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GIESSEN

Limitations of Structural Superlubricity:

Chemical Bonds versus Contact Size

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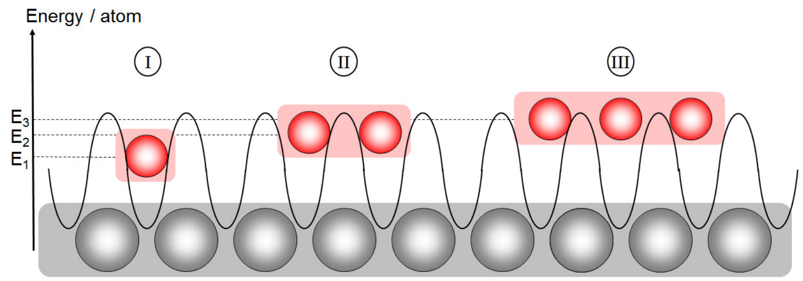
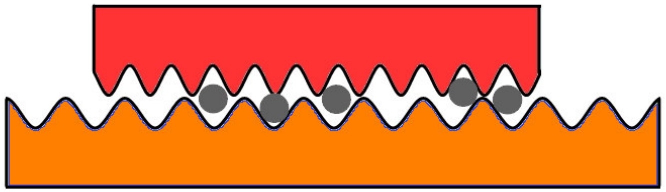
IAP

Structural Superlubricity of Nanoparticles

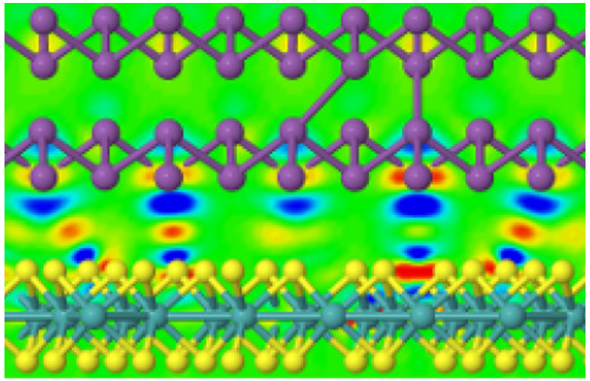
Structural Superlubricity Basics:
Concepts and Scaling



Limits of Structural Superlubricity
Case a) Mobile interface molecules

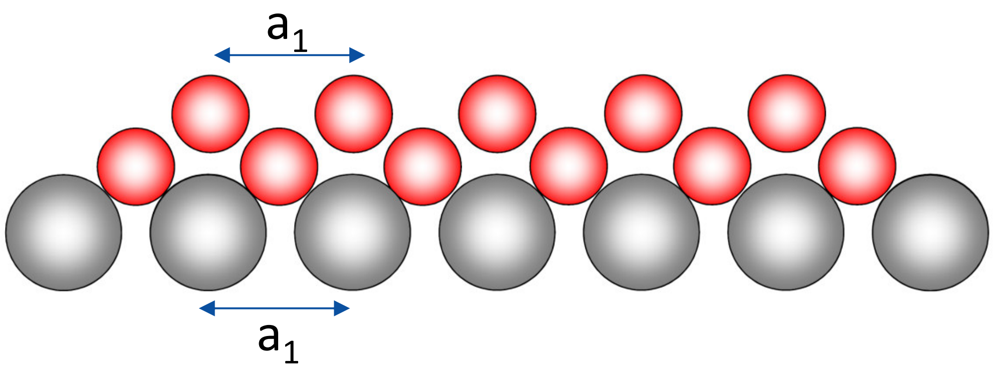


Limits of Structural Superlubricity
Case b) Size dependent break-down



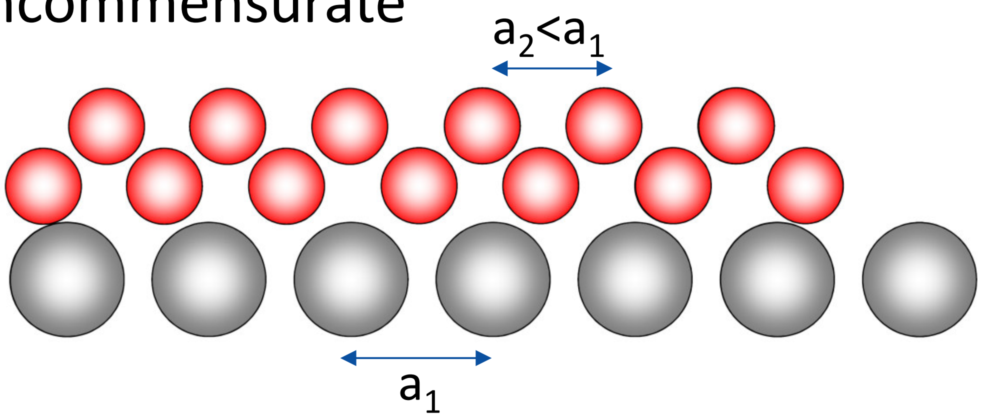
Structural Superlubricity: Commensurate vs Incommensurate

Commensurate



Interlocking of atomic potentials: Friction $\propto A_{contact}$

Incommensurate



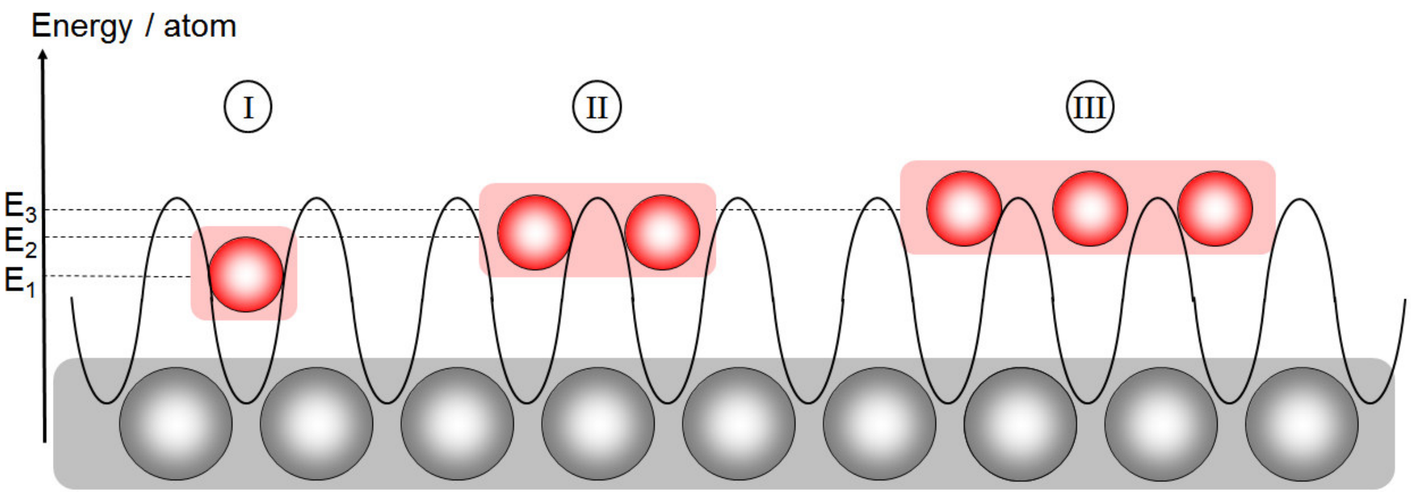
no interlocking of atomic potentials: structural lubricity ('superlubricity')

Hirano & Shinjo, PRB 41, 11 837 (1990)
Müser, Wenning, Robbins, PRL 86, 1295 (2001)
Dienwiebel et al., PRL 92, 126101 (2004)

Incommensurate Case: Friction Area Scaling

If particle and substrate have non matching lattice constants (**a≠b**)

Number of top atoms increases → Energy barrier per atom decreases



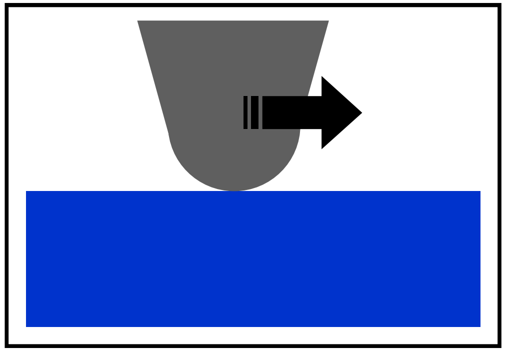
Theoretical
(calculations / simulations):
Energy barrier vs. particle size follows sublinear power law

$$\Delta E \propto N_{atom}^{\gamma} \quad (\gamma < 1)$$

deWijn, Phys. Rev. B. 86, 085429 (2012)
Müser, Wenning, Robbins, Phys. Rev. Lett. 86, 1295 (2001)
M. Müser in “Fundamentals of Friction and Wear at the Nanoscale”, Eds: E. Gnecco, E. Meier, Springer (2007)

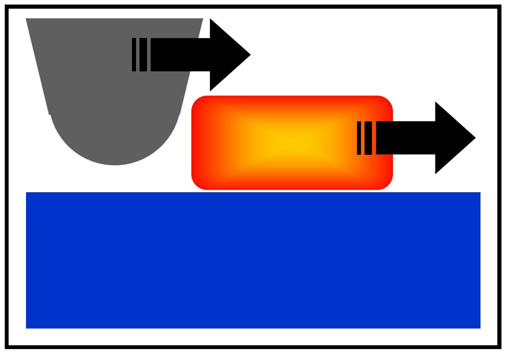
From Friction Force Microscopy to Particle Manipulation

