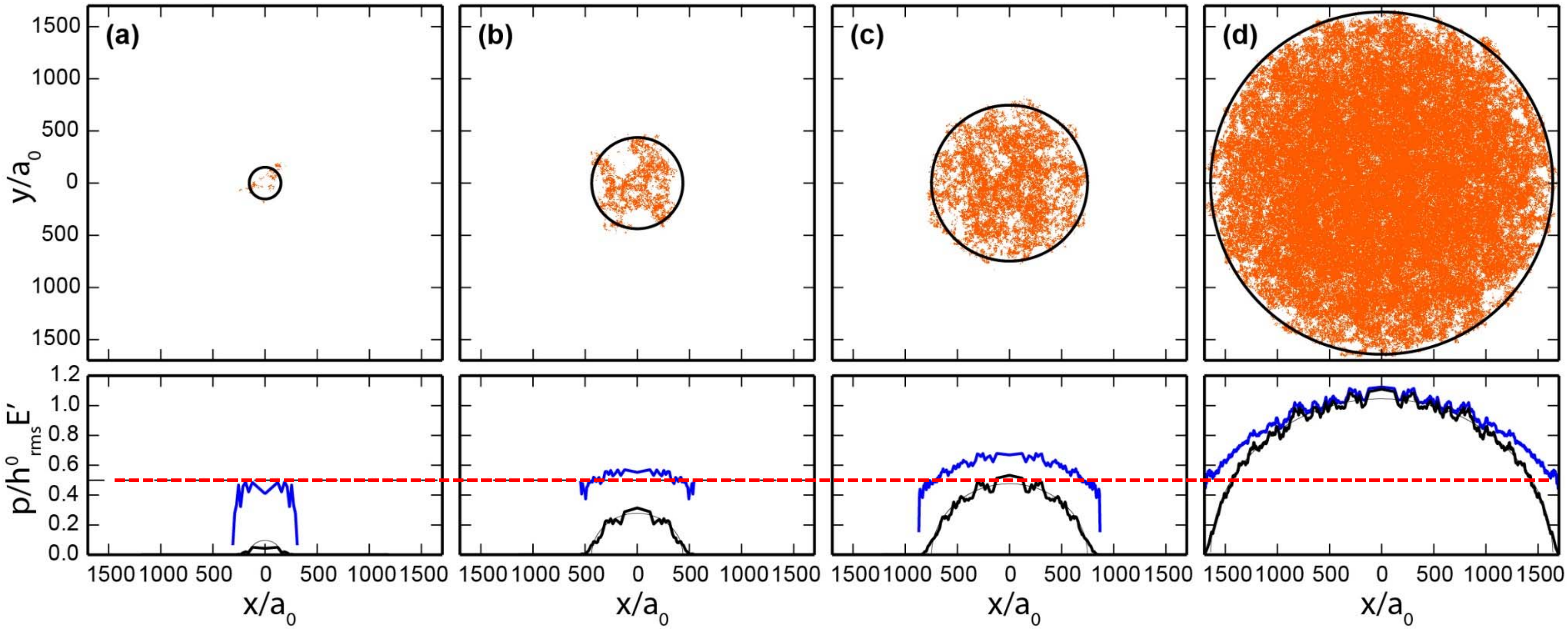
- Animals lower E‘ in 2 ways
  – independent stalks
  or sparse network of beams
  in compliant shell



- Elastomers – $\ell_a$=nm to μm vs. 3pm
  all atoms ⟶ w; E‘⟶ stretching between crosslinks
  $\ell_a/a_0 \sim n^3$ with n=# monomers between crosslinks
  Dahlquist criterion E‘<0.3MPa not big w

