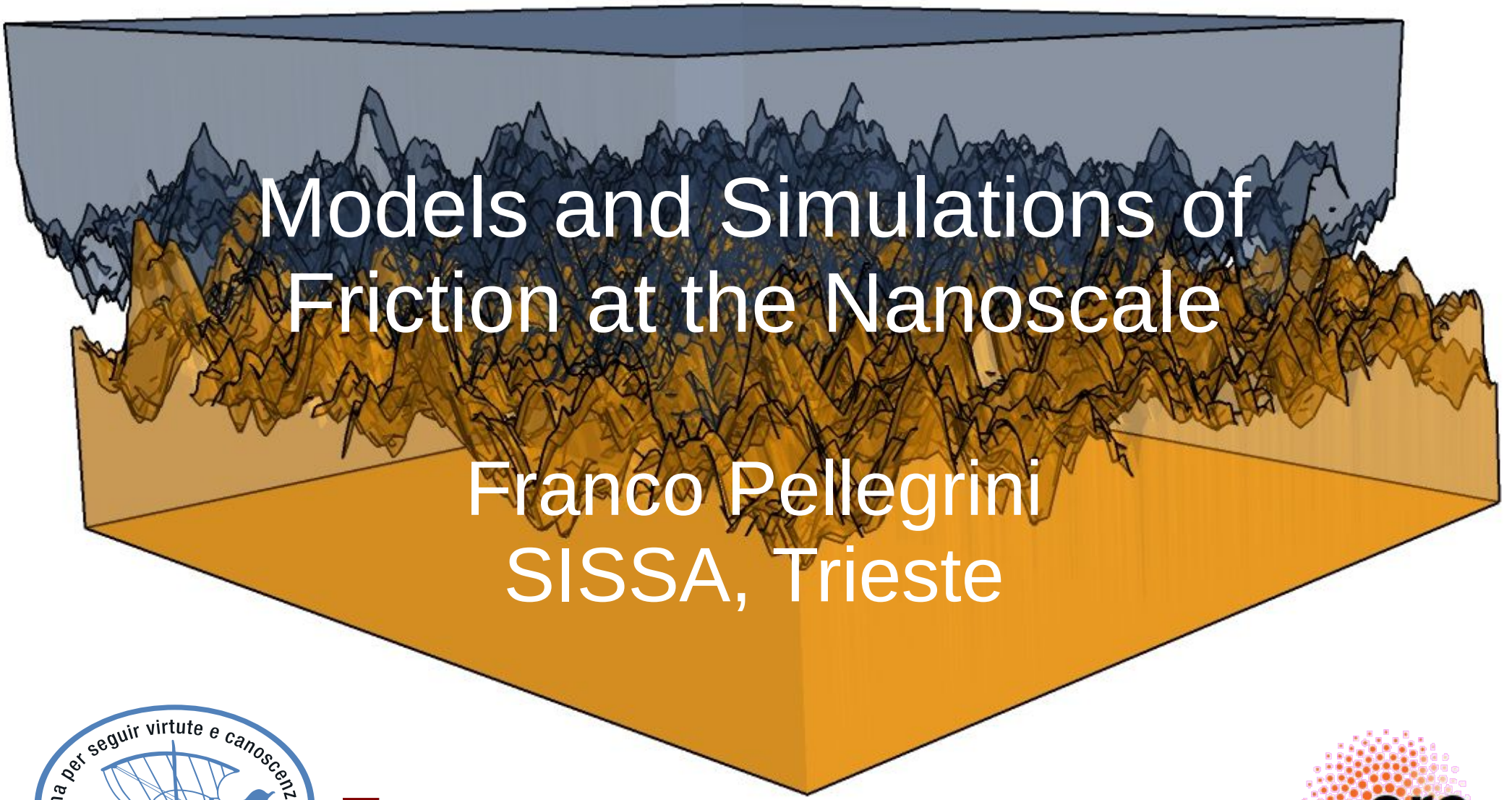


Models and Simulations of Friction at the Nanoscale

Franco Pellegrini
SISSA, Trieste

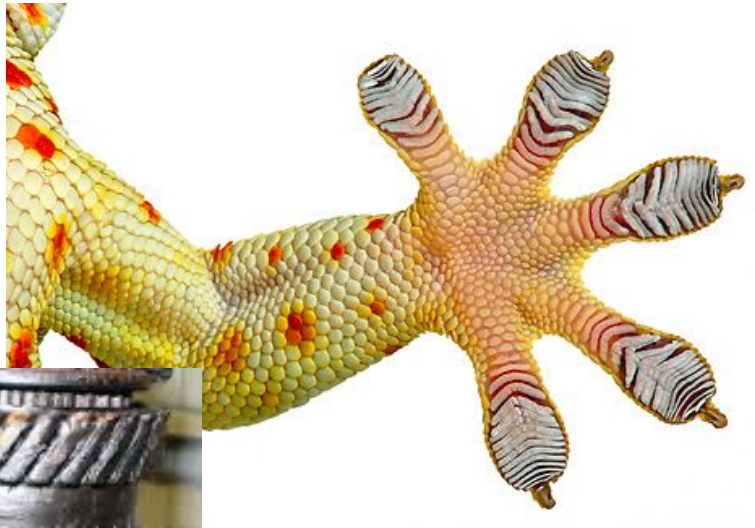
ma per seguir virtute e canoscenza
SISSA

iom
Istituto Officina dei Materiali

erc

Why Friction?

Friction: “Force resisting the relative motion of surfaces in contact”



Friction in physics 101

Static friction:

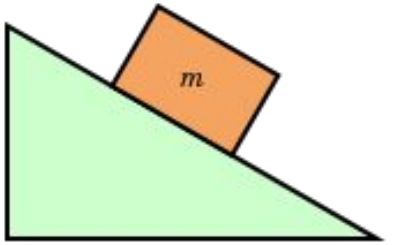
$$F_{max} = \mu_s N$$

Kinetic friction:

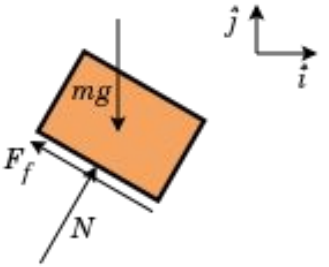
$$F = \mu_k N$$

Drag? F~v, F~v²

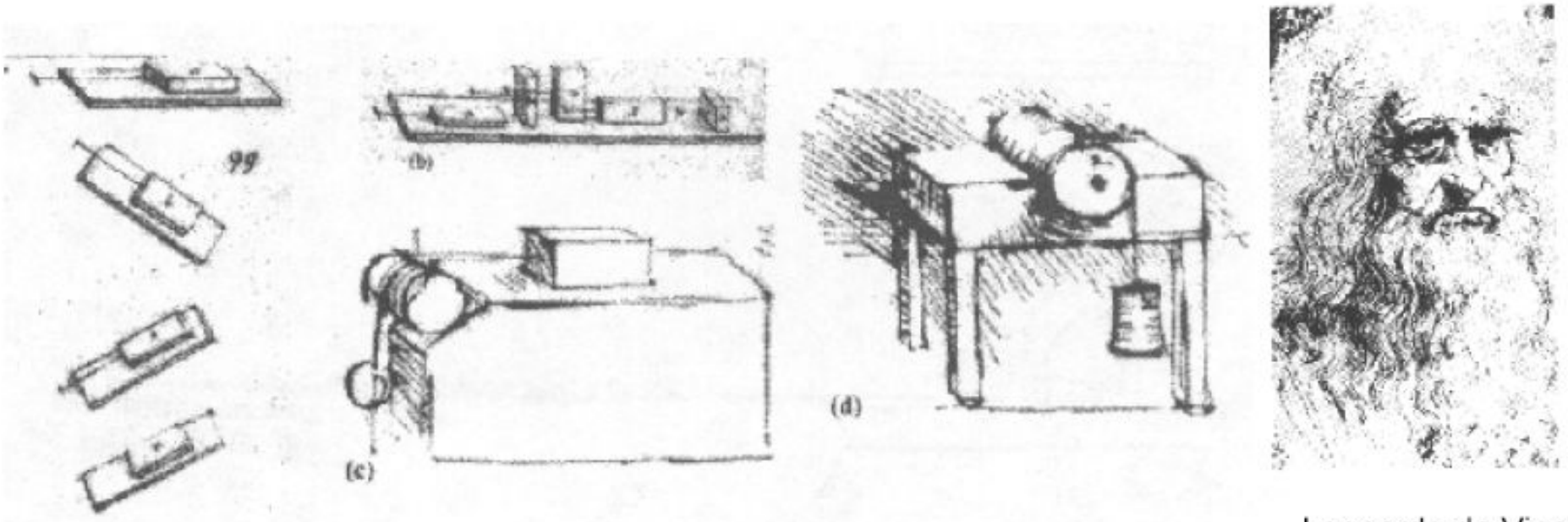
A block on a ramp



Free body diagram of just the block



History of tribology



Leonardo da Vinci
(1452-1519)

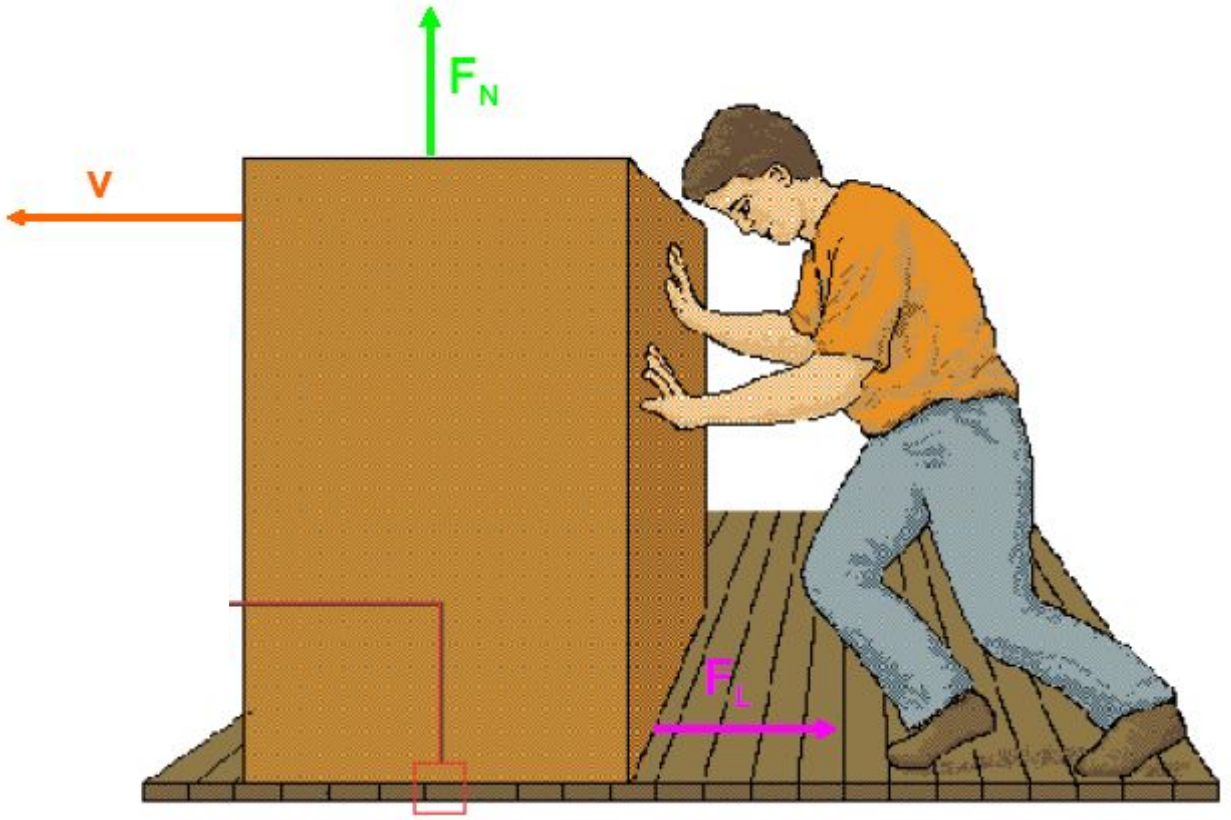
History of tribology

Amonton (1699):
- The force of friction is directly proportional to the applied load
- The force of friction is independent of the apparent area of contact

Coulomb (1785):
- Kinetic friction is independent of the sliding velocity

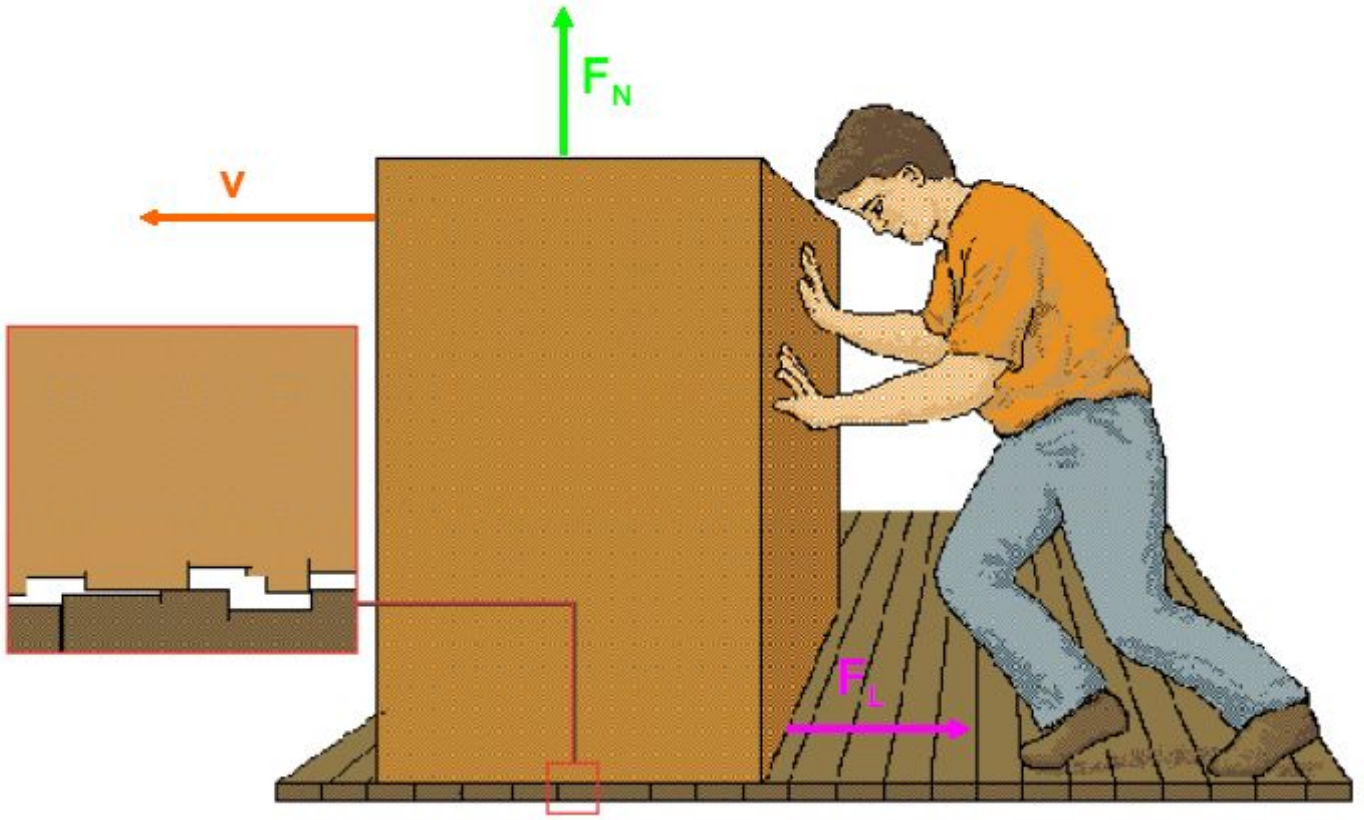
Microscopic theory

What is the area of contact?