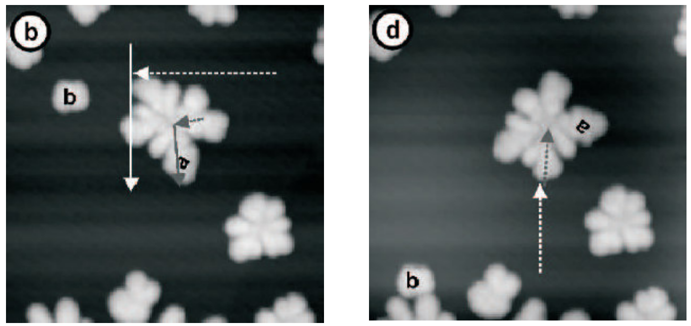
Vary tip apex by TEM preparation



Schwarz et al, Phys Rev B 56 (1997) 6987

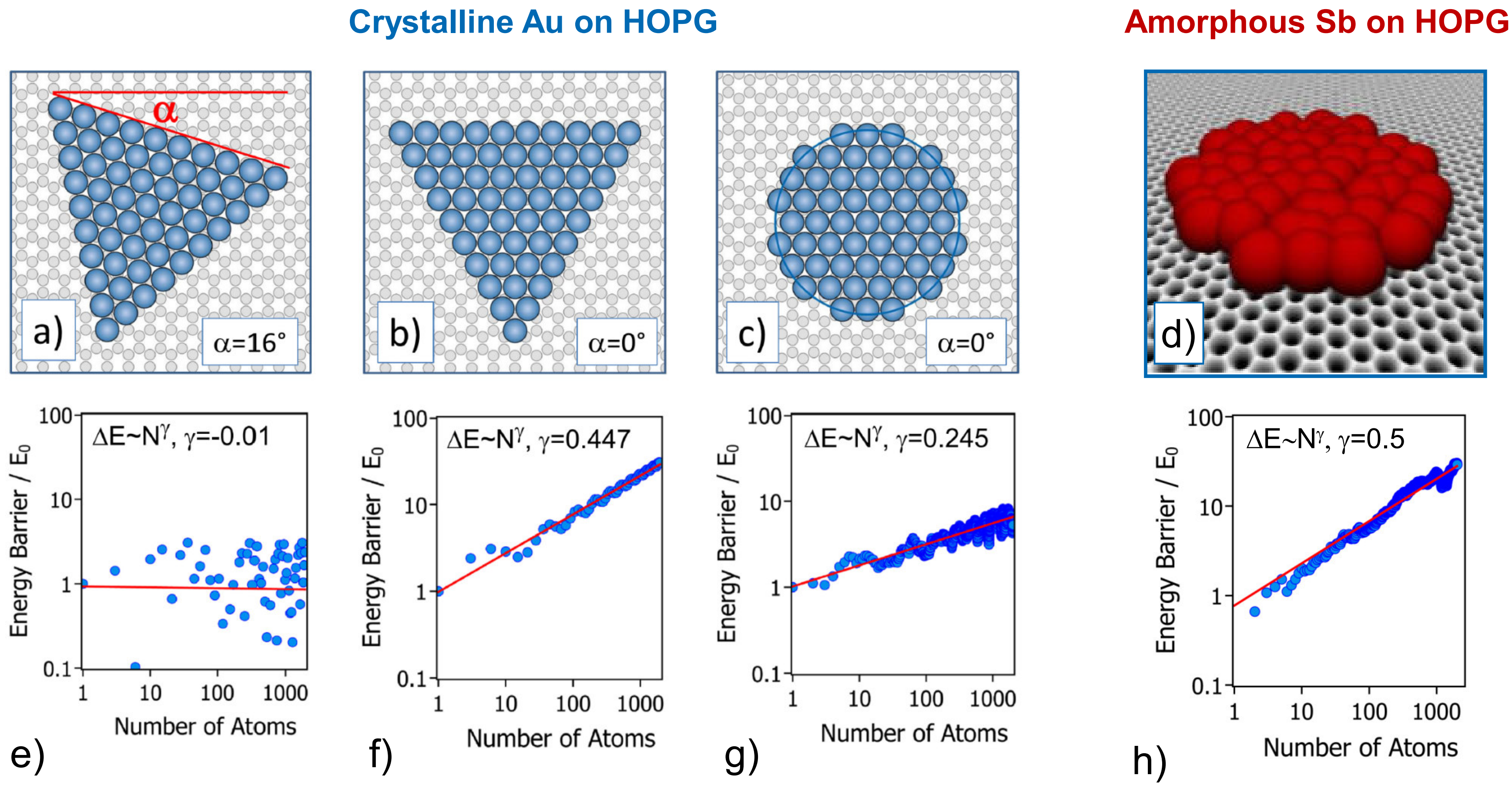
Use tip to push particles with varying size





Ritter et al., Phys. Rev. B **71**, 085405 (2005)

Theory: Calculation of Energy Barriers for Nanoparticles



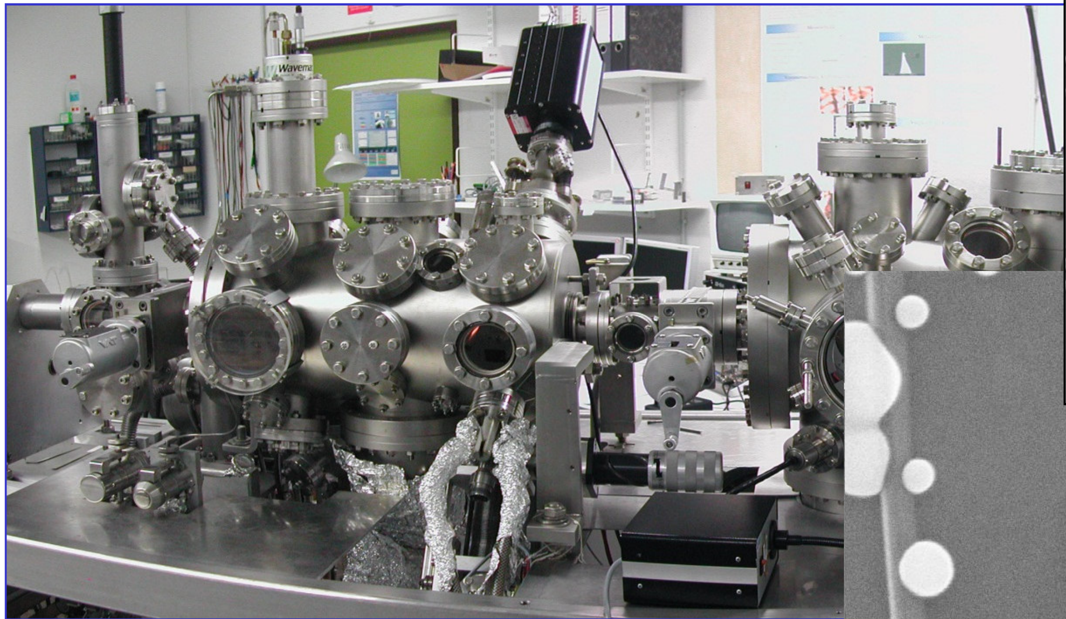
Gold Nanoparticles: Scaling depends on shape and orientation ($0<\gamma<0.5$)

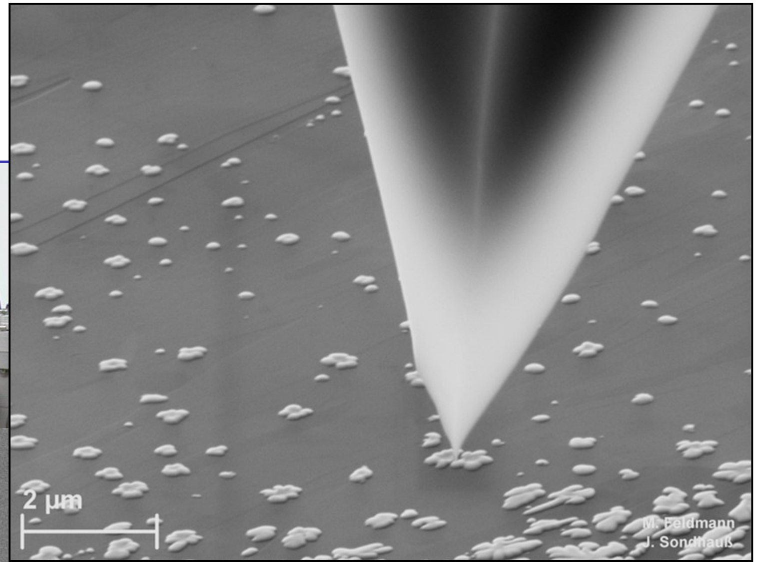
Antimony Nanoparticles: Scaling independent of shape and orientation ($\gamma=0.5$)

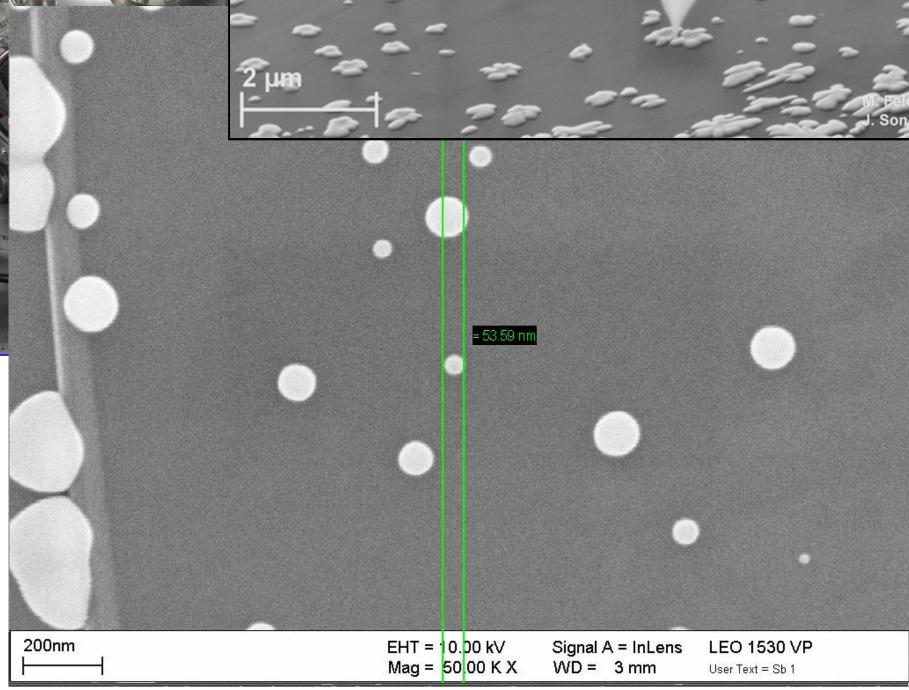
Dietzel et al., Phys. Rev. Lett. 111, 235502 (2013), Supplemental Material