# *Sphere on Flat*

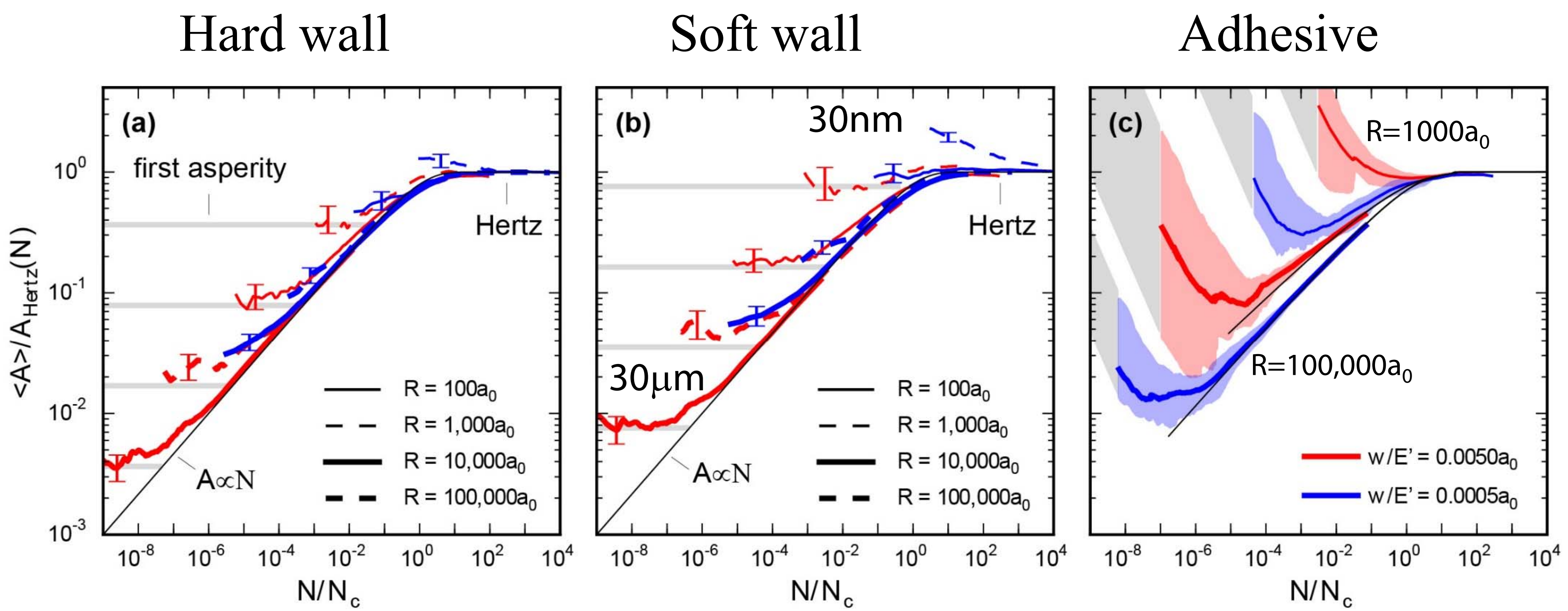
Parallel plates are hard to align ⟹ experiments use sphere-on-flat
Like parallel at small loads, Hertz at large loads
Top – contact in orange, solid=Hertz radius,




Bottom – black=mean pressure at a given radius
blue= mean pressure in contacting regions
red= flat surface prediction for $p_{rep}$

# *Area Divided By Hertz Prediction*

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




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

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.

# *What are Scales of Colloid Interactions?*

Double Layer Interactions

Poisson-Boltzmann – constant chemical potential

& constant local pressure $p=ck_BT-\varepsilon E^2/2$

Typically E=0, $p=c_0k_BT$ at midpoint between surfaces

This allows simple estimate of scale

1M solution of + and - $\Rightarrow p = 2 \cdot \frac{6\cdot 10^{23}}{(0.1m)^3} \cdot 4 \cdot 10^{-21} J$

$p = 48 \cdot 10^5 Pa$~5MPa

If p<<$p_{rep} = 0.5\, h'_{rms} E'$ have little effect on contact

Negligible for metals or ceramics

Marginal for very smooth plastics E'~1GPa

Interesting for rubber, gels

Need to include conformal nature of interaction,

range over wavelength

# *What are Scales of Colloid Interactions?*

Can also consider polymer brushes on surfaces.