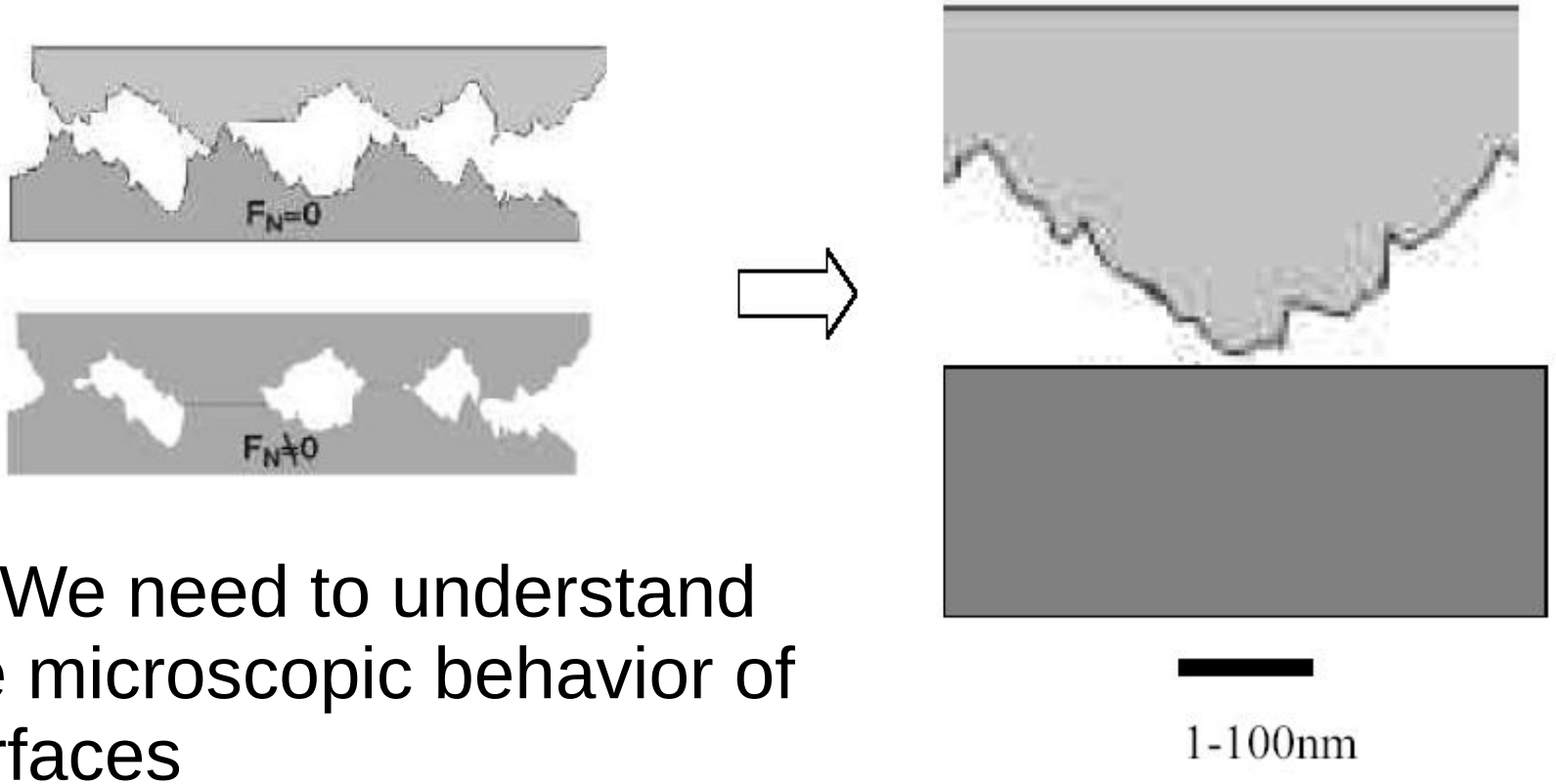
Microscopic theory

What is the area of contact?



Microscopic theory

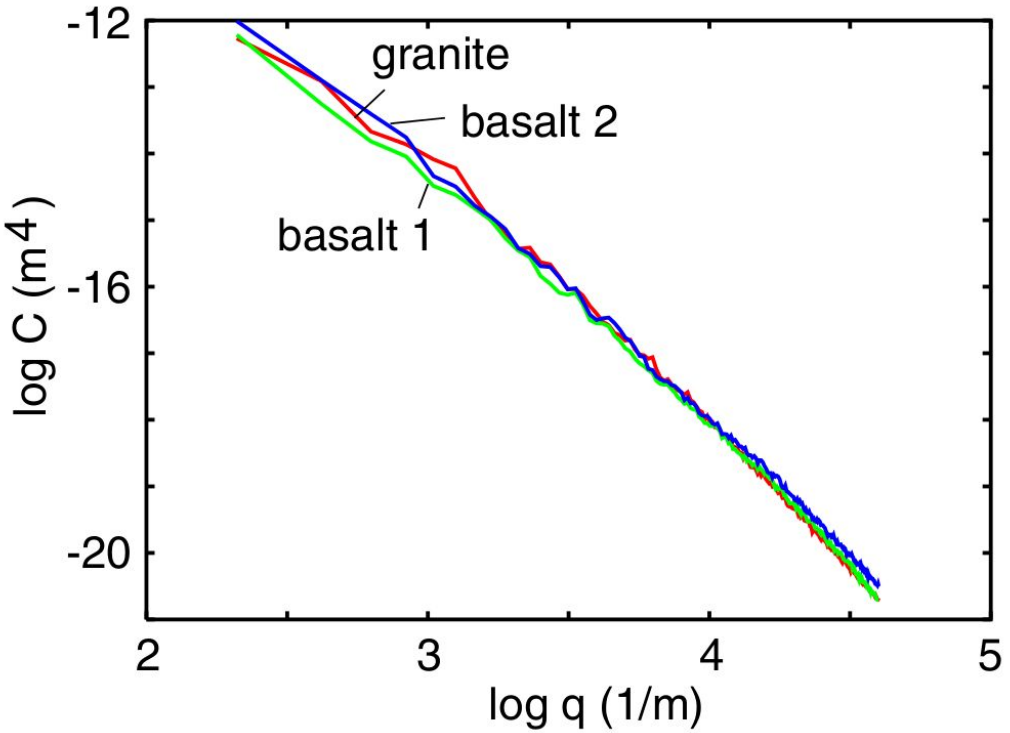
Bowden-Tabor (1950):
Friction **is** proportional to the **real** area of contact.
But area of contact is (mostly) proportional to load.

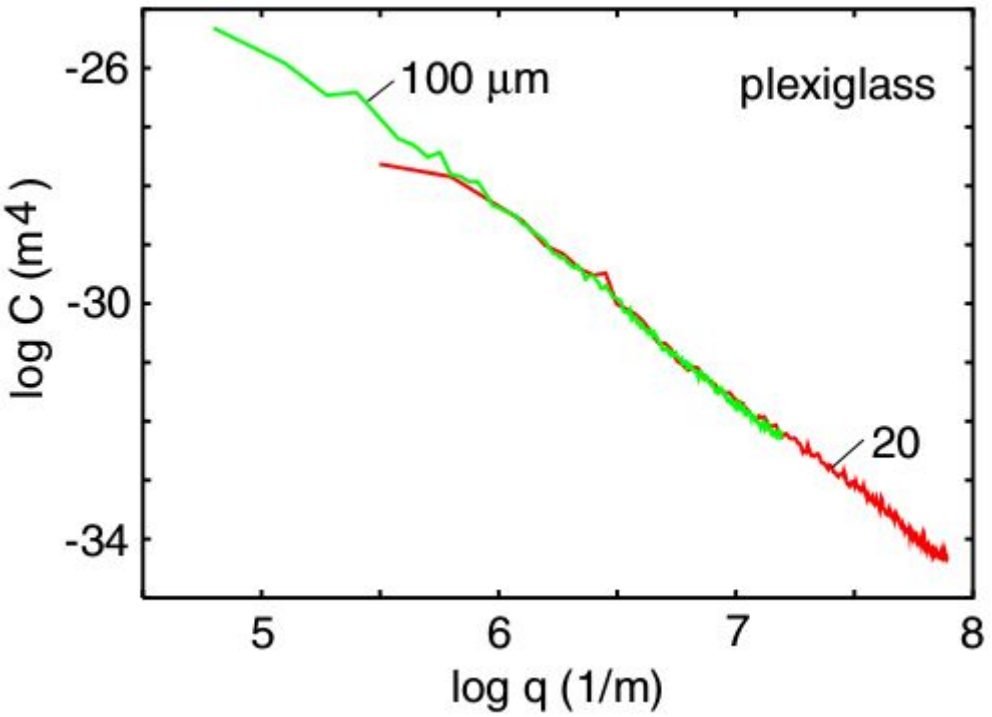


→ We need to understand the microscopic behavior of surfaces

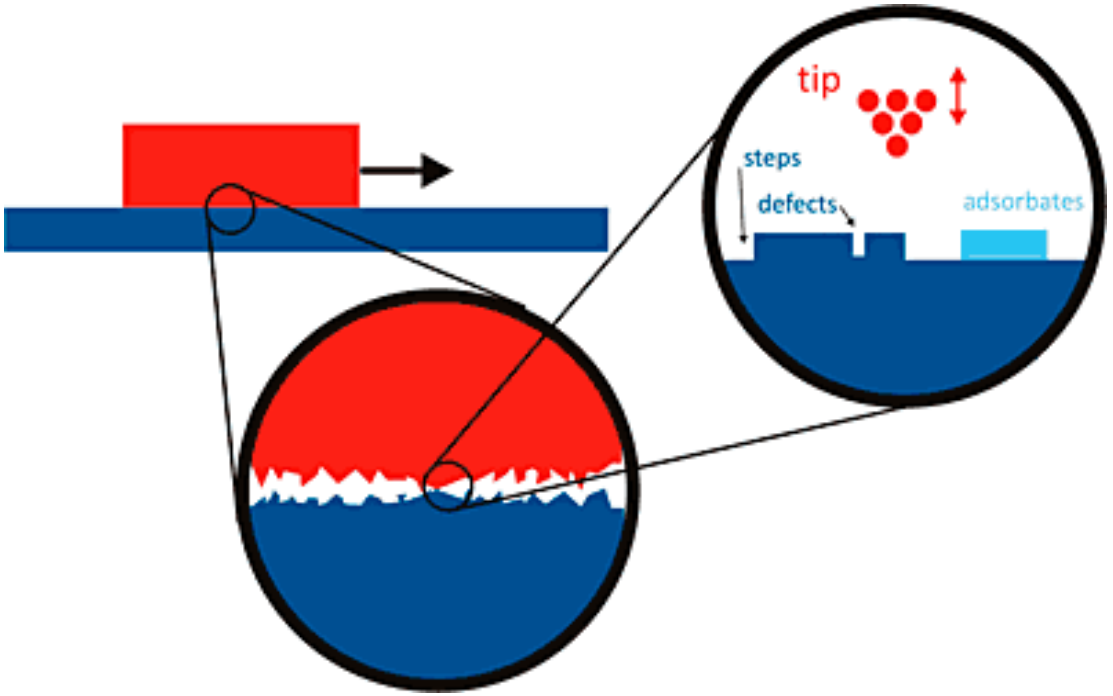
Surface roughness

Roughness power spectrum $C(q) = \frac{1}{(2\pi)^2} \int \mathrm{d}^2x \, \langle h(x)h(\mathbf{0})\rangle \mathrm{e}^{-\mathrm{i}q\cdot x}$