Metallic Antimony nanoscale islands by sublimation

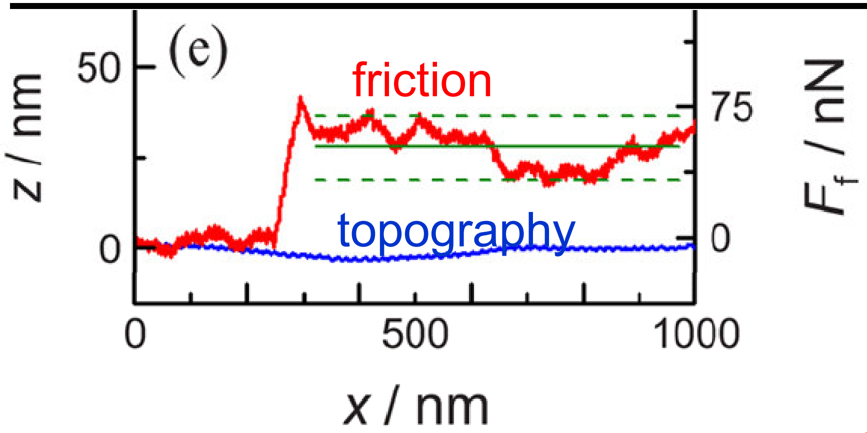
Omicron room temperature
AFM in UHV

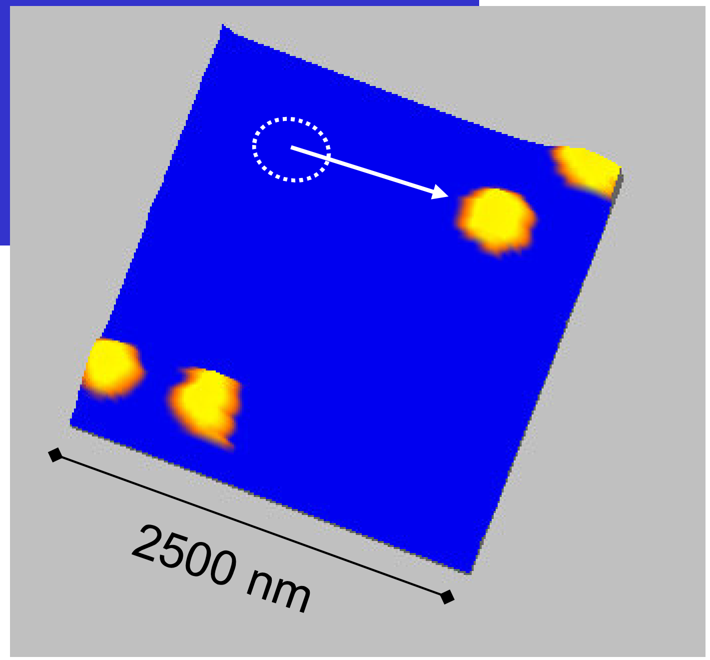






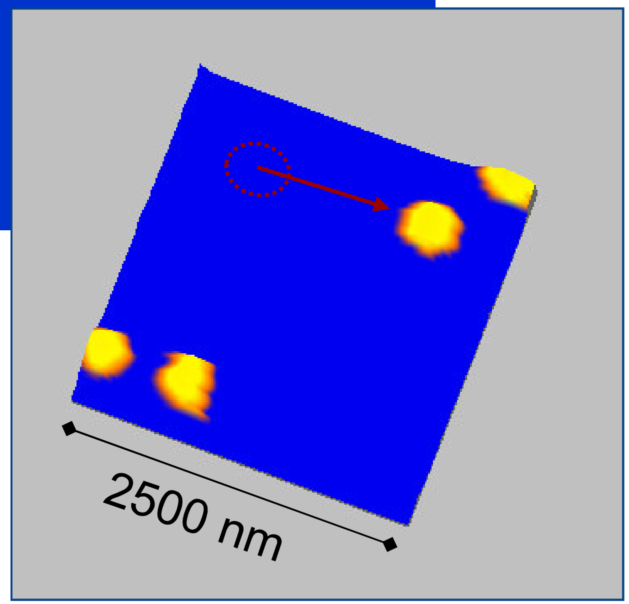
Moving Nanoparticles by Atomic Force Microscopy





Dietzel, Mönninghoff, Jansen, Fuchs, Ritter,
Schwarz, Schirmeisen, JAP 102 (2007) 084306

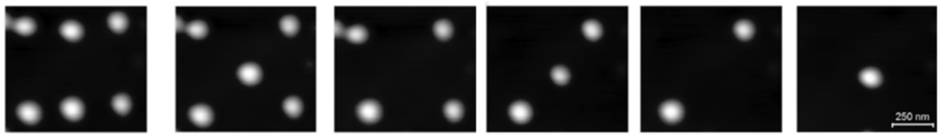
Moving Nanoparticles by Atomic Force Microscopy



D. Dietzel et al., J. Appl. Phys. 102, 084306 (2007)

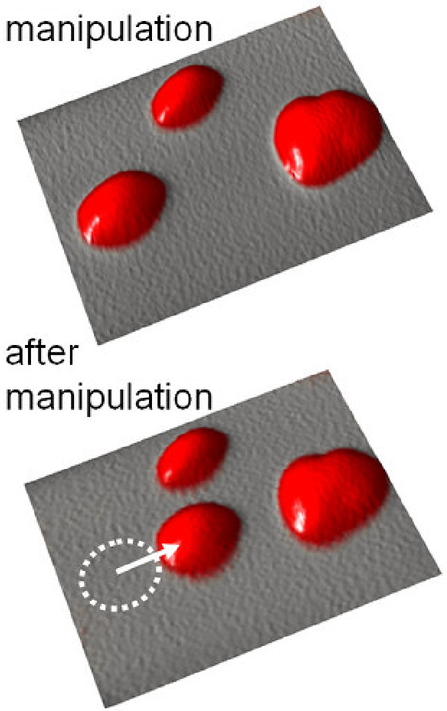
Full Control over particle positioning!

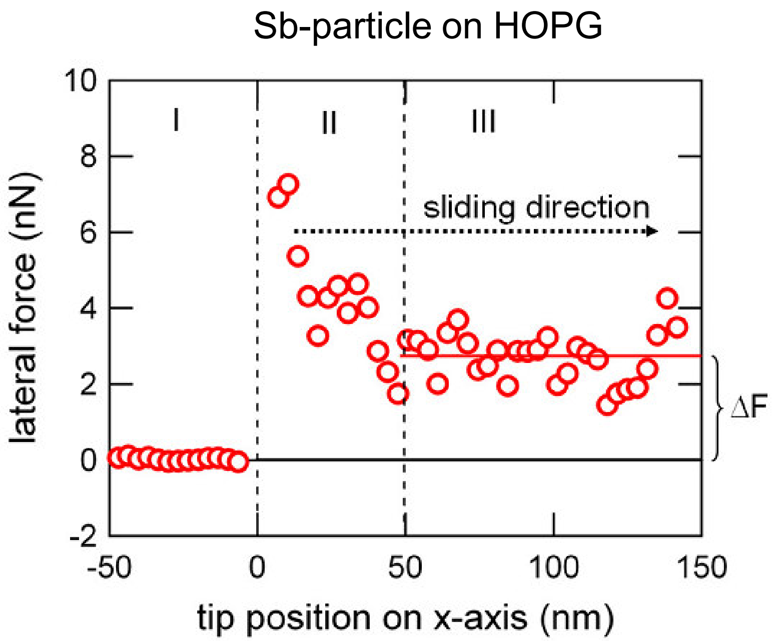
(Precision ≈ 30nm)



D. Dietzel et. al, Tribology Letters 39, 273-281 (2010)

Measuring Friction by Manipulation of Nanoparticles





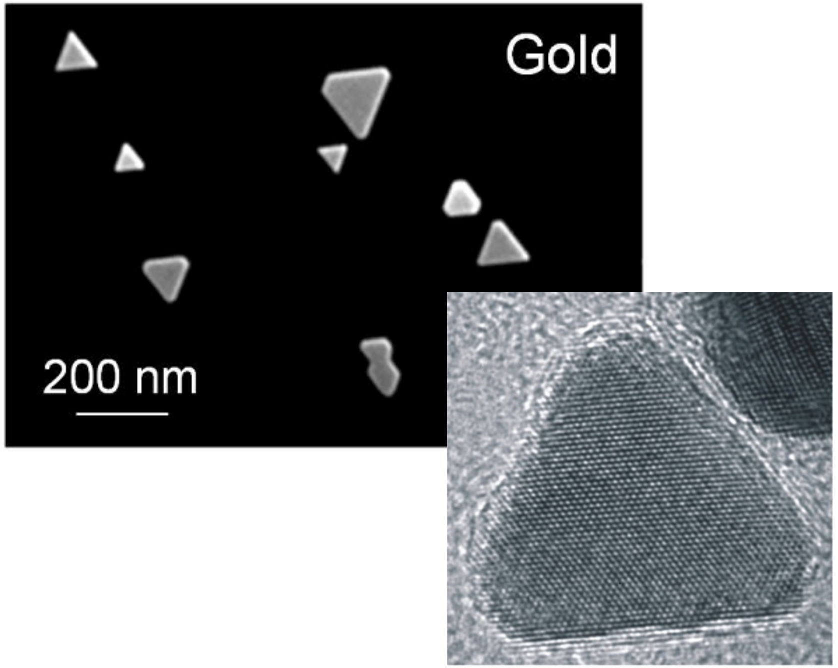
Manipulation by tip pushing from side:

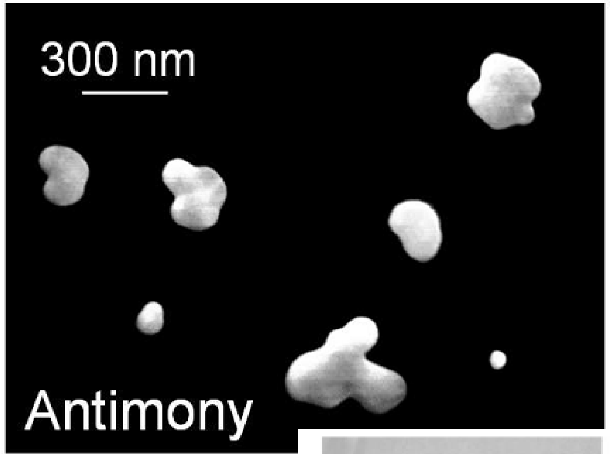
⇨ Quantitativ friction can be extracted from manipulation

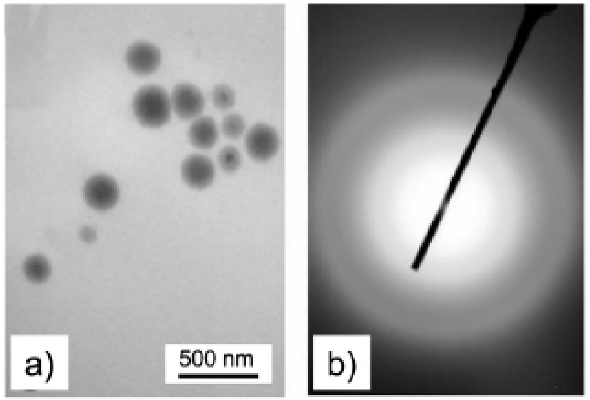
⇨ Fast manipulation of statistically significant number of particles of different size