Clearly long-range repulsion screens roughness prevents contact and minimizes friction

Basically pushes boundary lubrication regime to lower velocities & viscosities, higher loads.

Significant friction only from fraction of surface separated by ~1nm or less.

Need smooth surfaces or pressures ~ $p_{rep} = 0.5\, h'_{rms} E'$ that are much larger than typical colloidal forces

Questions:

Is behavior of silica spheres different than rubber spheres?

Is there a scale dependence? Larger hard to bring into contact.

# *Conclusions*

- Ignoring interactions between asperities gives qualitatively wrong spatial distribution of contacts changes adhesion, stiffness, conductance
- Small $A_{rep}/A_0 \longrightarrow A_{rep}$ proportional to load
  $N_{rep}=p_{rep}A_{rep}$; $p_{rep}=h'_{rms}E'/\kappa_{rep}$   $\kappa_{rep}\approx 2$
  $N_{att}=(w/\Delta r)A_{att}$
  $N=A_{rep}(1/\kappa_{rep}-1/\kappa_{att})h'_{rms}E'$
  $< 0 \longrightarrow$ adhesion

$$\frac{1}{\kappa_{att}}=\frac{\pi\ell_a}{2h'_{rms}}\left(\frac{2\Delta r}{h'_{rms}d_{rep}}\right)^{\frac{2}{3}}$$

- Make things stick by reducing E' not increasing w!
  Only very soft, smooth surfaces adhere
- Parameter-free theory for rough spheres
- Difficult to get large, constant shear stress in contact unless have mobile third bodies or have plastic deformation that produces excessive wear

# *Dimensional Analysis of Contact Stiffness*

Contacts often dominate macro stiffness → jet engine mounts

Electrical and thermal conductance scale like stiffness

Normal stiffness $k_N \equiv -dN/du$ with u=mean surface separation

Tangential stiffness $k_T = -dF/dx$ with x=lateral disp.

Dimensional analysis $k_N = N/\chi h_{rms}$ with $\chi$ a constant and $h_{rms}$=rms height → sensitive to system size

Integrate $-dN/du = N/\chi h_0 \Rightarrow N = \chi A_0 E' \exp(-u/\chi h_{rms})$

Isotropic continuum - lateral stiffness $k_T = k_N\, 2(1-n)/(2-n)$

Experiment:

Lateral - Berthoud, Baumberger, Proc. R. Soc. Lond. A454, 1615 ‘98.

Normal - Benz, Rosenberg, Kramer, Israelachvili, J. Chem. Phys. ‘06.

Lorenz and Persson. J. Phys. Condens. Matter 21, 015003 ’09.

Theory: Pei, Hyun, Molinari, Robbins, JMPS 53, 2385 (2005).

Persson, Phys. Rev. Lett. 99, 125502 (2007), Campana et al. (2011)

3D simulations of Lennard-Jones atoms (up to $10^{10}$)