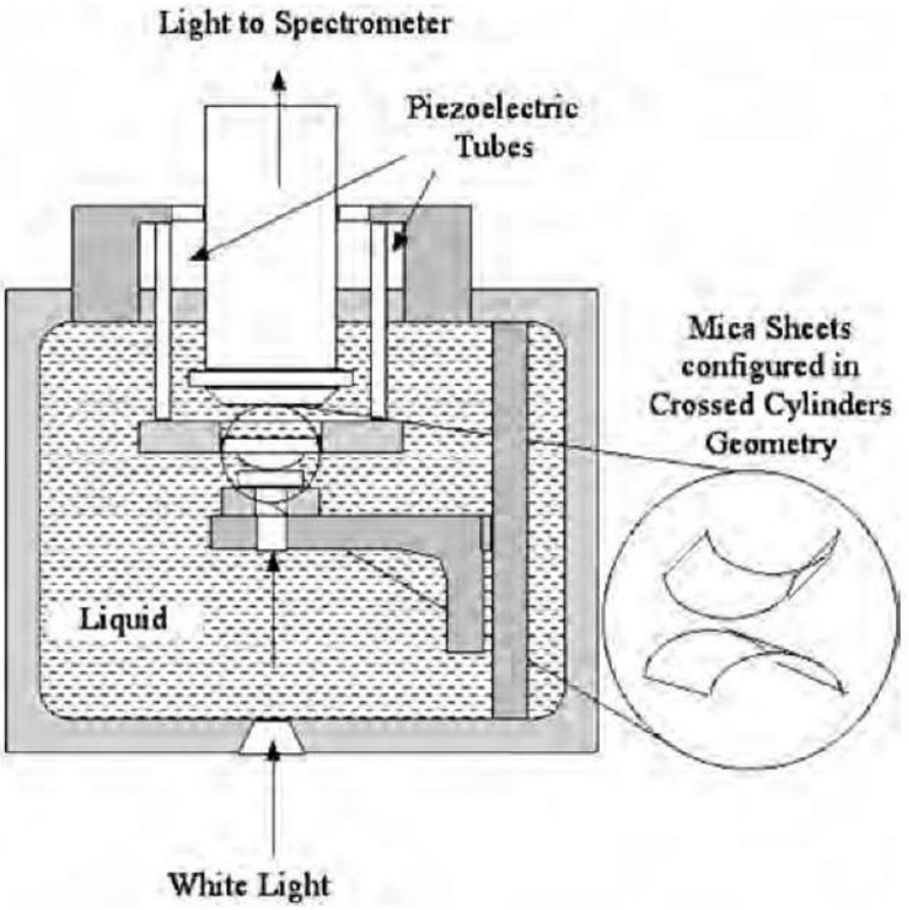




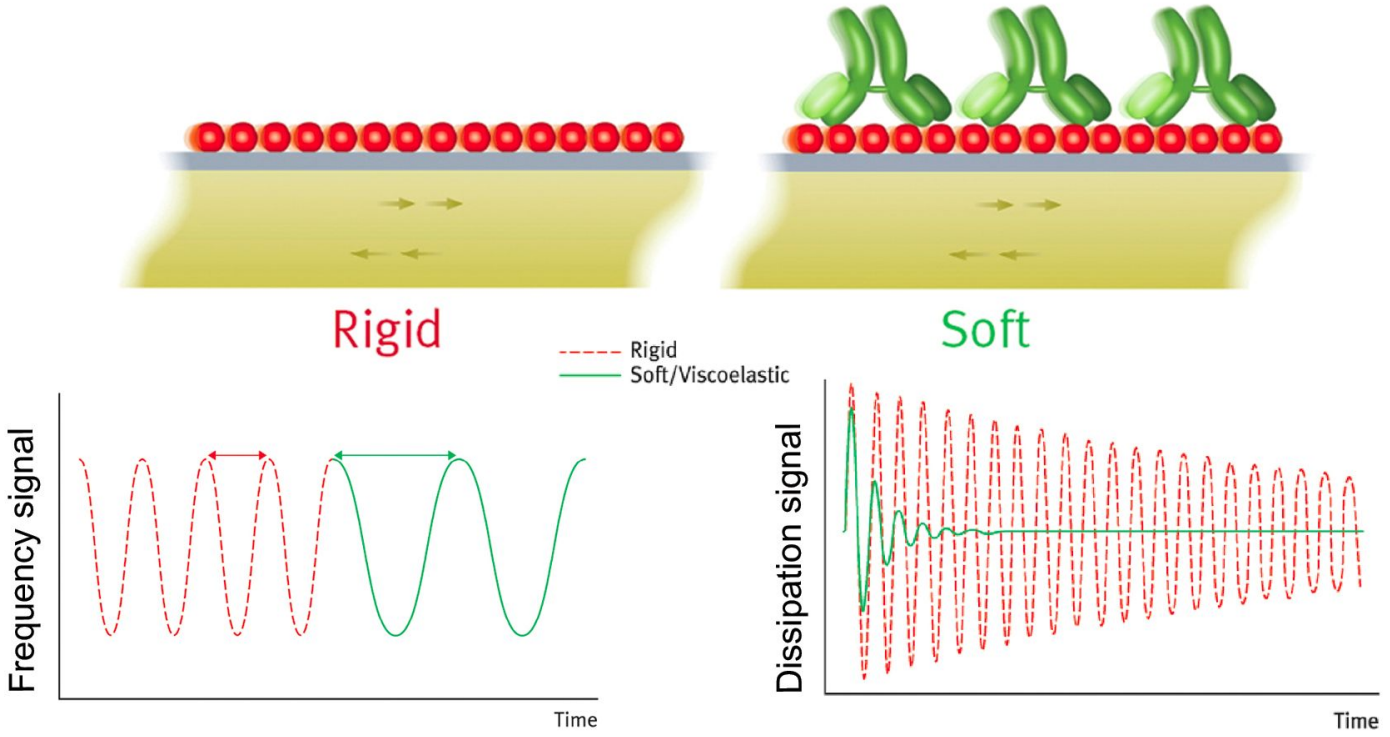
Experimental setups



Surface force apparatus

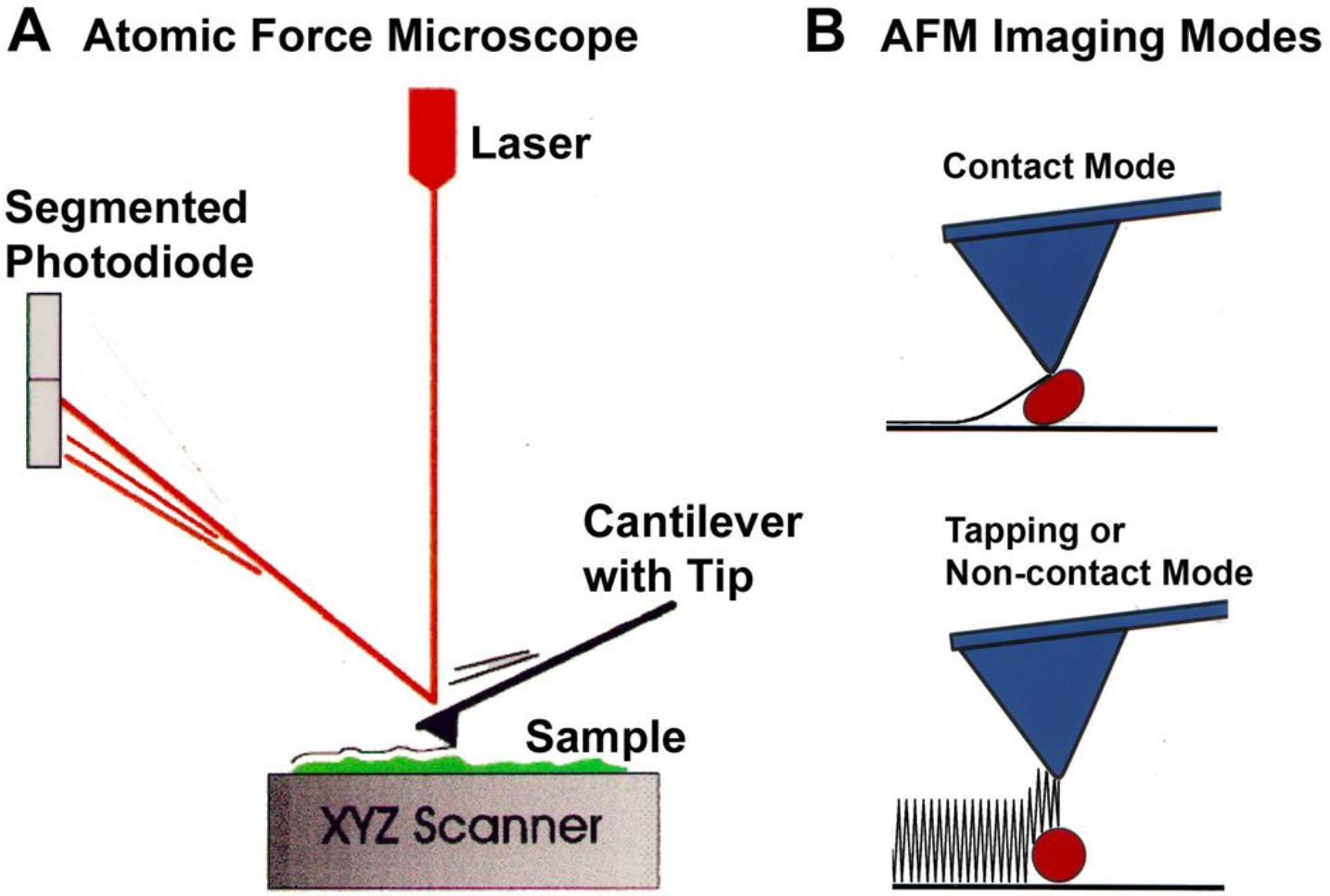


Quartz crystal microbalance

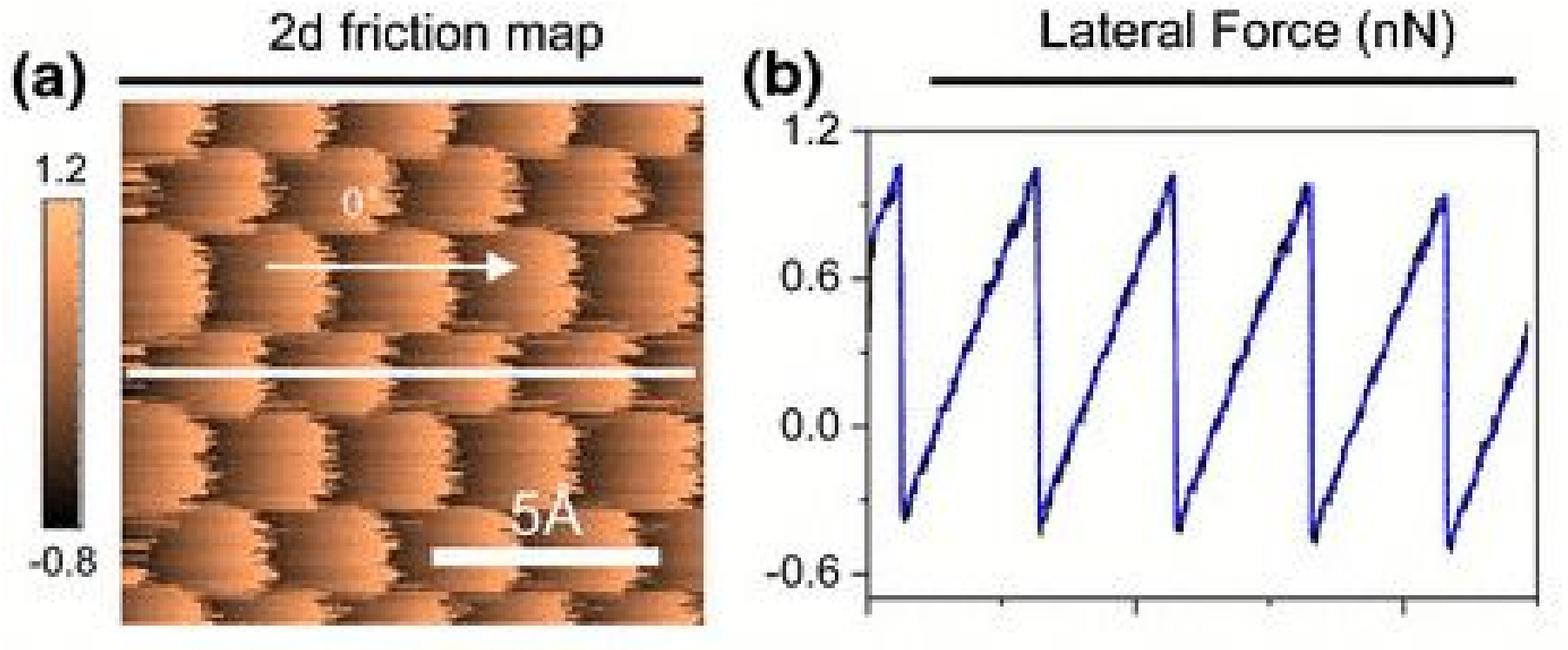


Atomic force microscopy

(and Friction force microscopy)