D. Dietzel et al., J. Appl. Phys. 102, 084306 (2007)
D. Dietzel et al., Phys. Rev. Lett. 101, 125505 (2008)

Metallic Nanoscale Islands by Sublimation







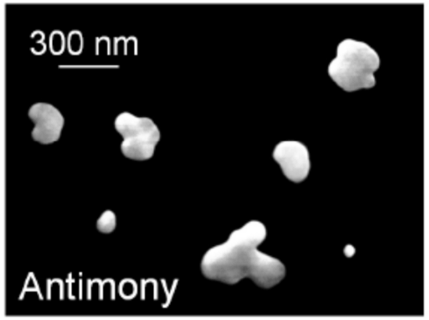
Preparation of metallic nanoparticles by thermal evaporation of Sb and Au under **UHV (ultrahigh vacuum)** conditions

- Substrate: HOPG
- Antimony nanoparticles ⇨ amorphous
- Gold Nanoparticles ⇨ crystalline

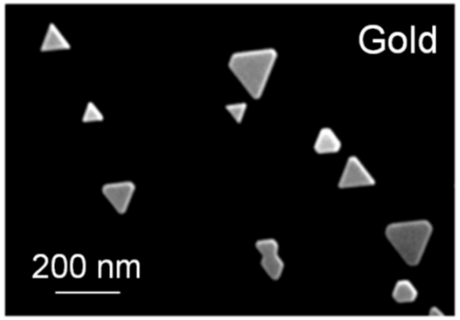
Characterization Sb-particles: B. Stegemann et al., J. Phys. Chem. B 108, 14292 (2004), D. Dietzel et al., Phys. Rev. B 82, 035401 (2010)

Contact Area Dependence of Nanoparticle Friction

amorphous
antimony

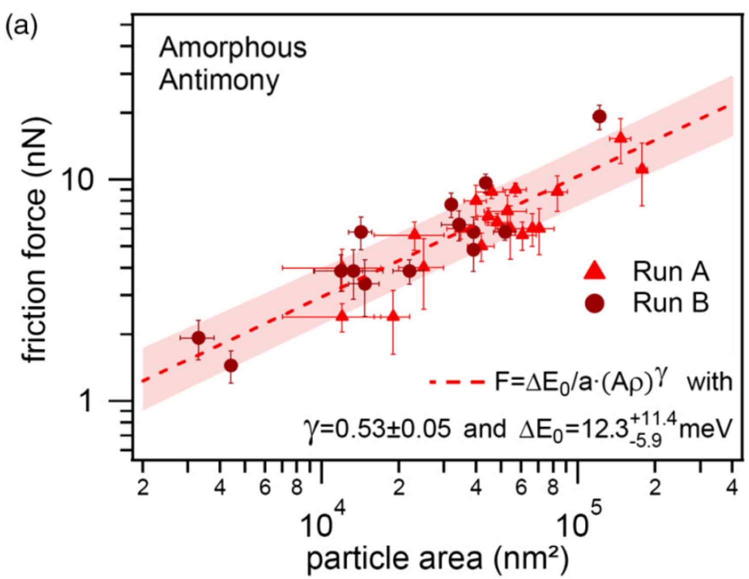


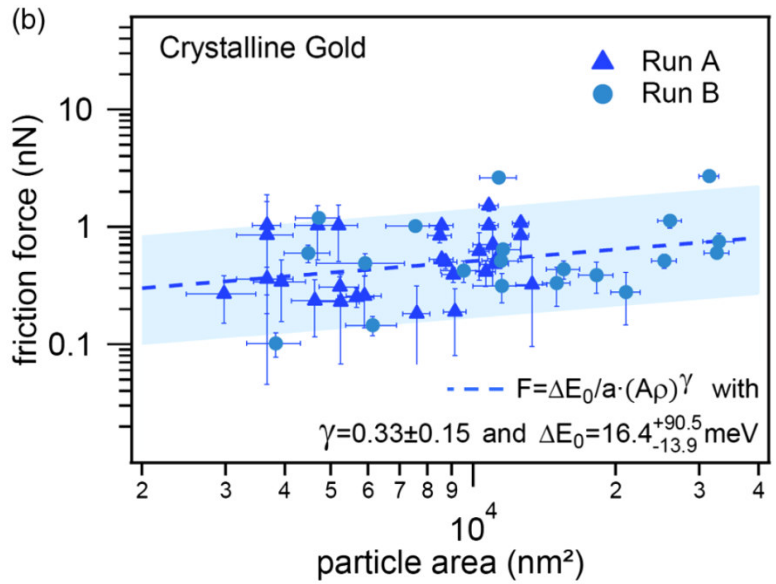
crystalline
Gold



$F \sim A^{0.53}$

$F \sim A^{0.33}$





Sublinear friction vs. area scaling
is experimentally confirmed!

Dietzel et al., Phys. Rev. Lett. 111, 235502 (2013)

Atomic Diffusion Energy: Upscaling to Nanoparticle Friction

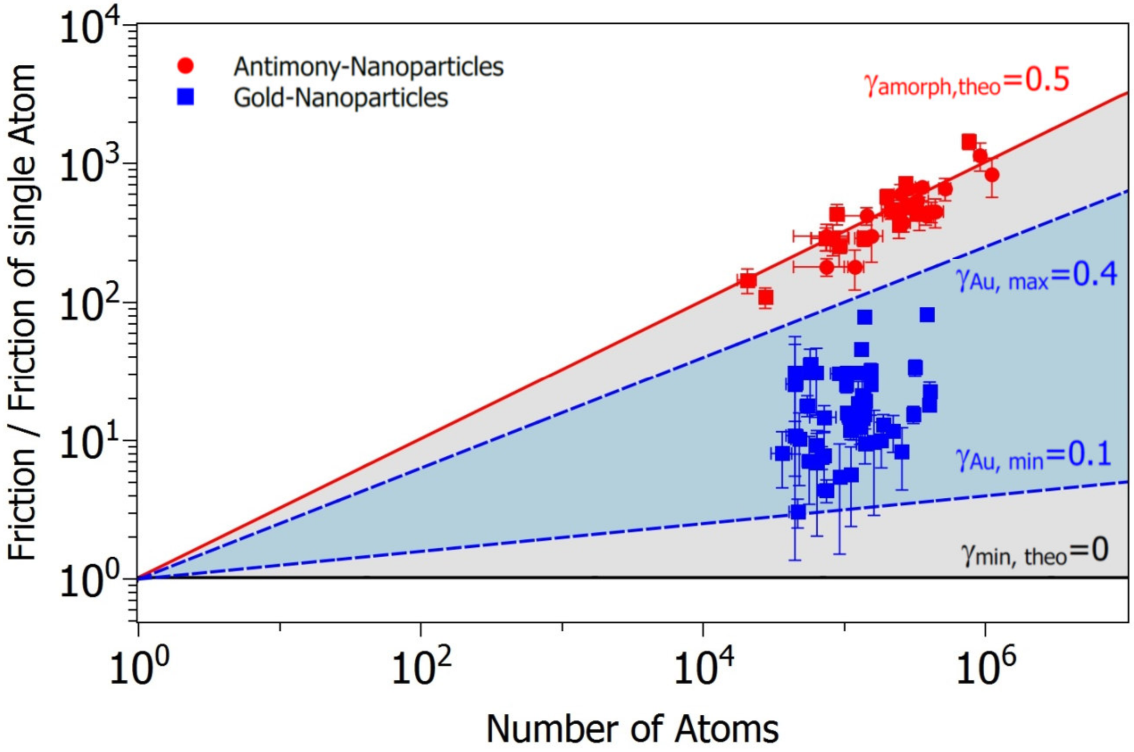
Simple model:
Diffusion energy barrier yields single atom friction:

$$F_{atom} = \frac{\Delta E}{a}$$

$$F_{particle} = \frac{\Delta E}{a} \cdot N^{\gamma}$$

normalize

$$F_{particle} / F_{atom} = N^{\gamma}$$



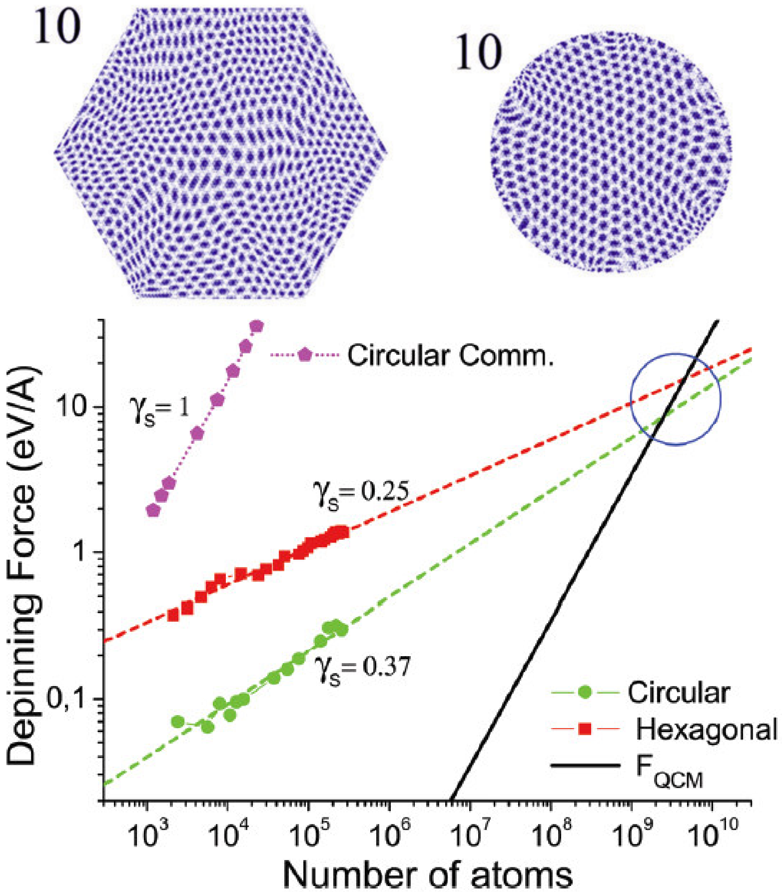
- Amorphous Sb particles: good agreement with theory (γ=0.5)
- Crystalline Au particles: No Uniform scaling due to variety of particle configurations
- Data can best be described by range of scaling (0.1<γ<0.4)
- No “perfect“ triangles => specific expectations for triangle γ=0 or γ=0.5 not met

Dietzel et al., Phys. Rev. Lett. 111, 235502 (2013)