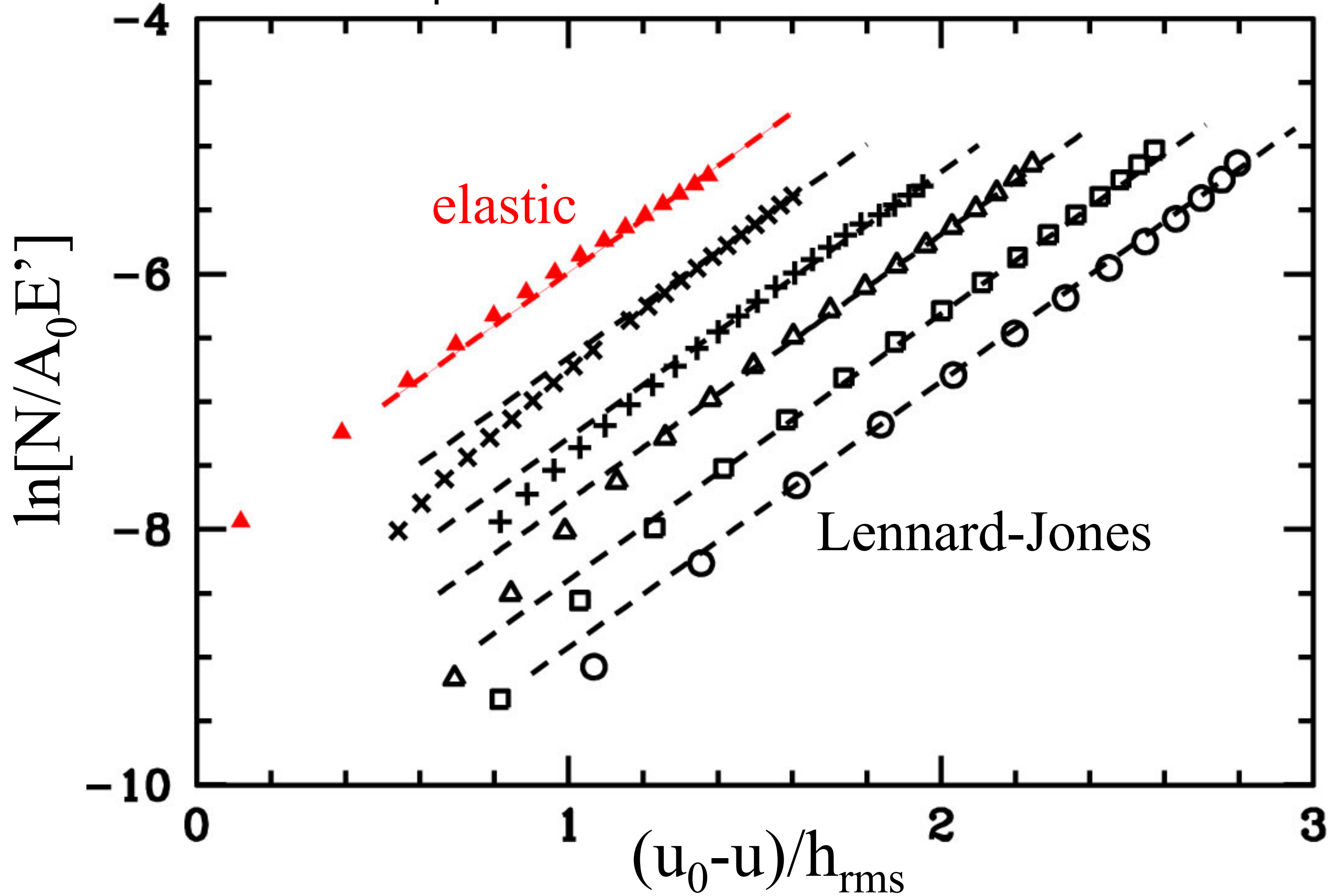
Akarapu, Sharp, Robbins PRL 106, 001504301 (2011), Pastewka, Prodanov, Lorenz, Müser, Robbins and Persson, Phys. Rev. E87, 062809 (2013).

# *Load Varies Exponentially With Separation u*

Find $F_N = \chi A_0 E' \exp(-u/\chi h_{rms})$ with $\chi$=0.48 $\rightarrow k_N = N/ch_{rms}$