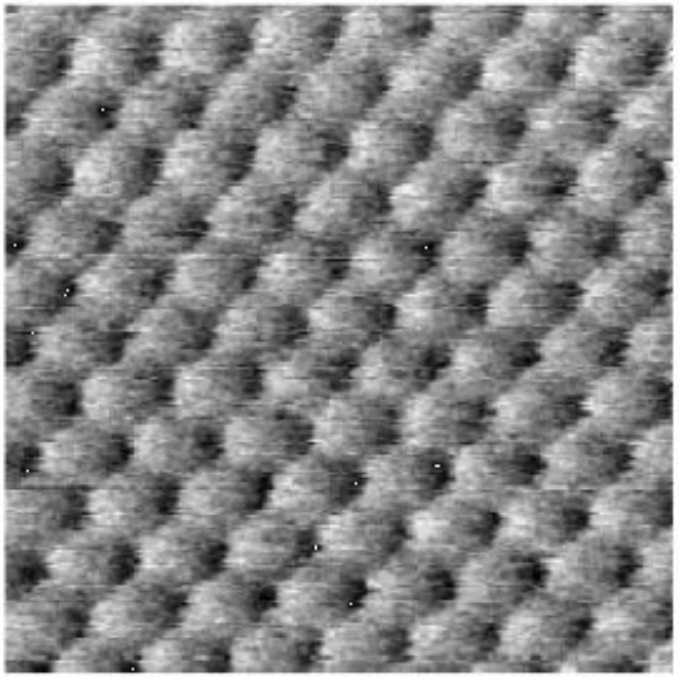


Stick-slip

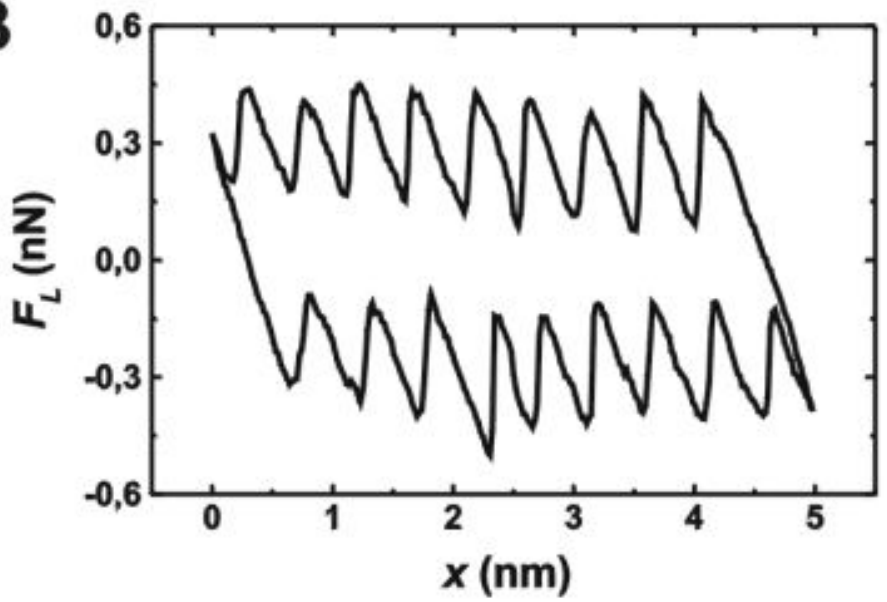


Hysteresis

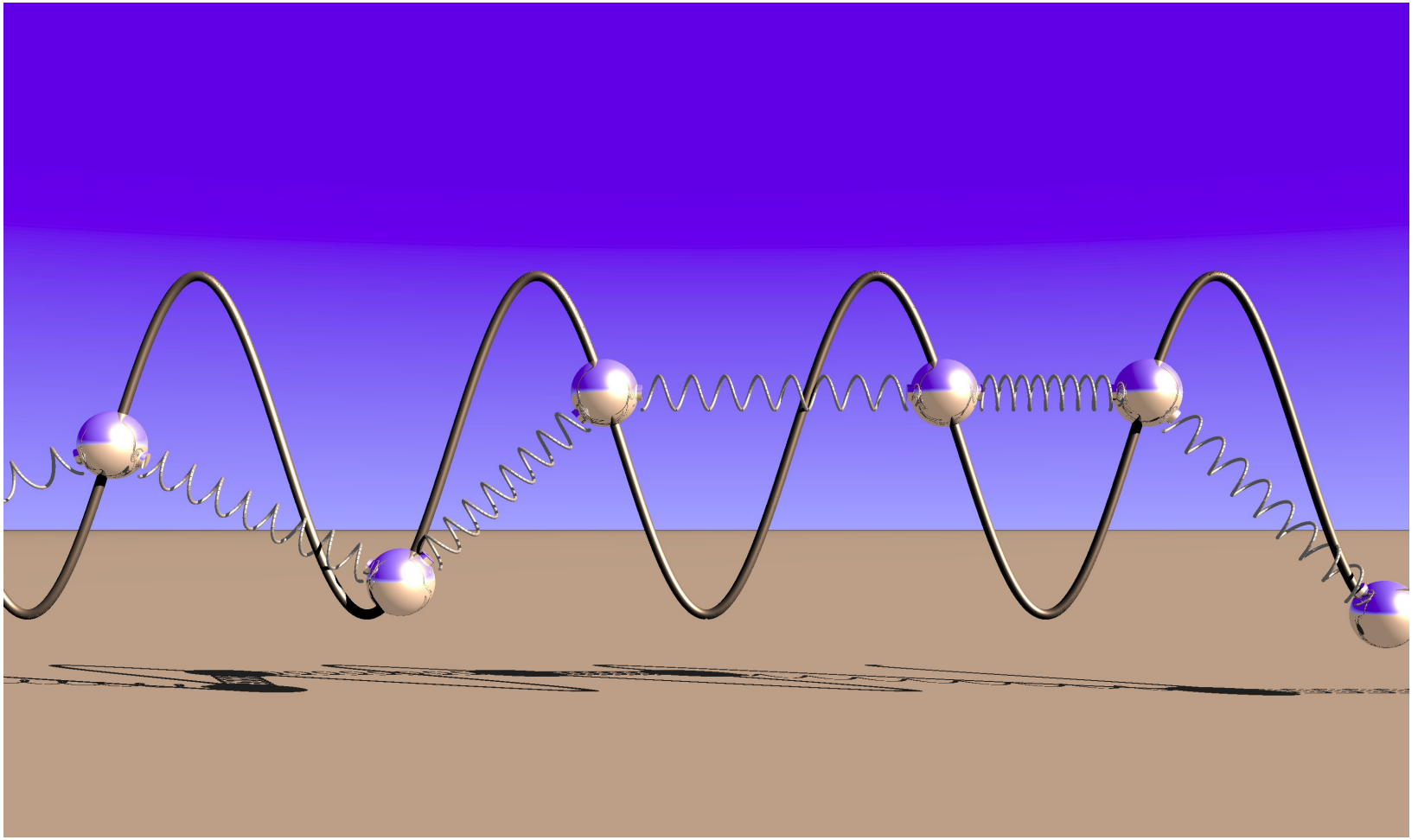
A



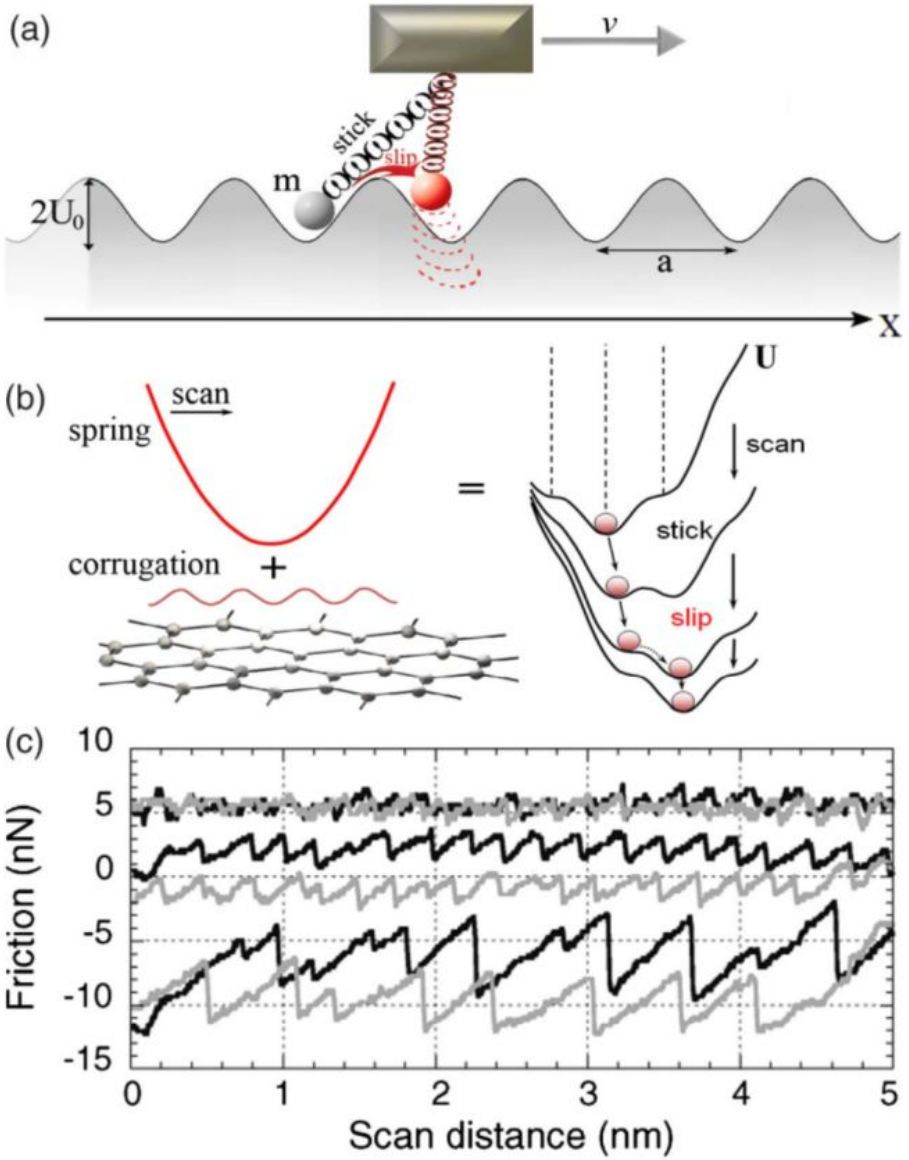
B



Toy Models



The Prandl-Tomlinson model (1928)



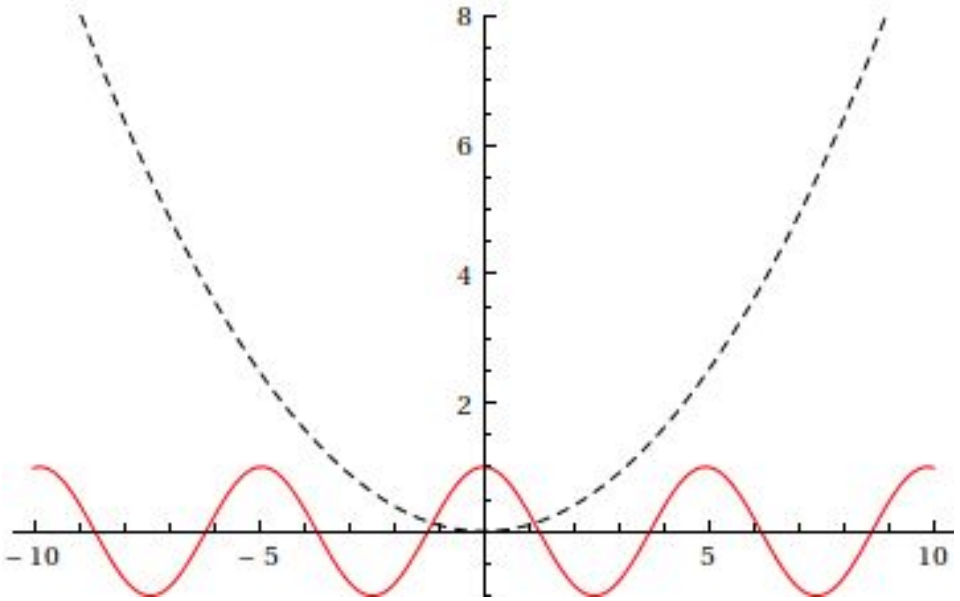
$$U(x,t) = U_0 \cos\left(\frac{2\pi}{a}x\right) + \frac{K}{2}(x - vt)^2$$

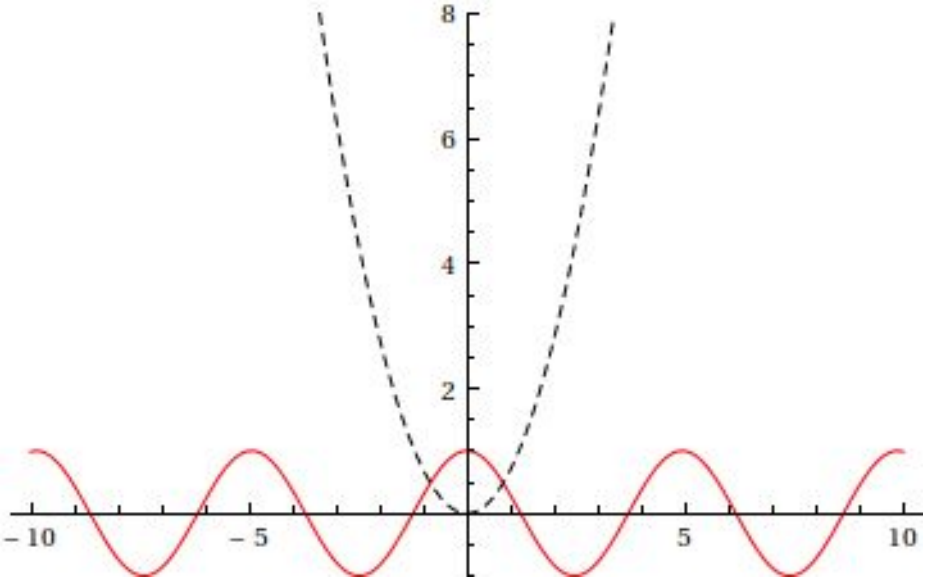
$$m\ddot{x} + m\gamma\dot{x} = -\frac{\partial U(x,t)}{\partial x} + \hat{f}(t)$$

Depending on K/U_0, transition from smooth sliding to stick-slip

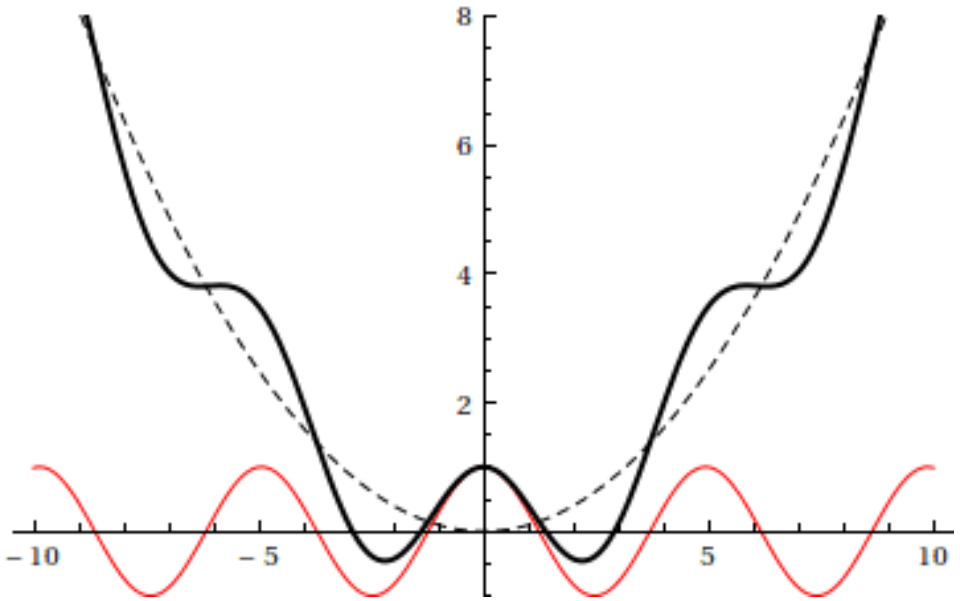
In stick-slip regime F~log v

The Prandl-Tomlinson model (1928)

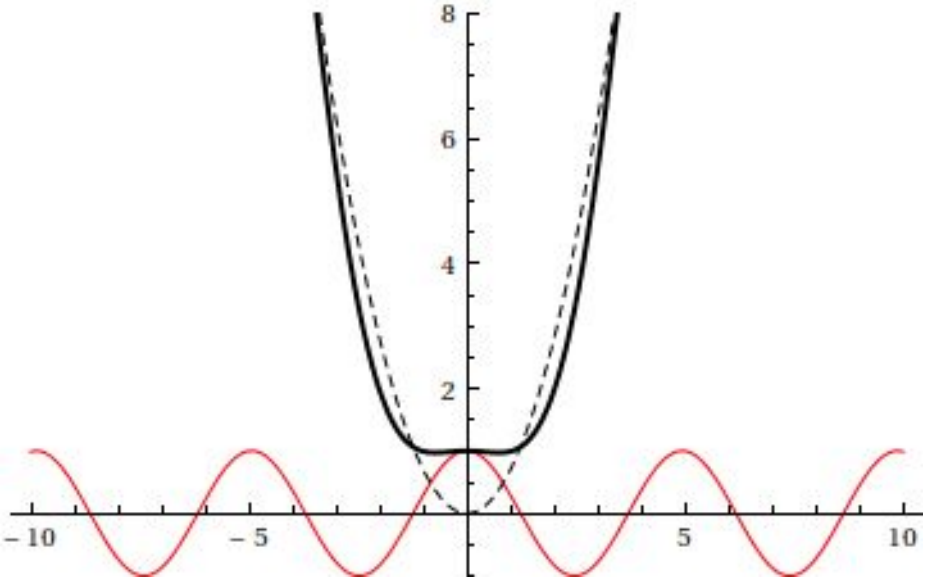




The Prandl-Tomlinson model (1928)