Sub-linear Scaling: A Fingerprint of Superlubricity

Physisorbed islands - Simulation

Varini et al., Nanoscale, 7 (2015) 2093

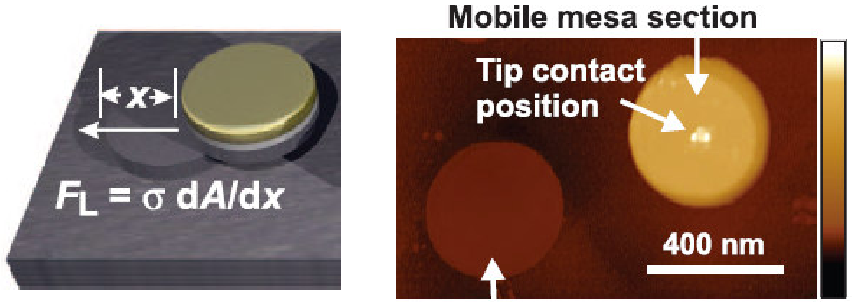


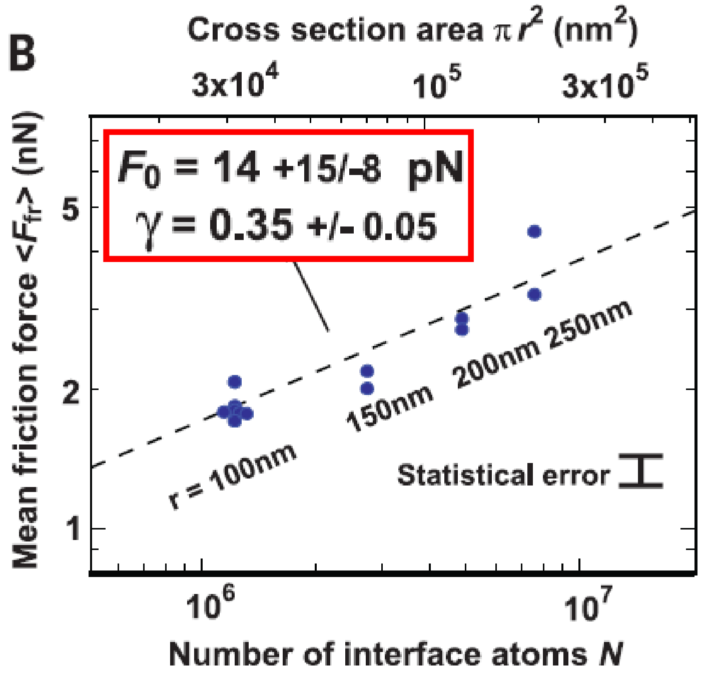
Again, incommensurate islands scale with

$$F \propto N_{atoms}^{\gamma} \qquad (\gamma < 0.5)$$

Graphite Interfaces - Experiments

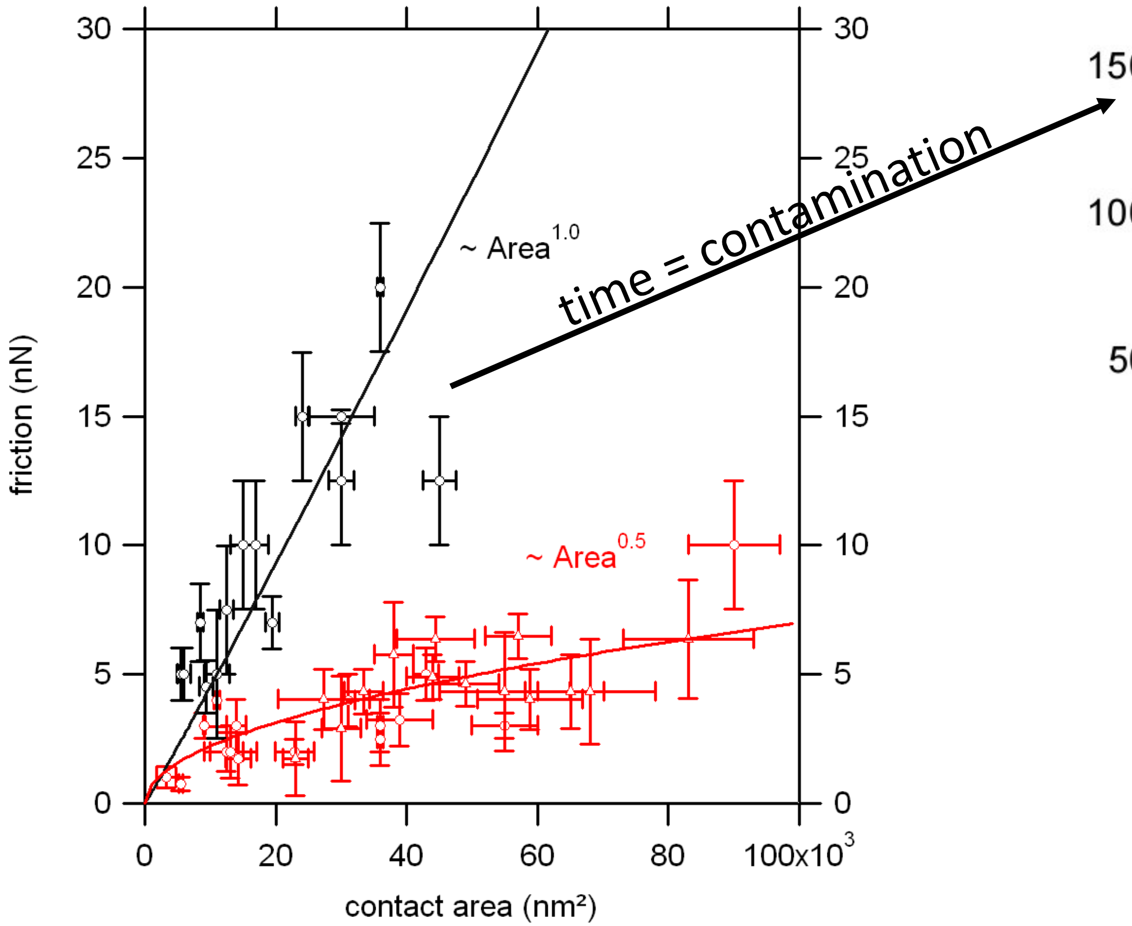
Koren et al., Science, 348 (2015) 679

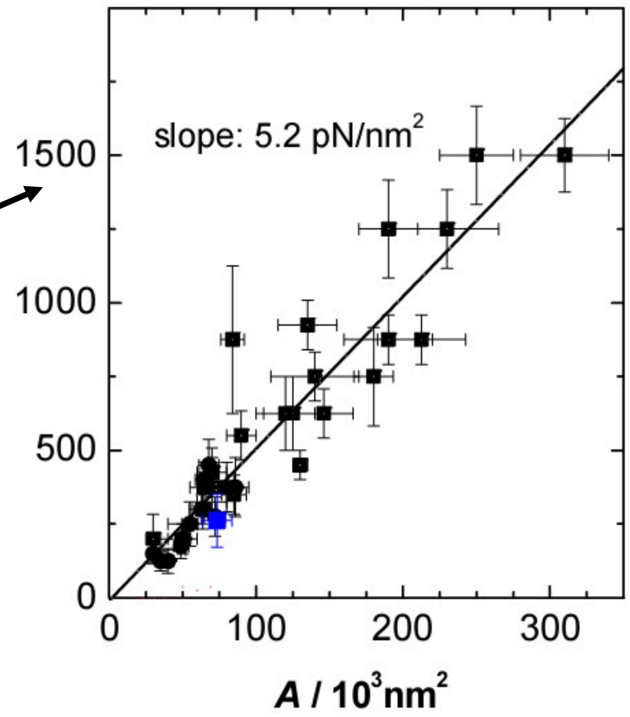




The Break-Down of Superlubricity: a) Interface Contamination

Antimony: Friction versus Area





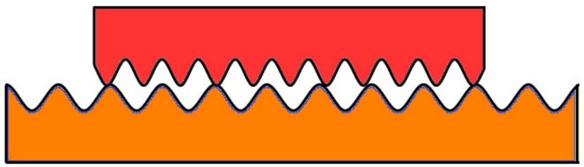
After weeks of storage in vacuum chamber

$F = \tau \cdot \text{area}$!

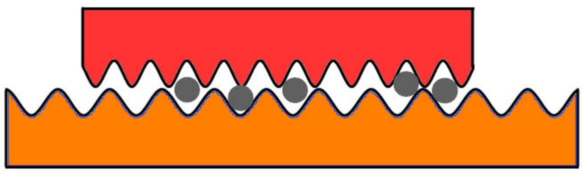
(almost exclusively)