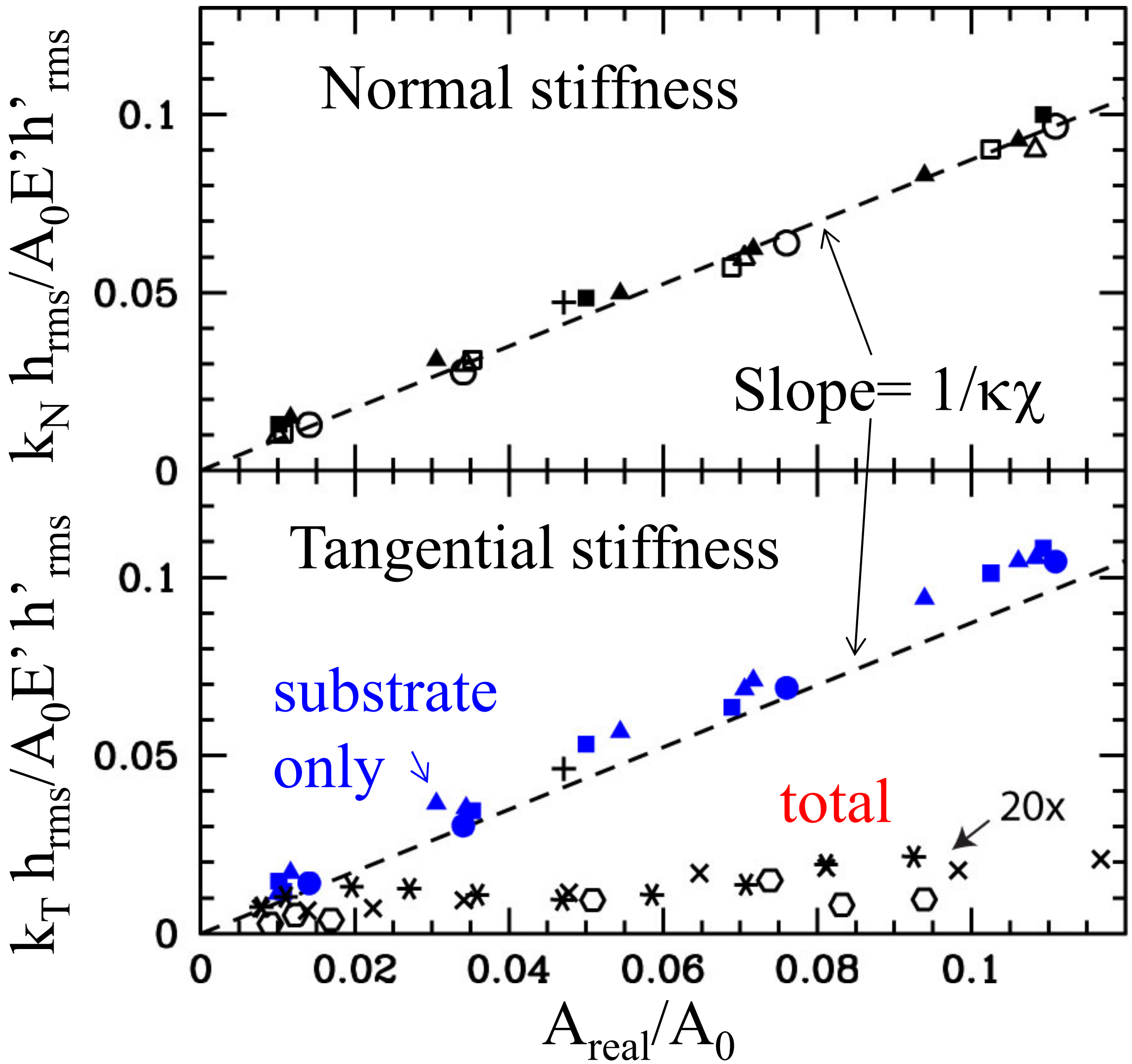
For all H, n, system size, continuum & Lennard-Jones

Adhesion: $1/\kappa \rightarrow 1/\kappa_{rep} - 1/\kappa_{att}$.



# *Normal Stiffness ∝ Load ∝ Area*

Predict and measure $(k_N / A_0 E') (h_{rms} / h'_{rms}) = (\kappa\chi)^{-1} A_{real} / A_0$




Results for $k_N$ with different H, L, xtal structure collapse with $\chi$~0.5

Tangential stiffness ~100 times smaller

Contribution from substrate ~$k_N$

Lateral motion between atoms on opposing interfaces dominates total $k_T$ !

$k_T$ varies with xtal surface, atomic spacing

Adhesion: $1/\kappa \rightarrow 1/\kappa_{rep} - 1/\kappa_{att}$