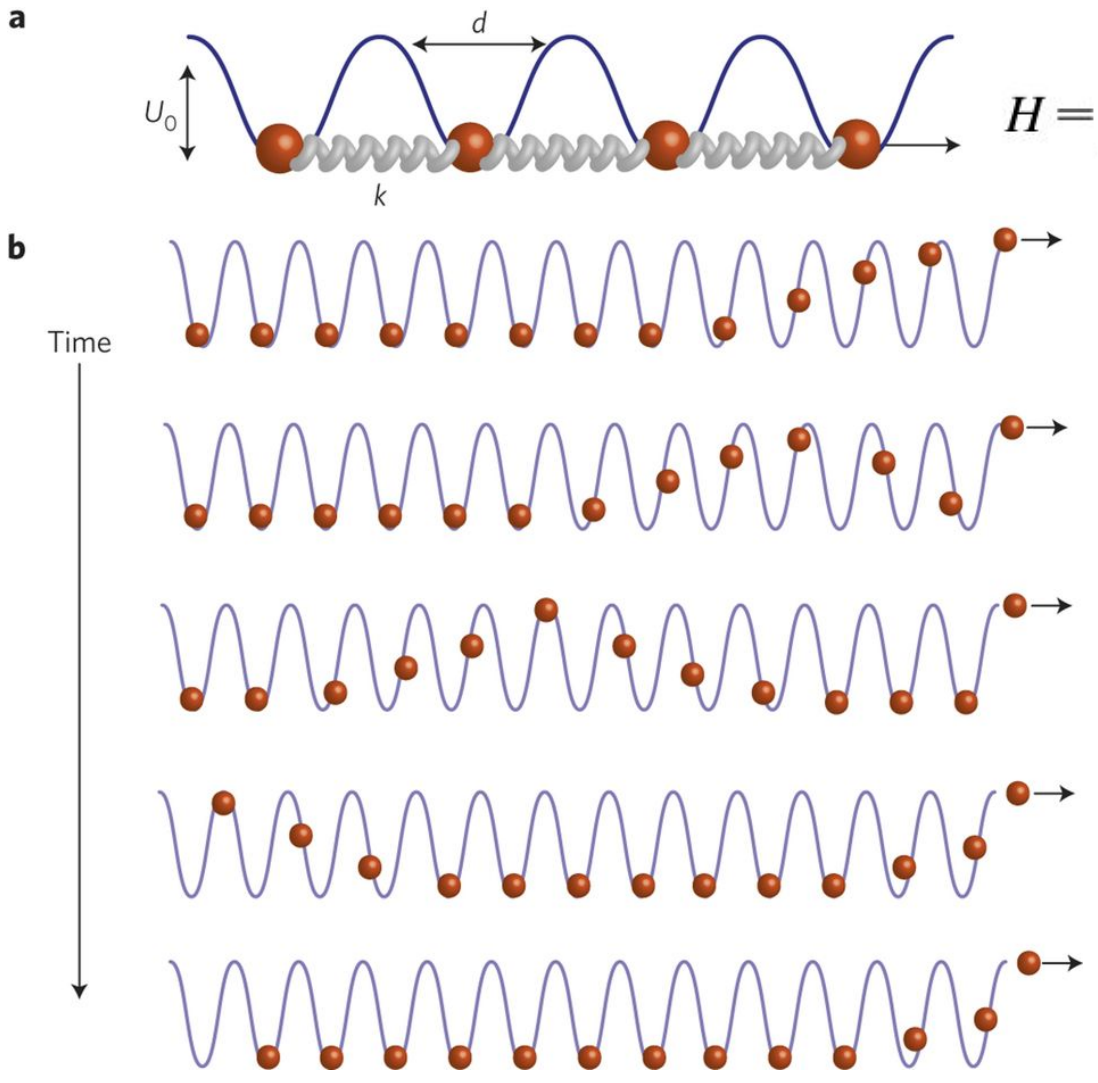


Stick-slip



Smooth sliding

Frenkel-Kontorova model (1938)



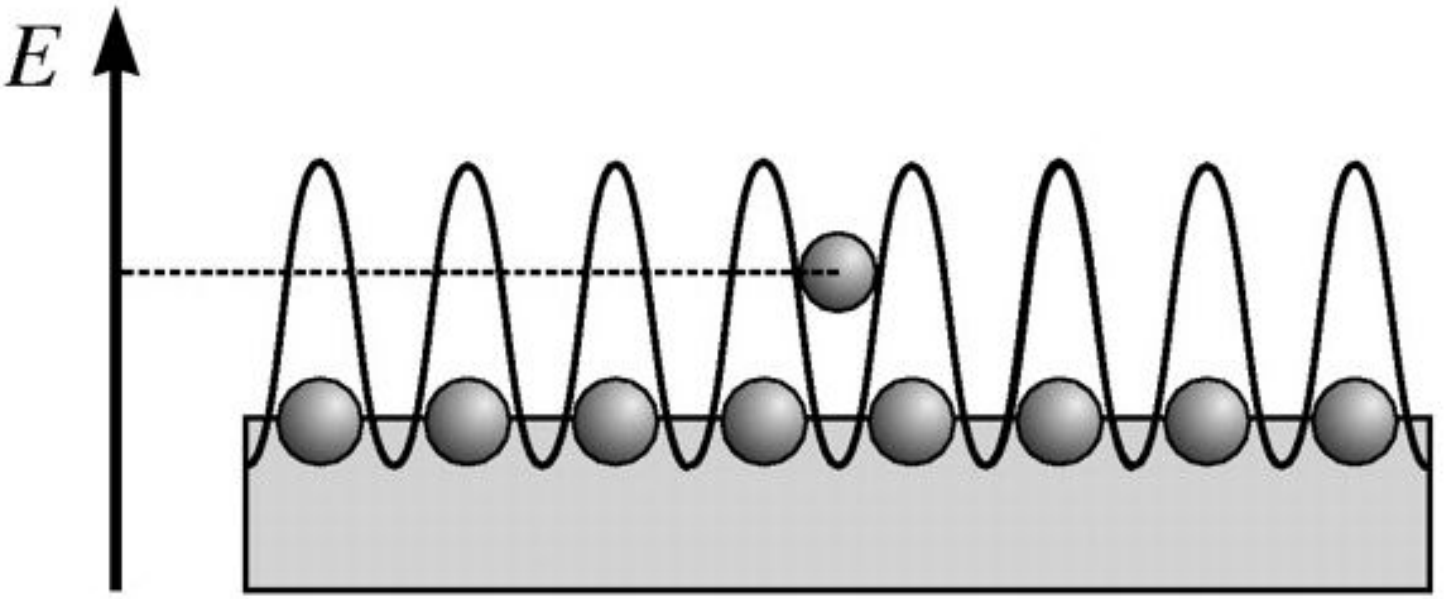
$$H = \sum_i \left[\frac{p_i^2}{2m} + \frac{K}{2}(x_{i+1} - x_i - a_c)^2 + \frac{U_0}{2}\cos\frac{2\pi x_i}{a_b} \right]$$

At given a_b/a_c ratio, behavior depends on K/U_0 (Aubry transition)

Formation of solitons (kinks)