D. Dietzel et al., Phys. Rev. Lett. 101, 125505 (2008)

MD Simulation: Friction and Contamination

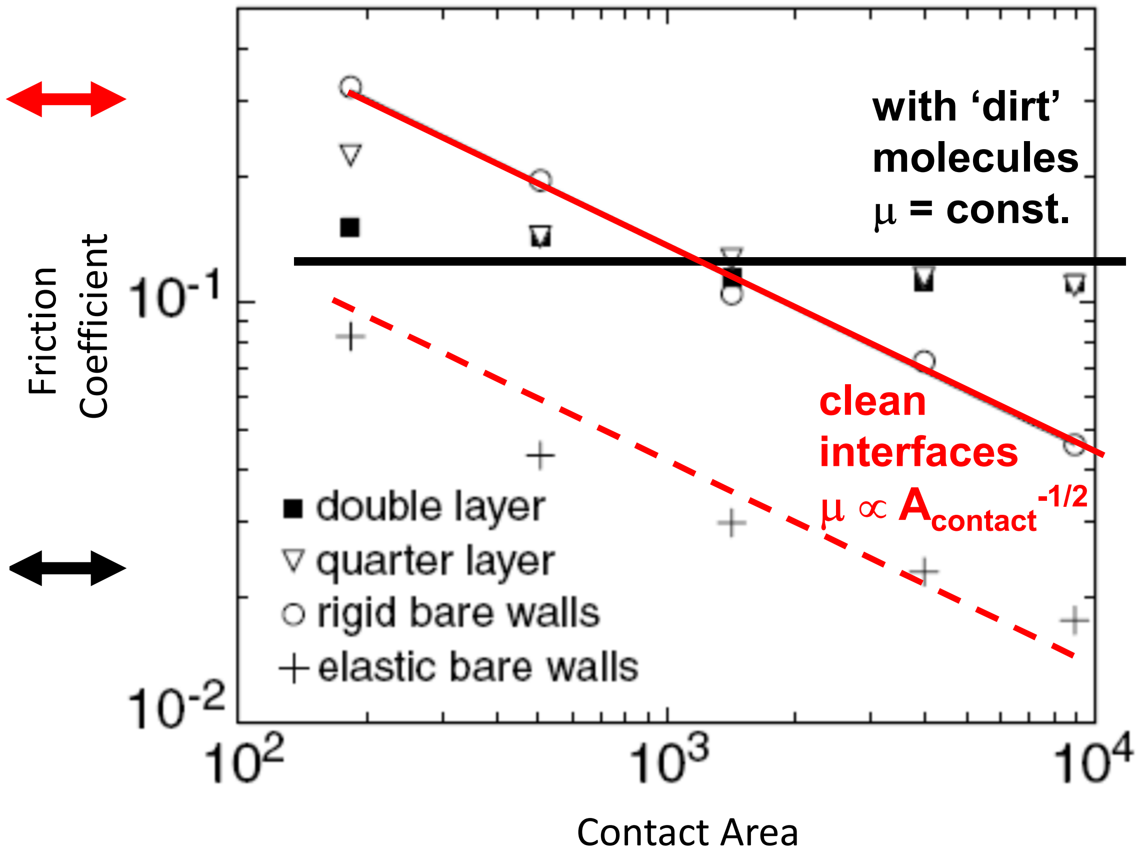


clean interface



contaminated interface

Friction coefficient versus contact area

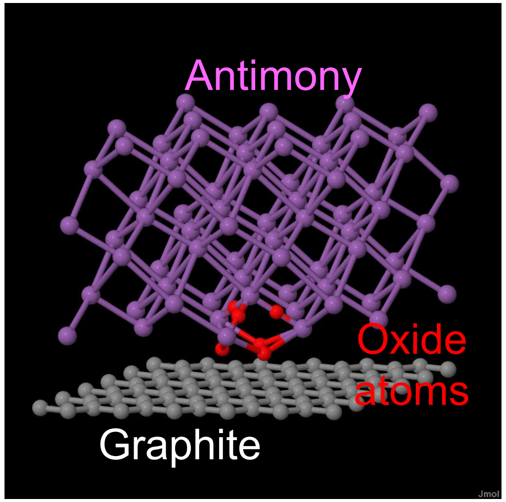


M. Müser et al., Phys. Rev. Lett. 86, 1295 (2001)

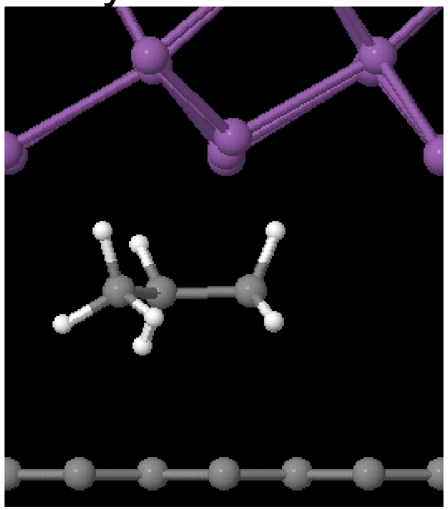
Mobile ‘dirt’ molecules mediate friction

Typical Interface Contaminations – Ab-Initio Simulations

Interface oxidation



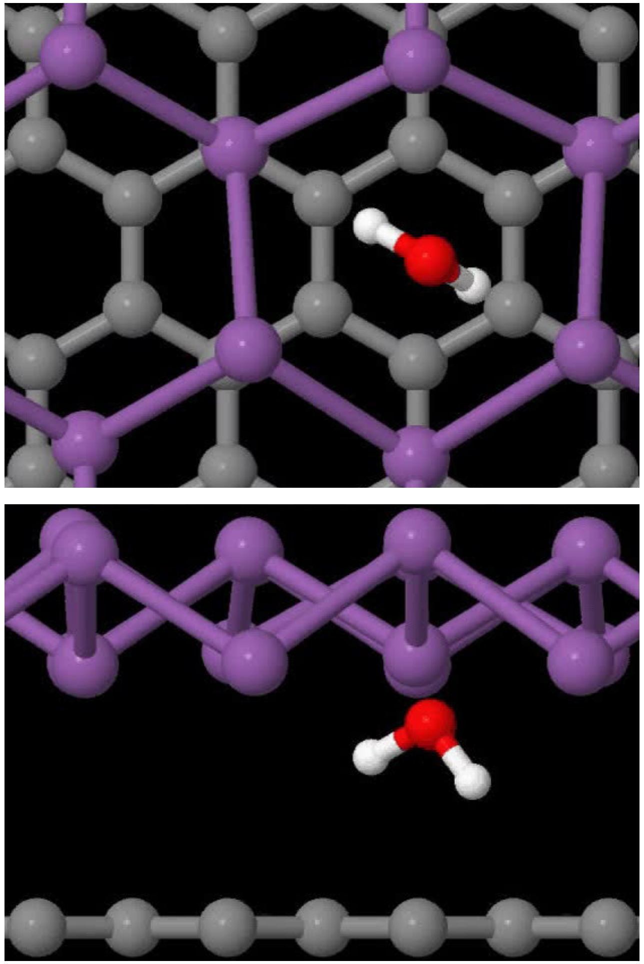
Hydrocarbons



Water molecules

Top view

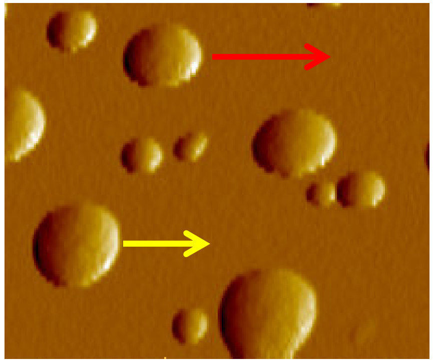
Side view

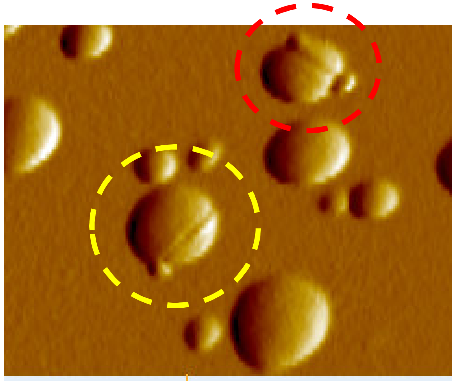


J. Brndiar, R. Turansky, D. Dietzel, A. Schirmeisen, I. Stich, Nanotechnology 22, 085704 (2011)

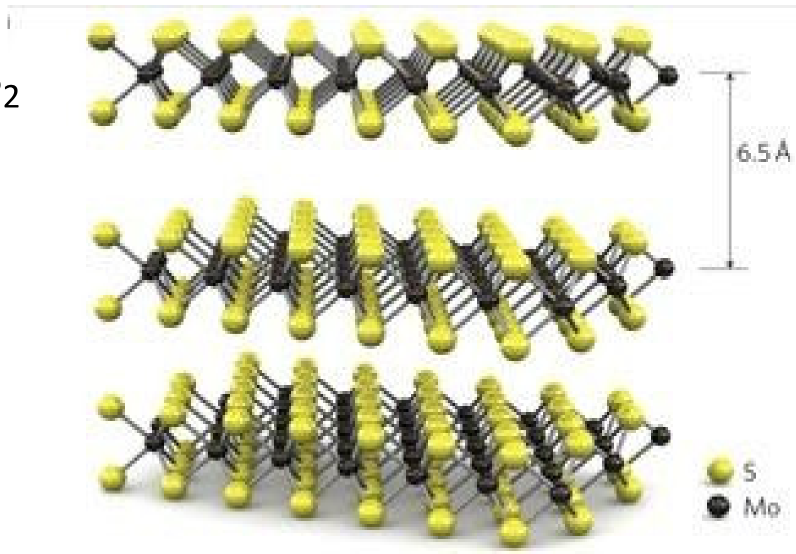
The Break-Down of Superlubricity: b) Relaxations/Dislocations

Nanomanipulation Experiments
Sb-particles on MoS_2





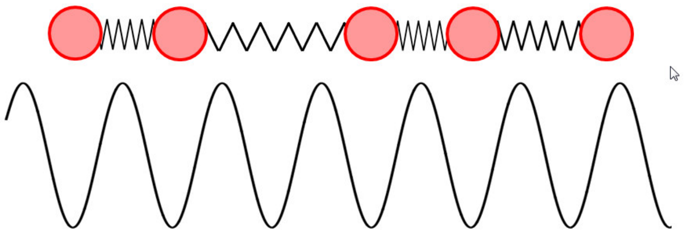
MoS_2



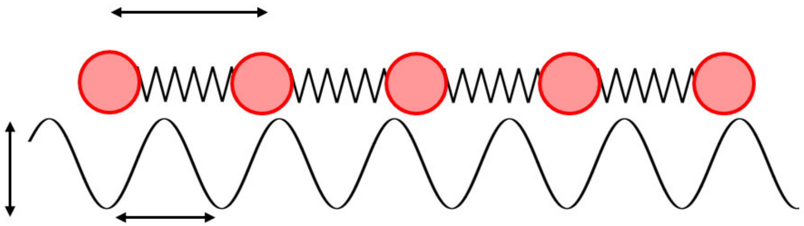
The Break-Down of Superlubricity: b) Relaxations/Dislocations

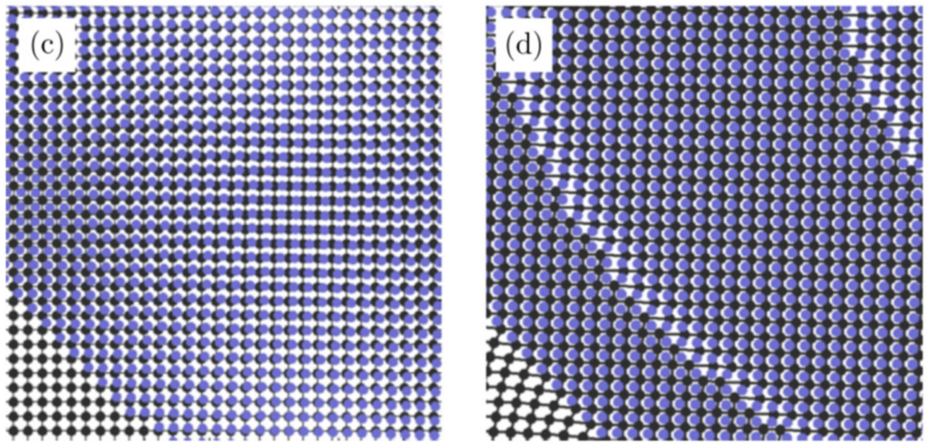
1D: Frenkel-Kontorova

interface energy τ_{max} large:
break-down of superlubricity



interface energy τ_{max} small:
superlubricity





For 3d islands: Transition from superlubric to ‚break-down' with dislocations, if island exceeds certain size limit b_{core}

$$b_{core}/d = G/\tau_{max}$$

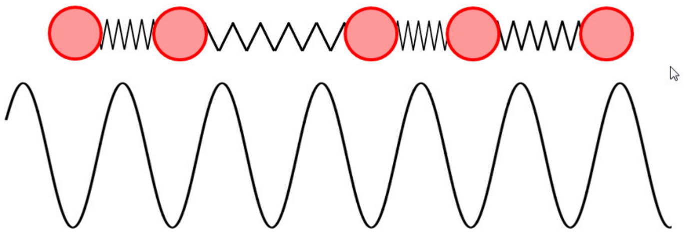
d: lattice constant; G: shear modulus; τ_{max}: maximum shear stress