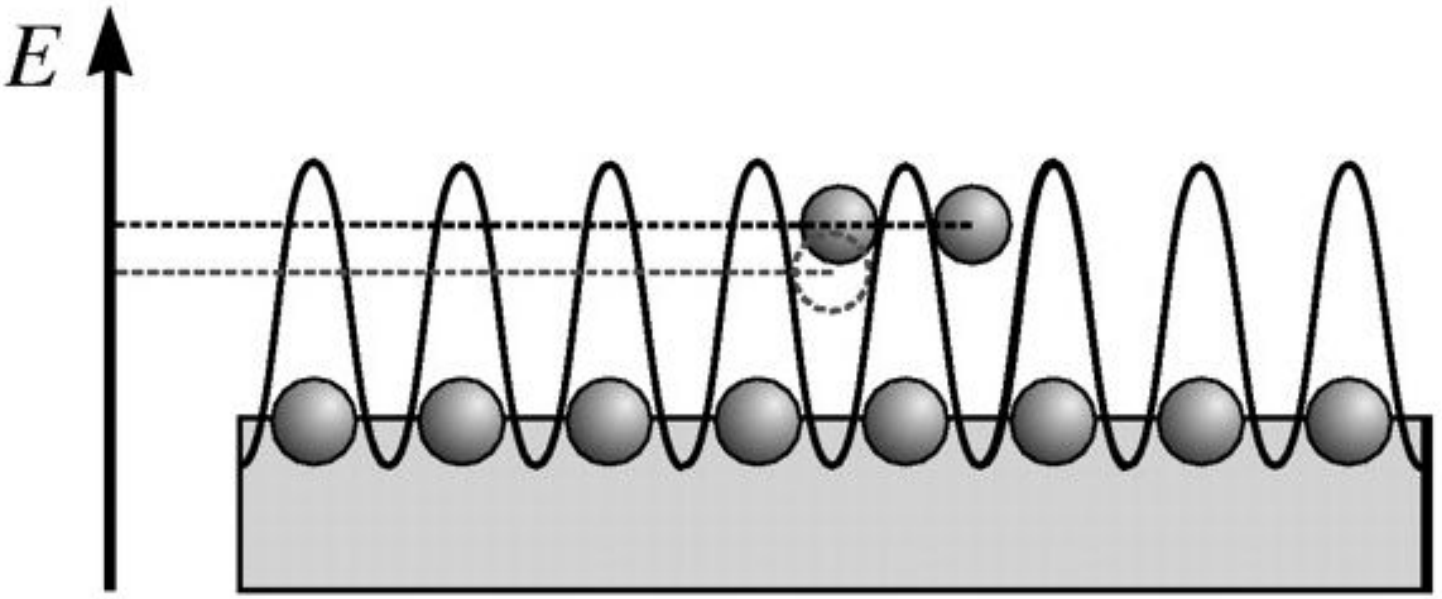
Aubry transition

From Tomlinson to FK



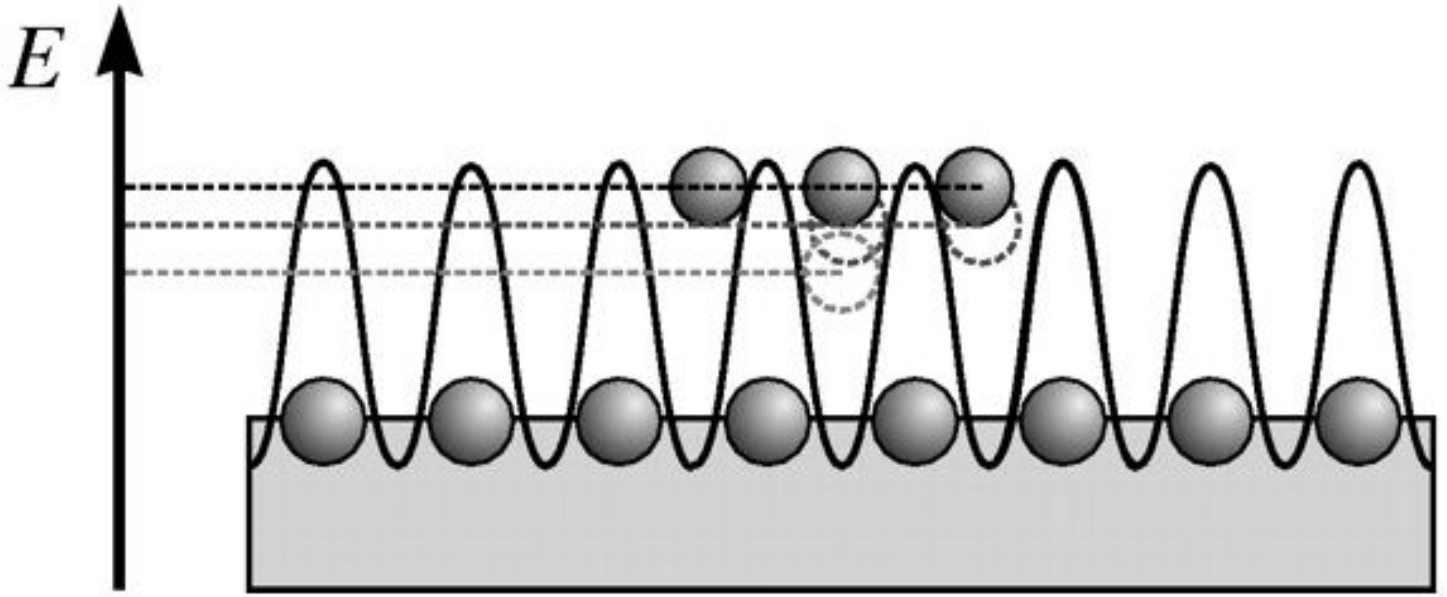
Aubry transition

From Tomlinson to FK



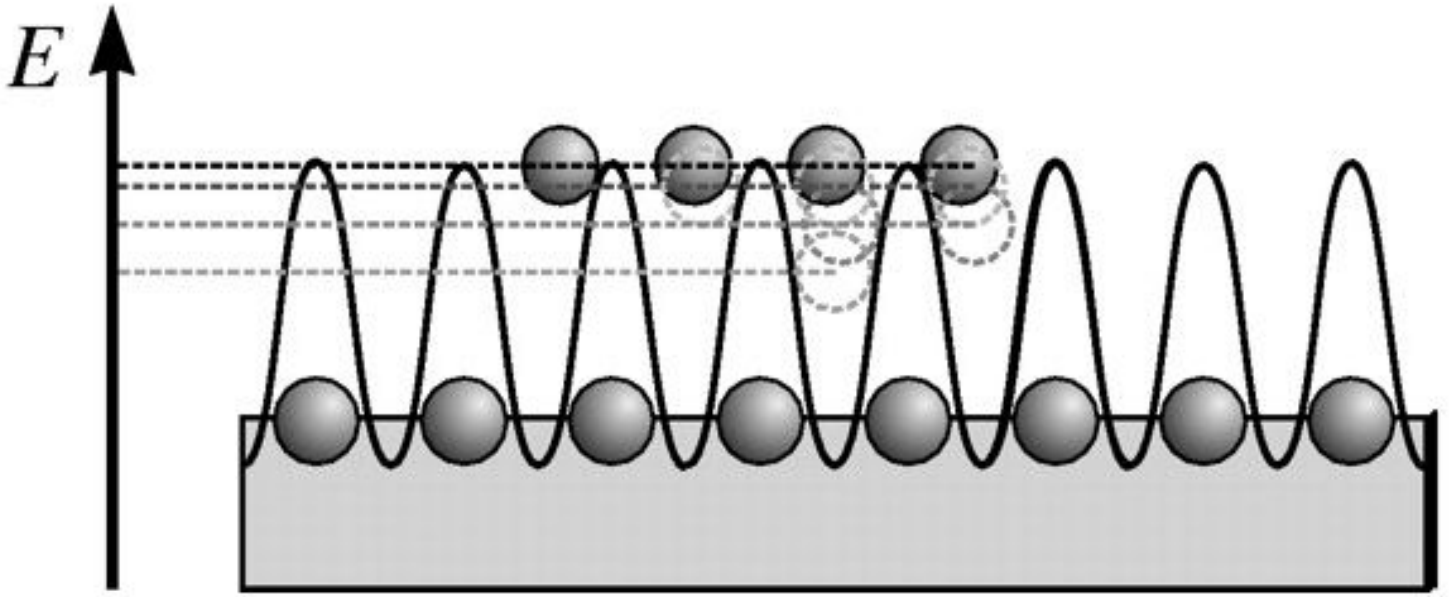
Aubry transition

From Tomlinson to FK



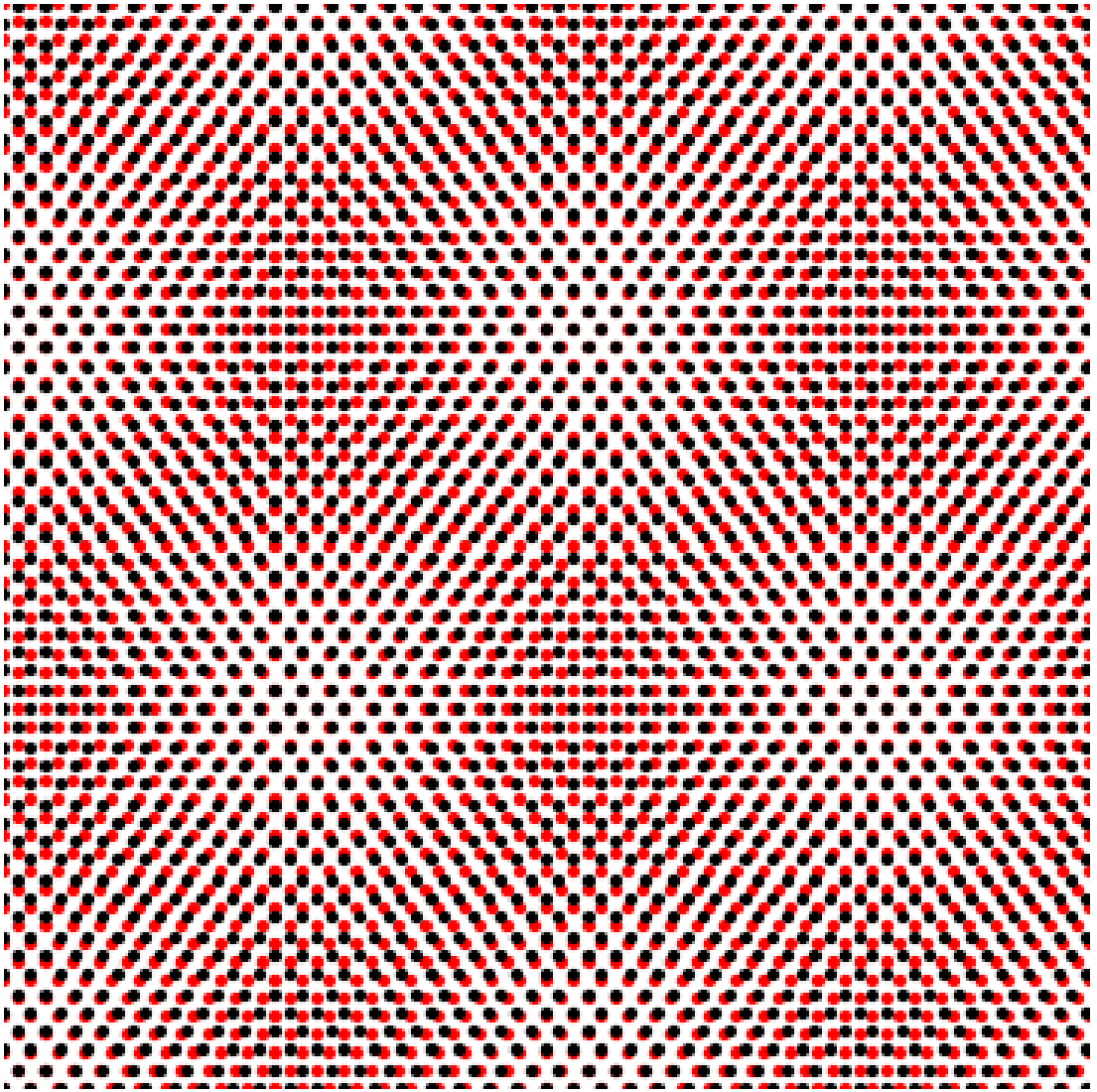
Aubry transition

From Tomlinson to FK

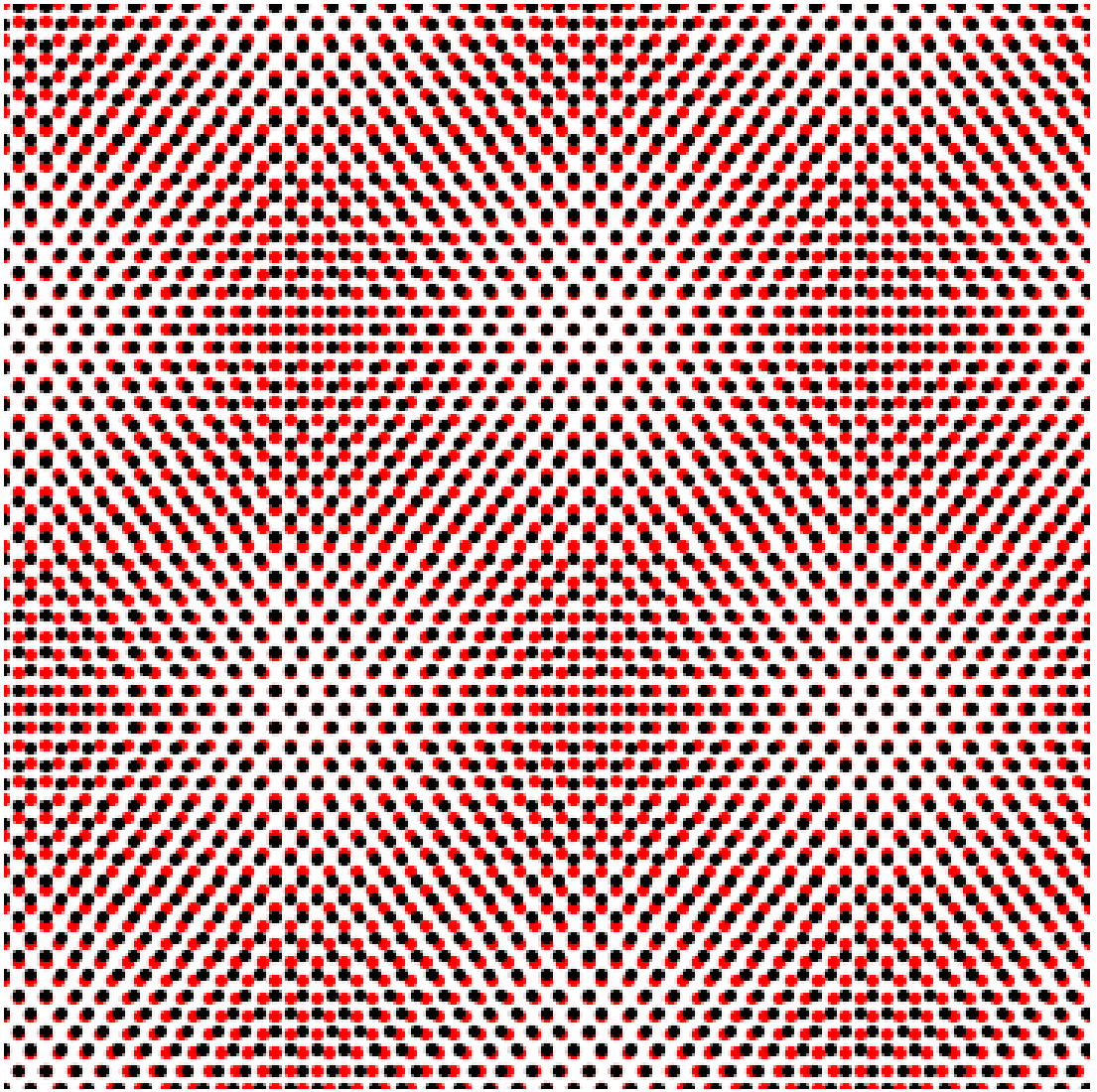


Depending on a_b/a_c ratio at different K/U_0 there is transition from pinned to free sliding (Aubry transition)