Sharp, Pastewka, Robbins, PRB 93 (2016) 121402R

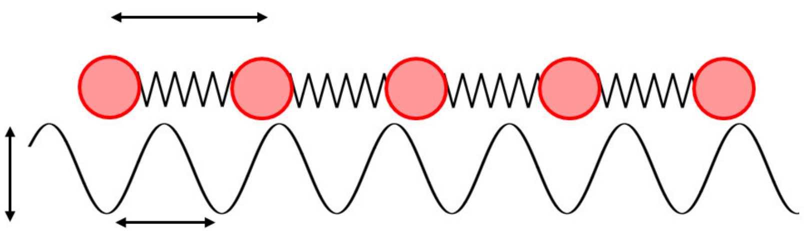
The Break-Down of Superlubricity: b) Relaxations/Dislocations

1D: Frenkel-Kontorova

interface energy τ_{max} large:
break-down of superlubricity

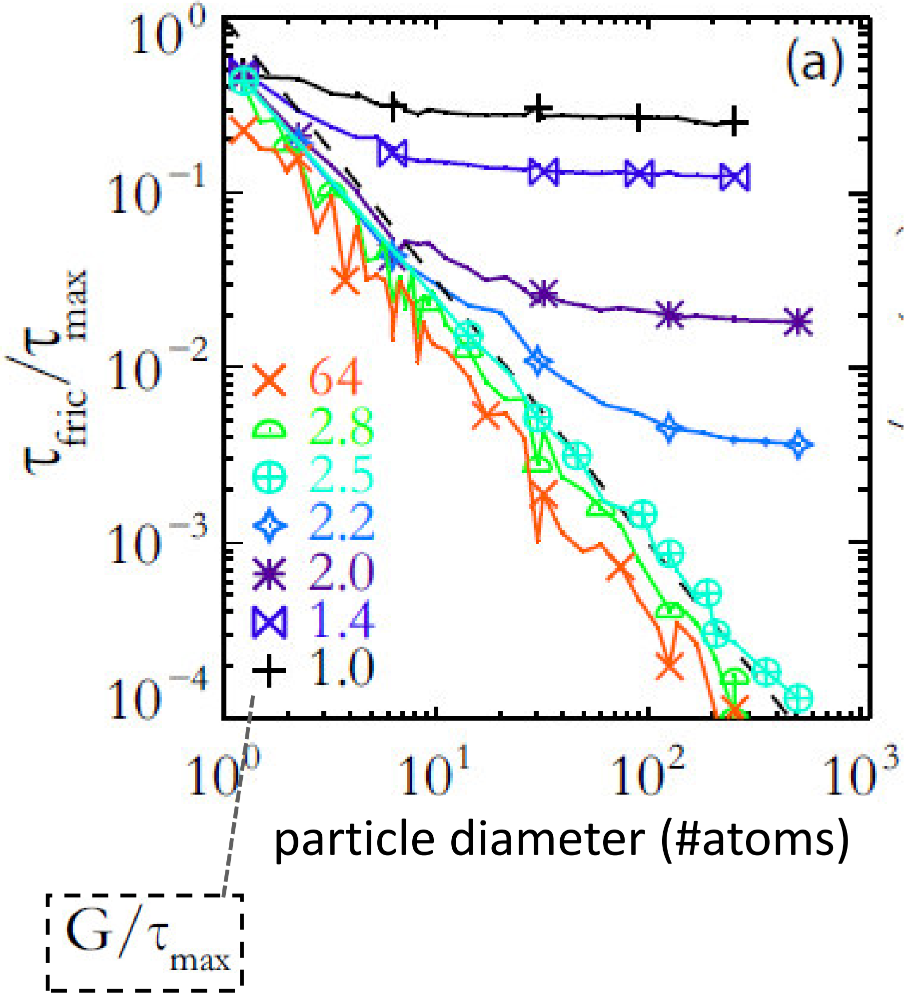


interface energy τ_{max} small:
superlubricity



2D: Peierls-Nabarro Transition

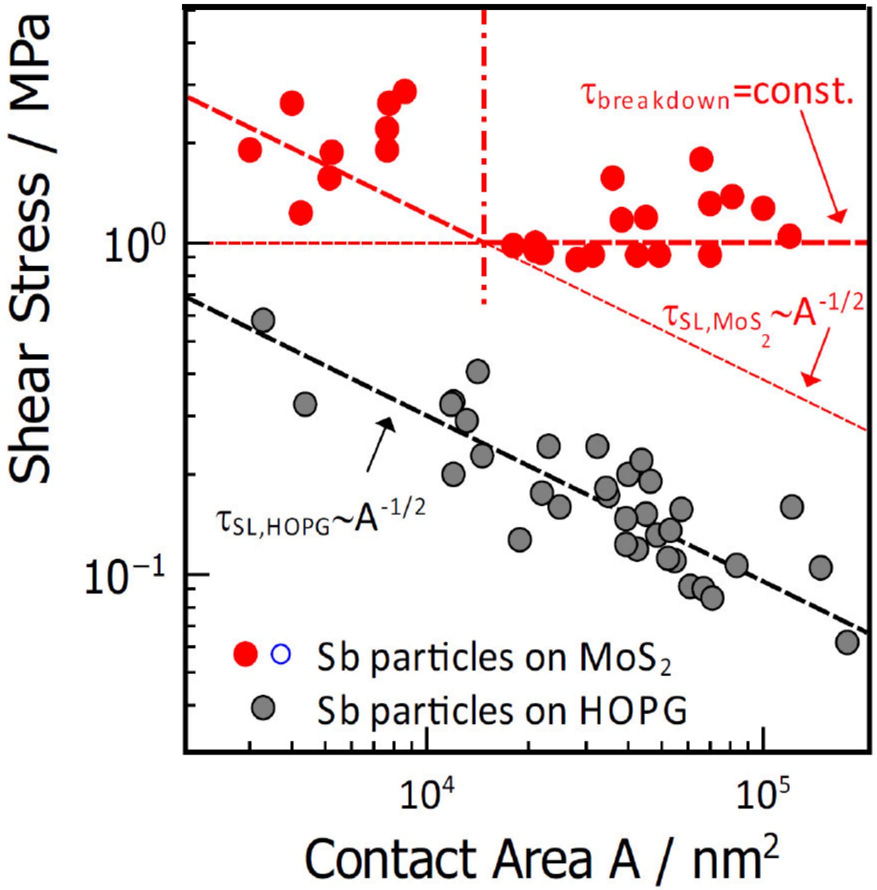
3d atomistic simulation: Friction per atom



Sharp, Pastewka, Robbins, PRB 93 (2016) 121402R

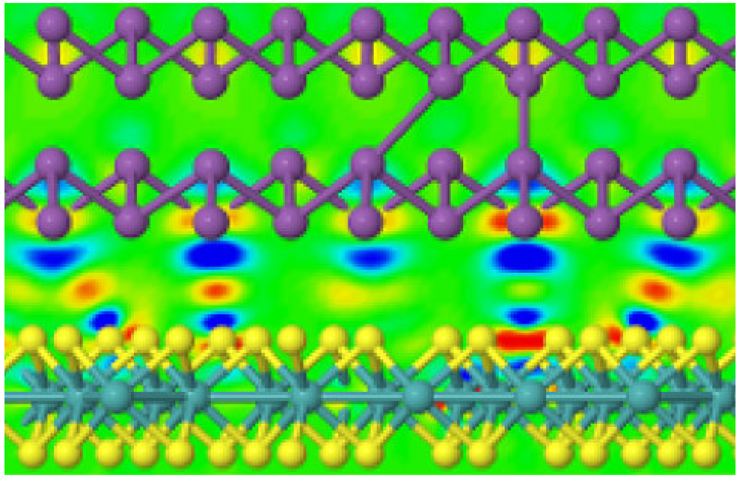
The Break-Down of Superlubricity: b) Relaxations/Dislocations

Expt.: Friction of particles: MoS_2 vs HOPG

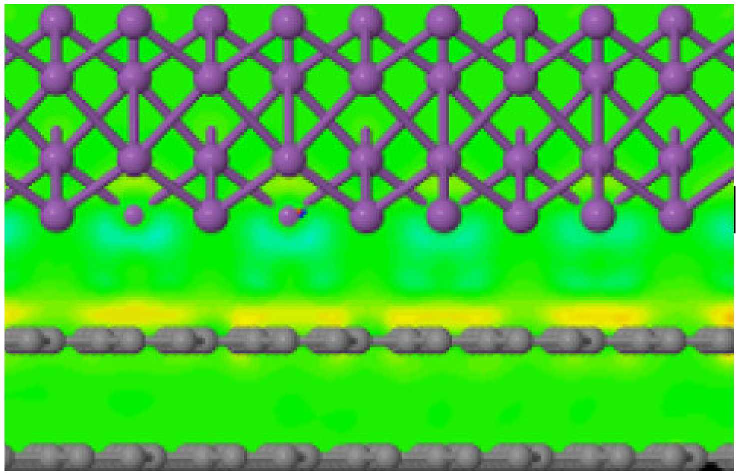


Dietzel, Brndiar, Stich, Schirmeisen, ACS Nano 11 (2017) 7642

Sb on MoS_2



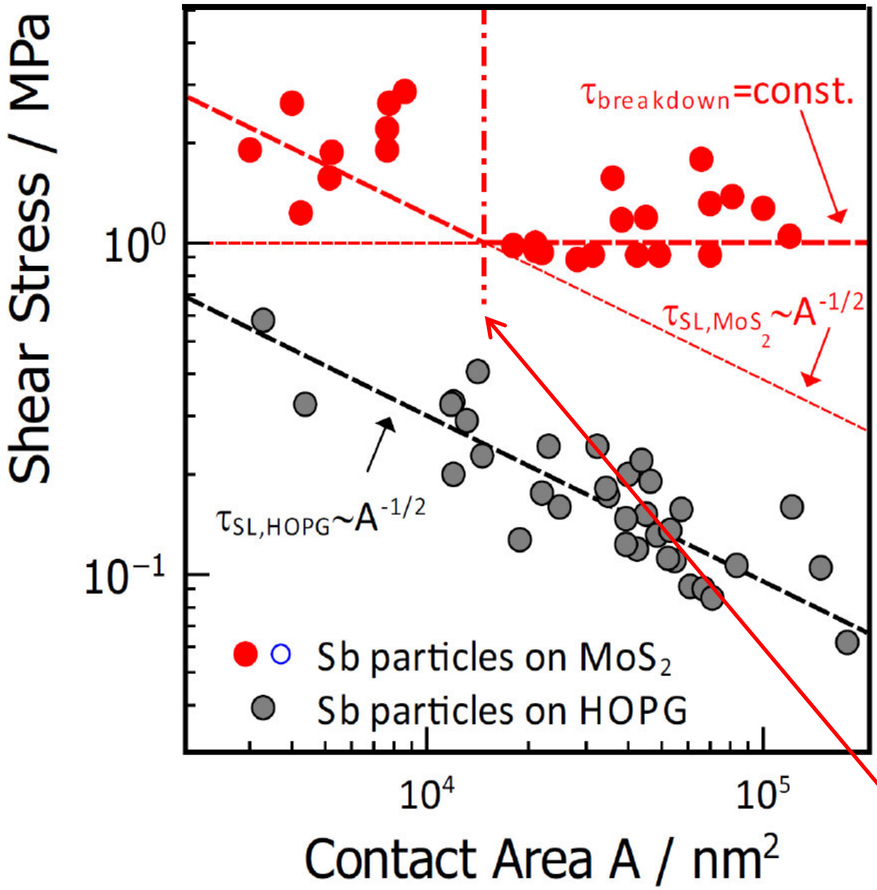
Sb on HOPG



Ab initio simulations: I. Stich, J. Brndiar

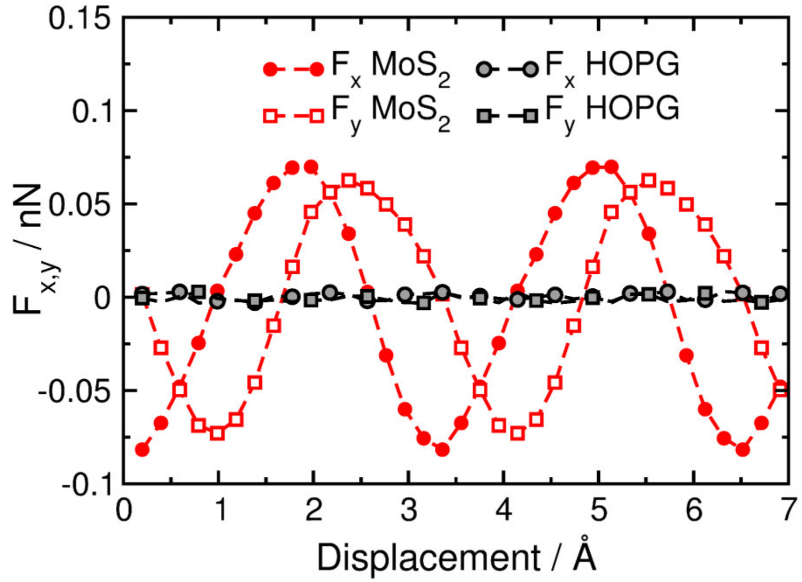
The Break-Down of Superlubricity: b) Relaxations/Dislocations

Expt.: Friction of particles: MoS_2 vs HOPG



Dietzel, Brndiar, Stich, Schirmeisen, ACS Nano 11 (2017) 7642

Force acting on Sb atom during sliding



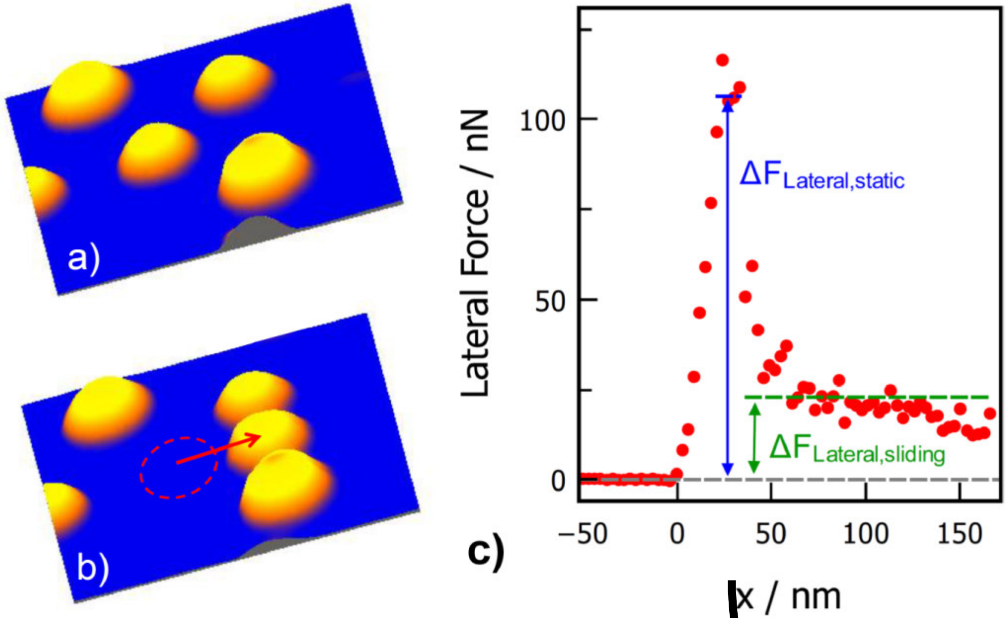
using $b_{core}/d = G/\tau_{max}$

(with τ_{max} = 290 MPa, G = 20 GPa)

⇨ $b_{core} = 30$ nm

Experiment: $r_{critical}$ = 50 – 80 nm

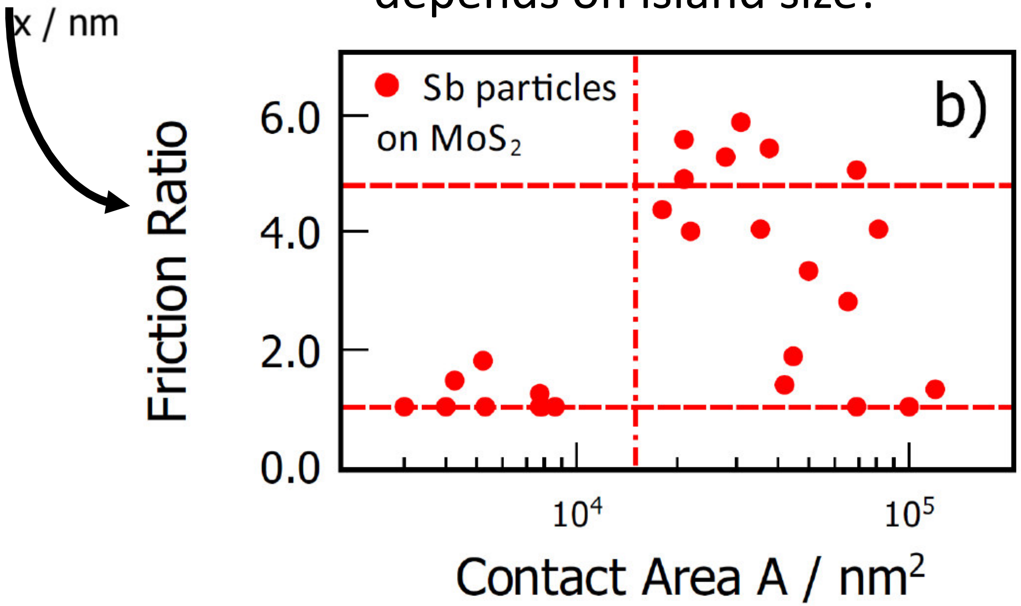
The Break-Down of Superlubricity: b) Relaxations/Dislocations



Experiments:

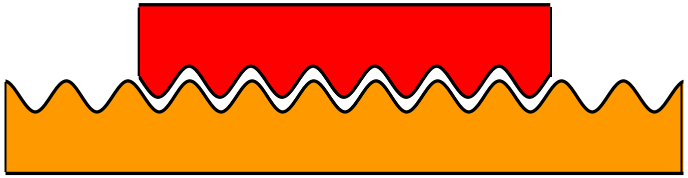
Sb islands on MoS_2 in UHV

Static/sliding friction ratio depends on island size!

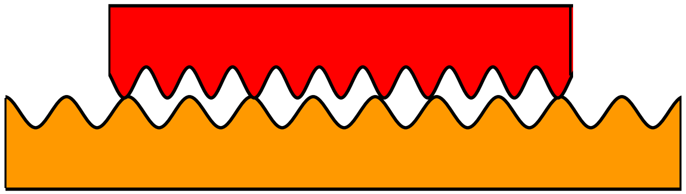


Dietzel, Brndiar, Stich, Schirmeisen, ACS Nano 11 (2017) 7642

Structural Superlubricity - Categorization



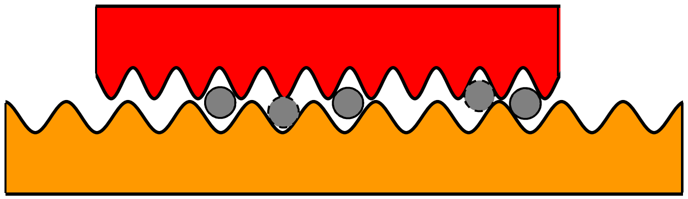
Interlocking of atomic potentials
friction $\propto$ area



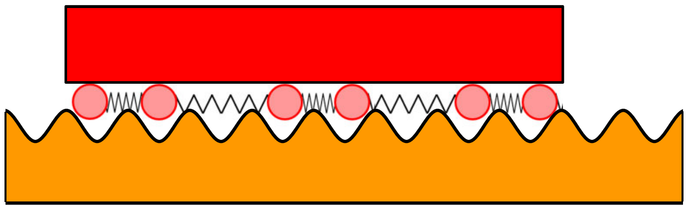
No interlocking of atomic potentials: Low friction "Superlubricity"

$$F = \Delta E / a(A\rho)^{\gamma}$$

with $\gamma \leq 0.5$



Mobile molecule mediated interlocking of atomic potentials
friction $\propto$ area



Critical size threshold for interface dislocations
friction $\propto$ area

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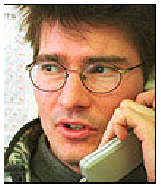
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