Superlubricity

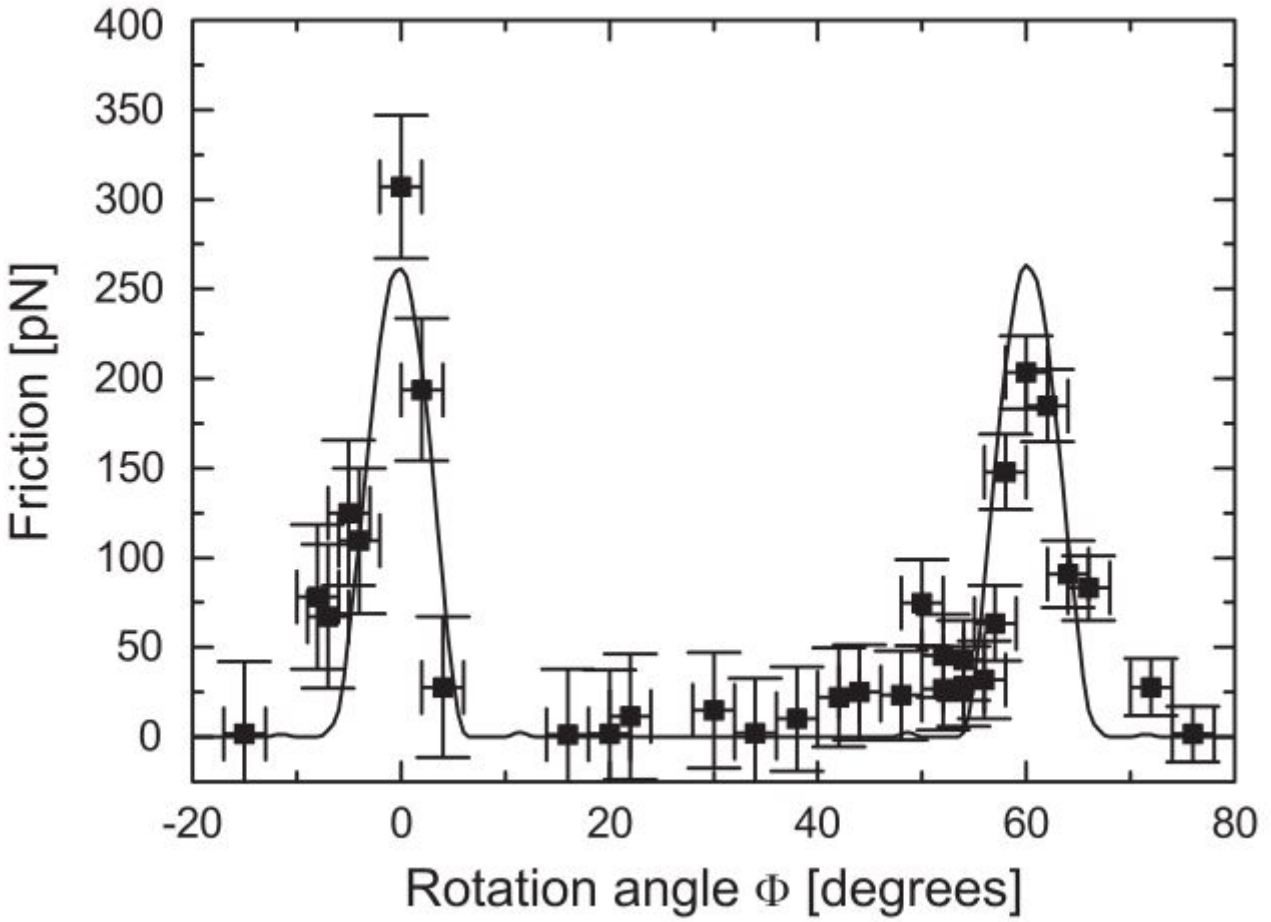


Superlubricity

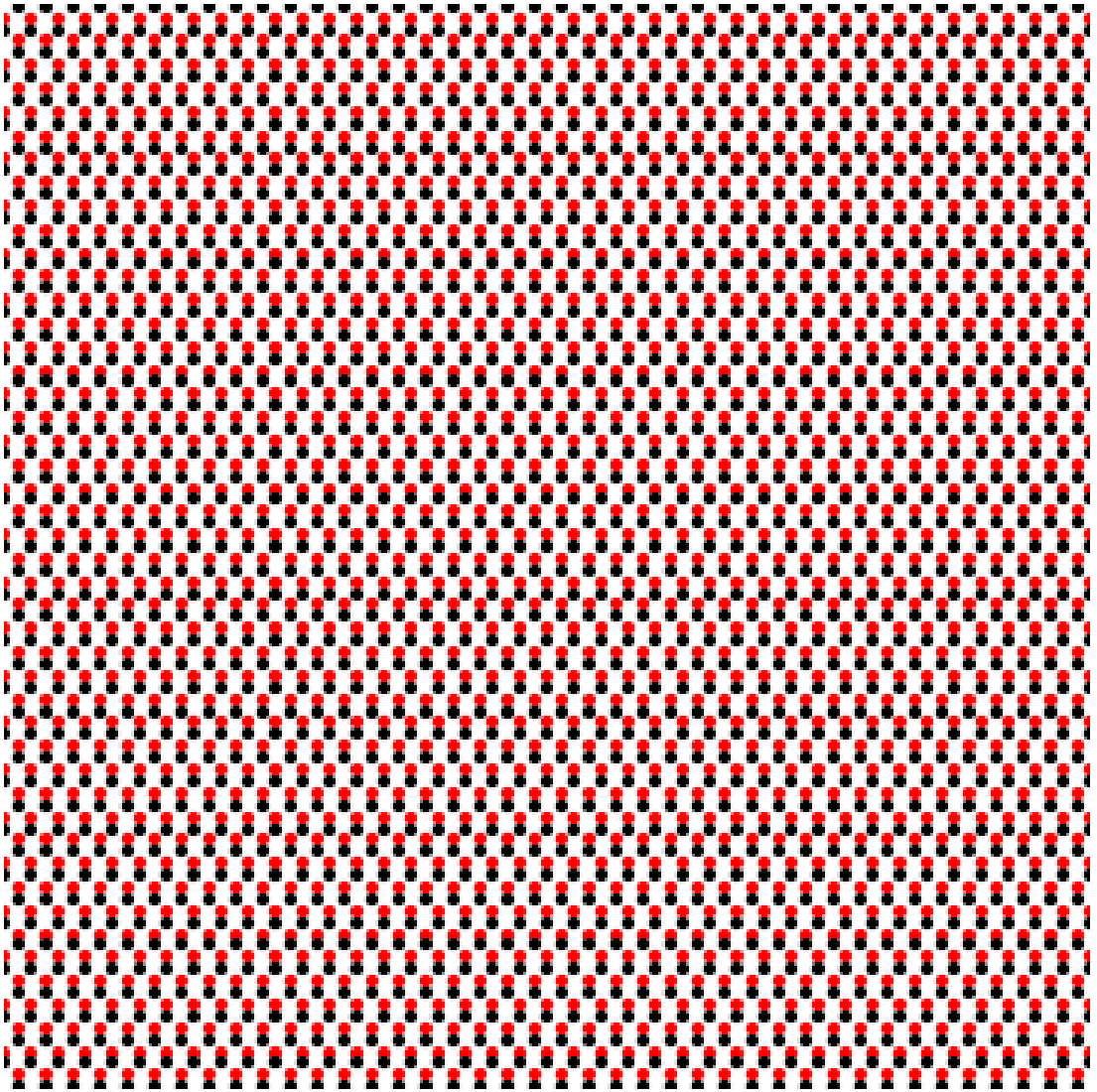


Superlubricity

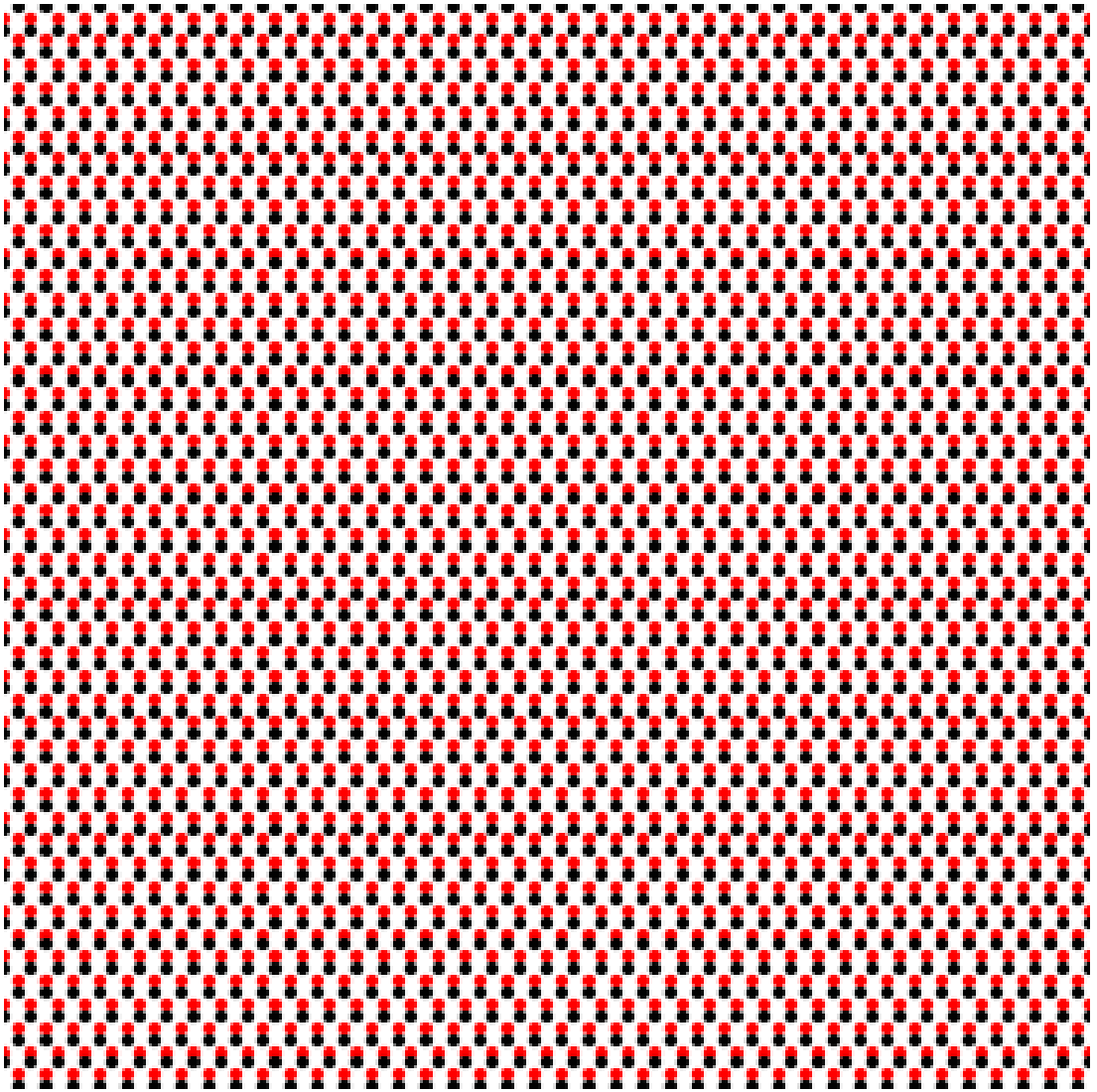
Graphene flake on graphene



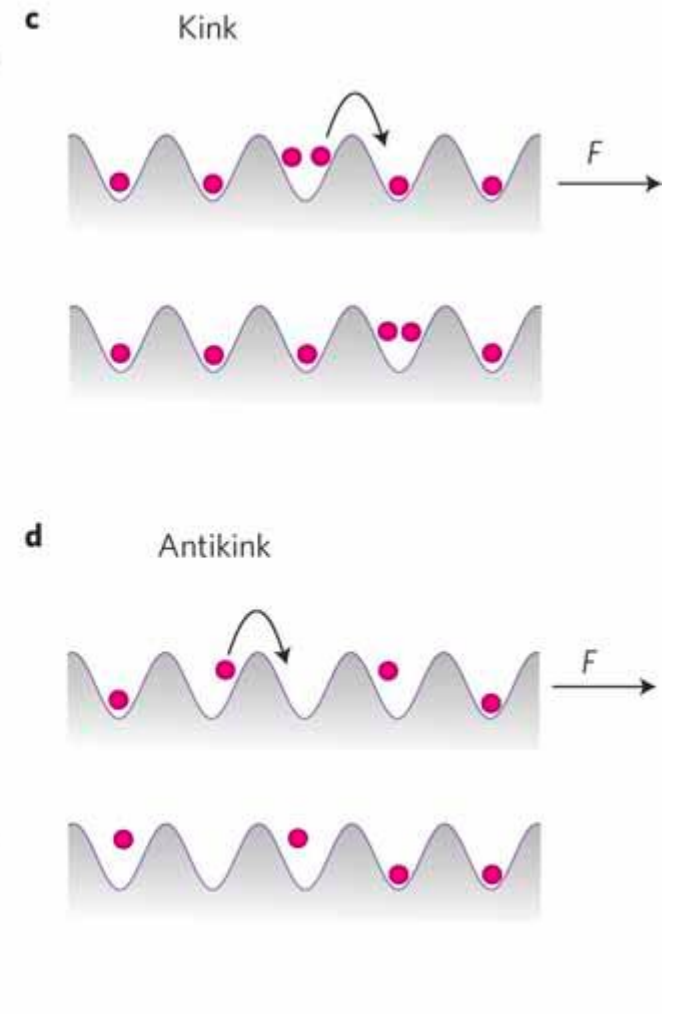
Superlubricity



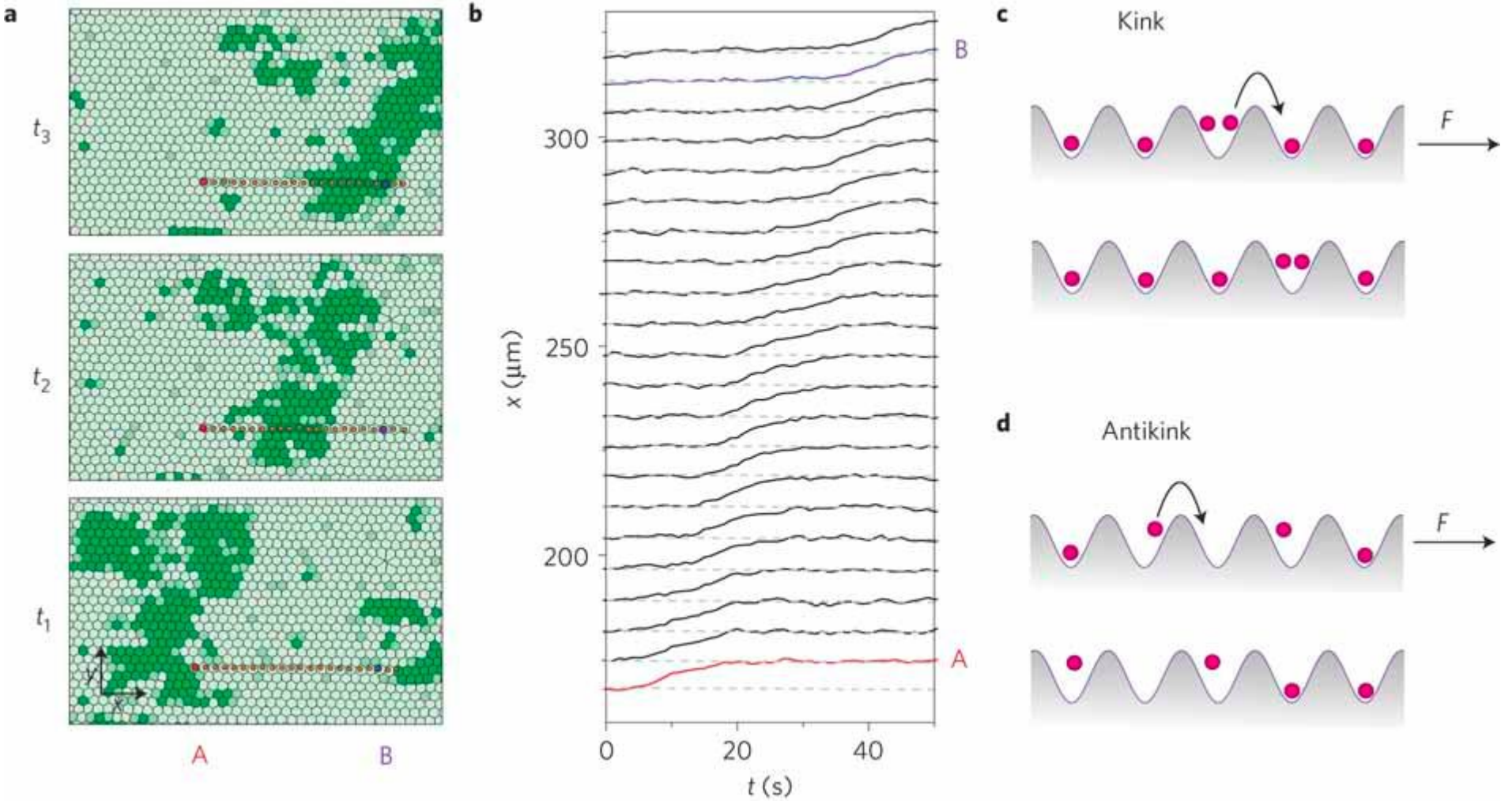
Superlubricity



Kinks & anti-kinks

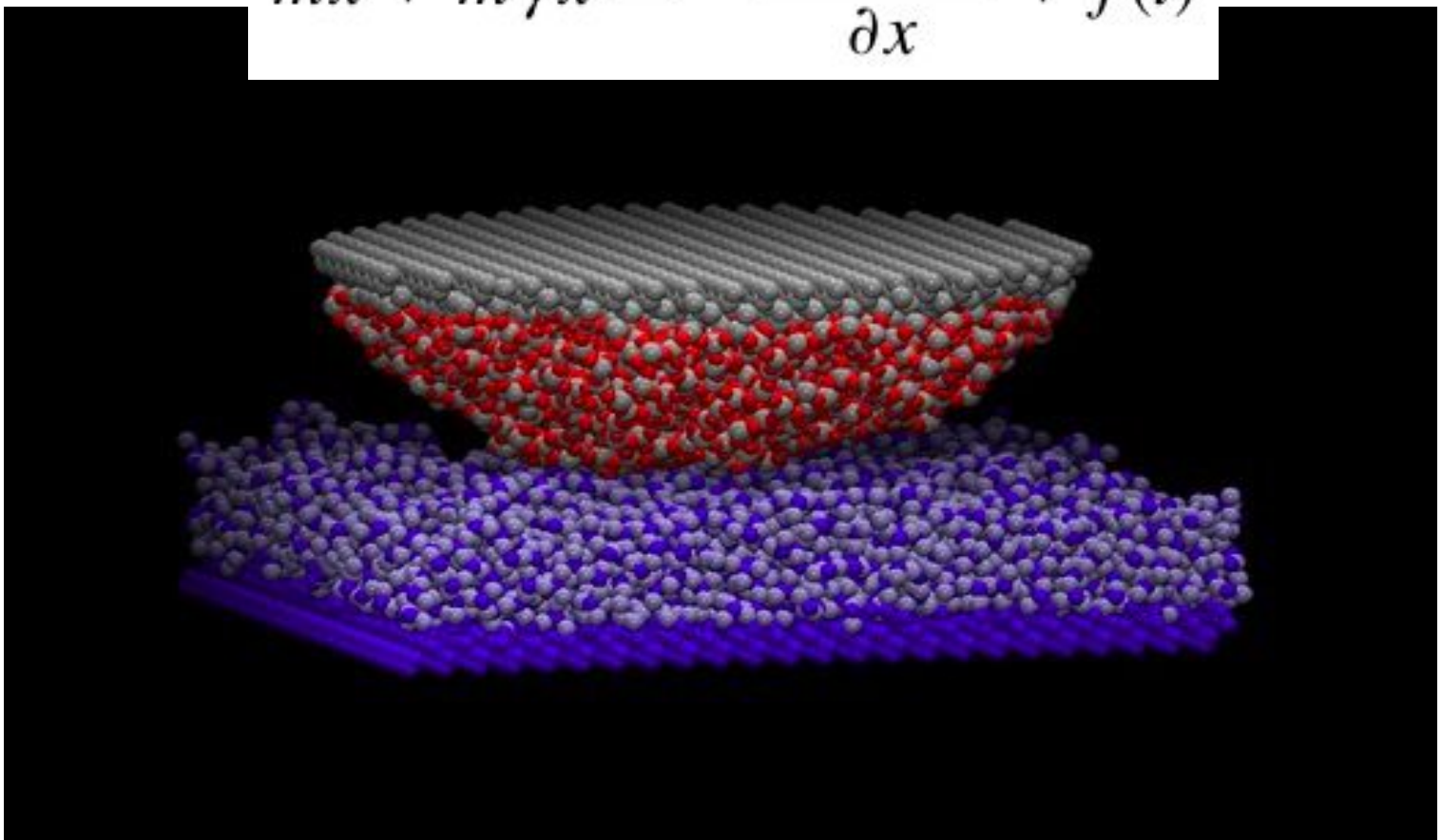


Kinks & anti-kinks



MD and Langevin

$$m\ddot{x} + m\gamma\dot{x} = -\frac{\partial U(x,t)}{\partial x} + \hat{f}(t)$$



MD and Langevin

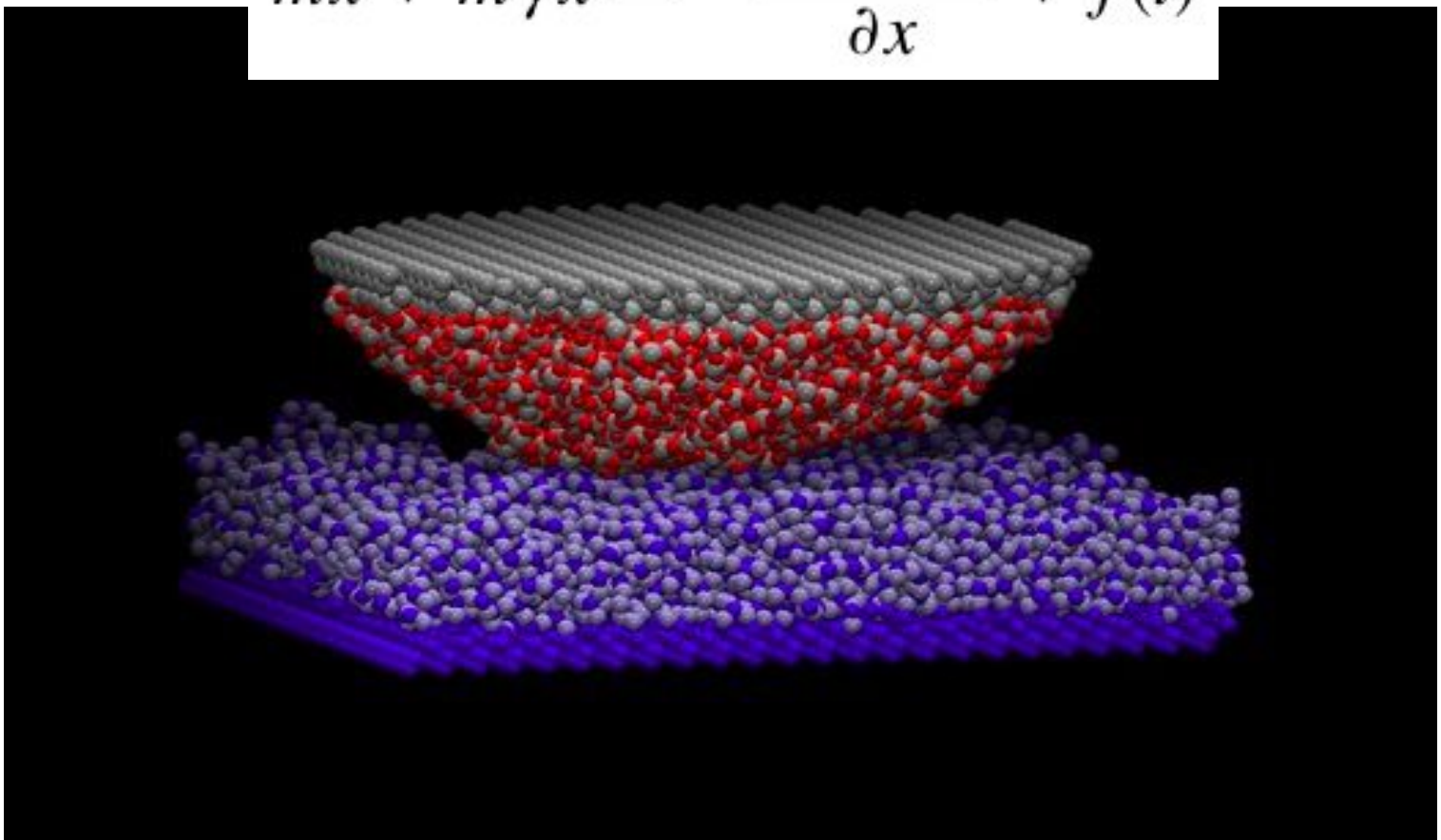
Dissipation?

Driving

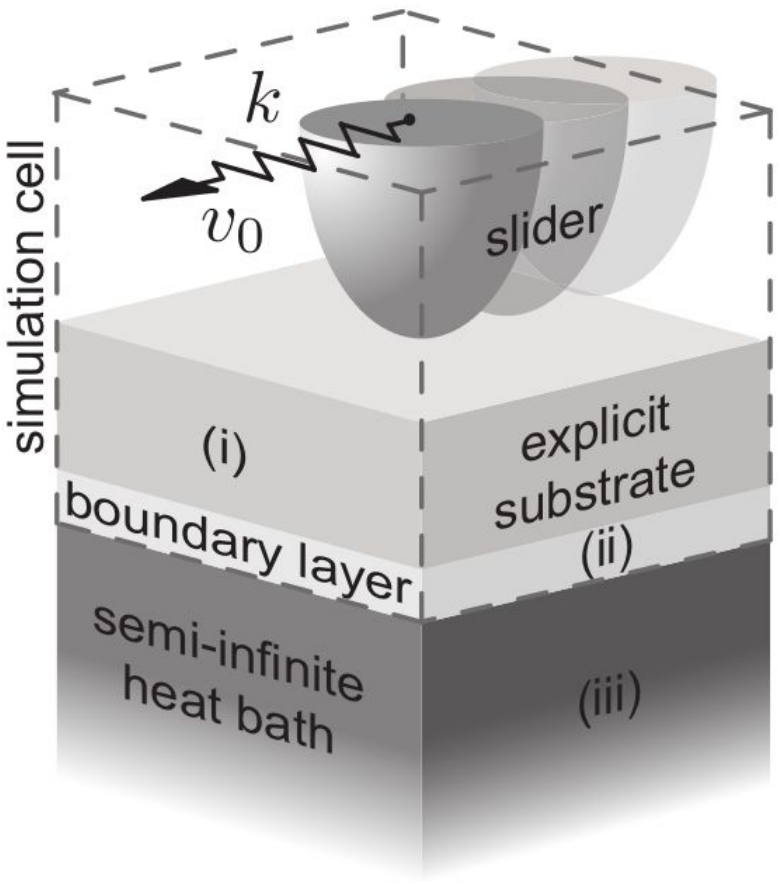
Inertia

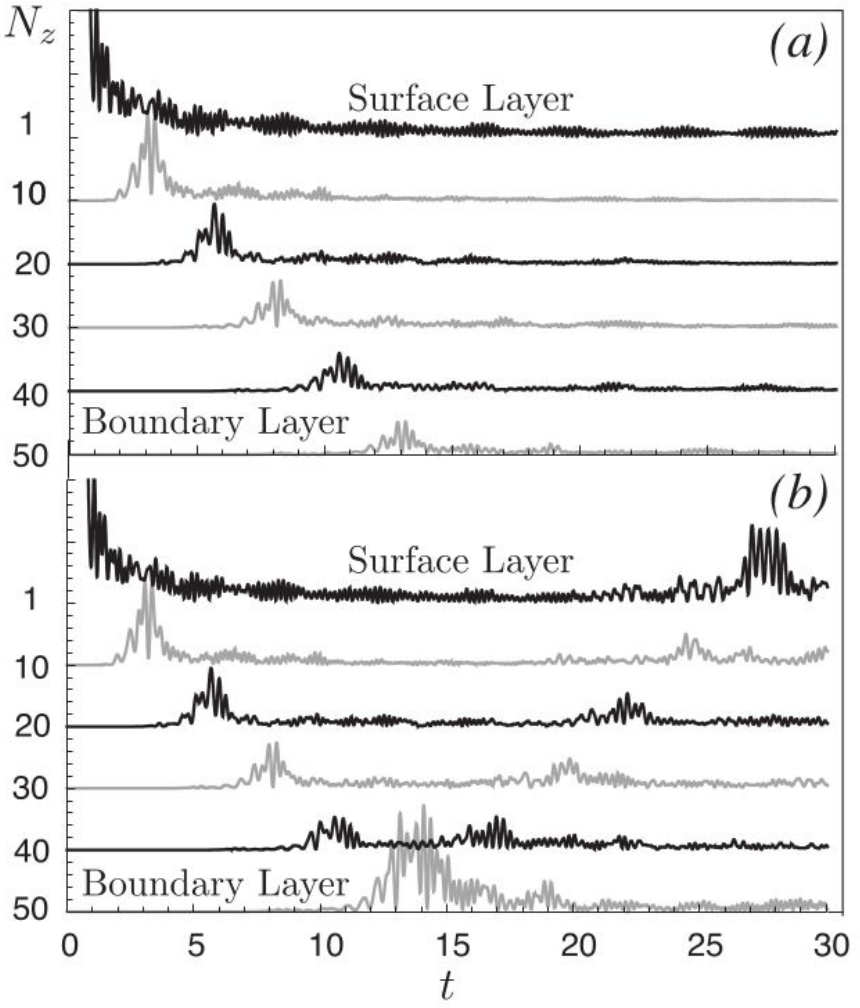
Noise

$$m\ddot{x} + m\gamma\dot{x} = -\frac{\partial U(x,t)}{\partial x} + \hat{f}(t)$$

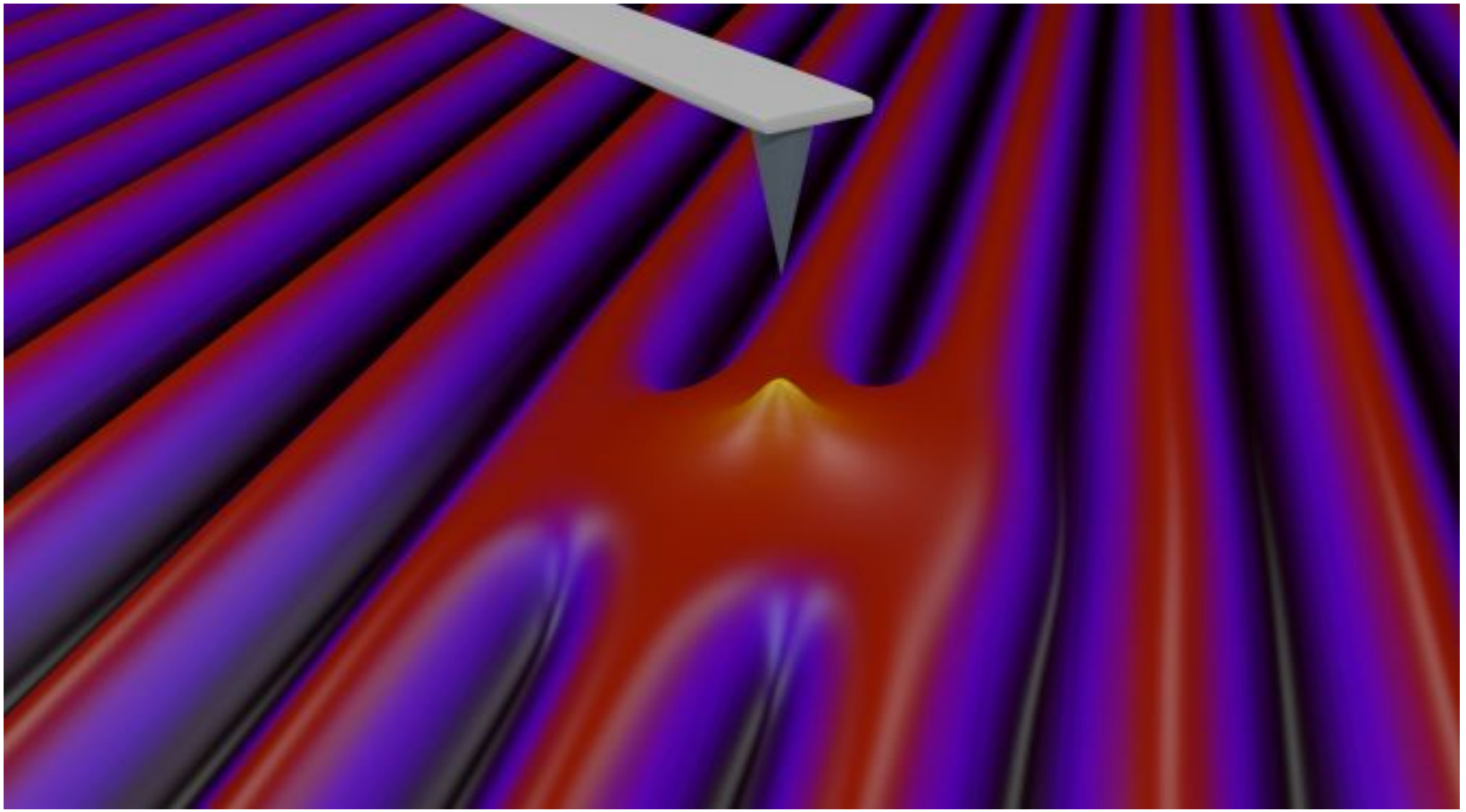


MD and Langevin

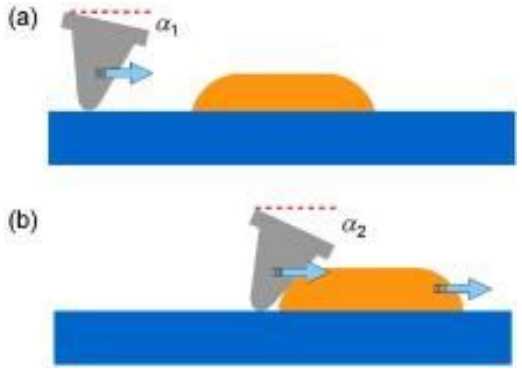


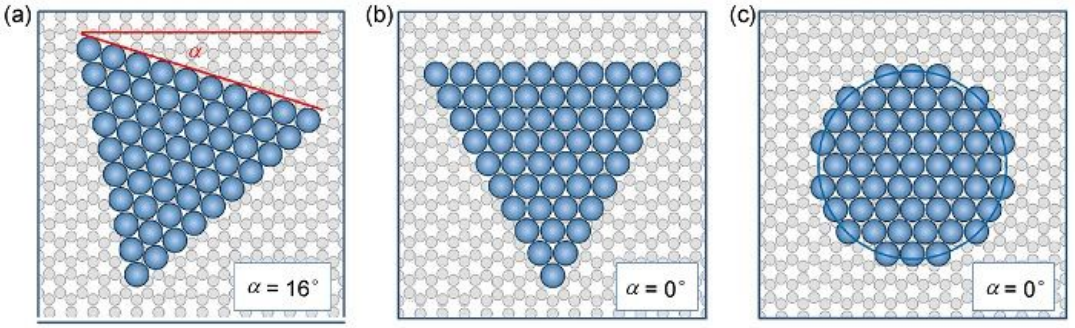


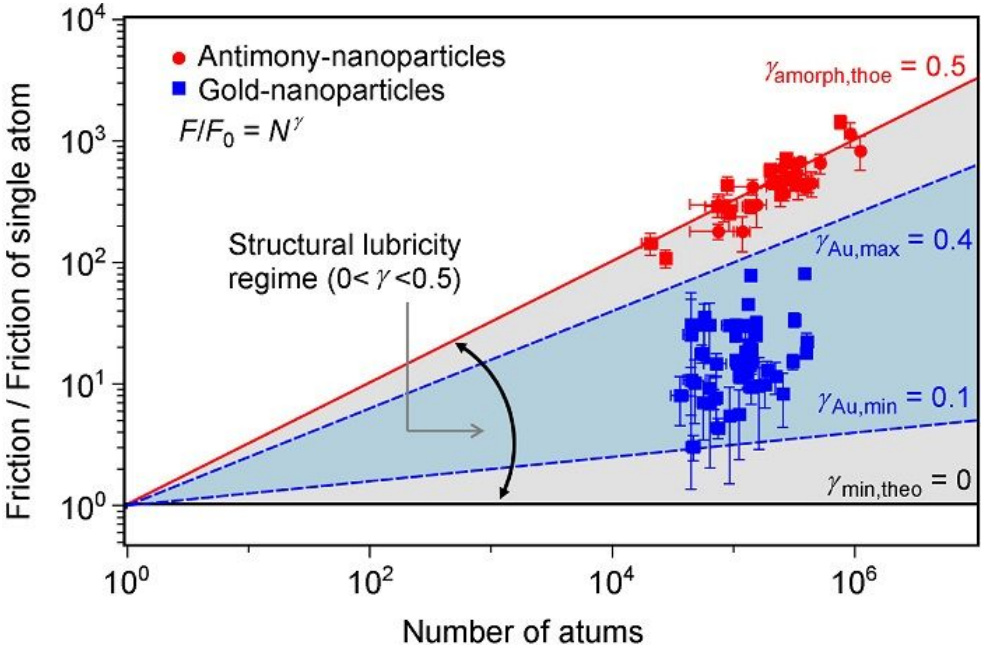
Interesting effects

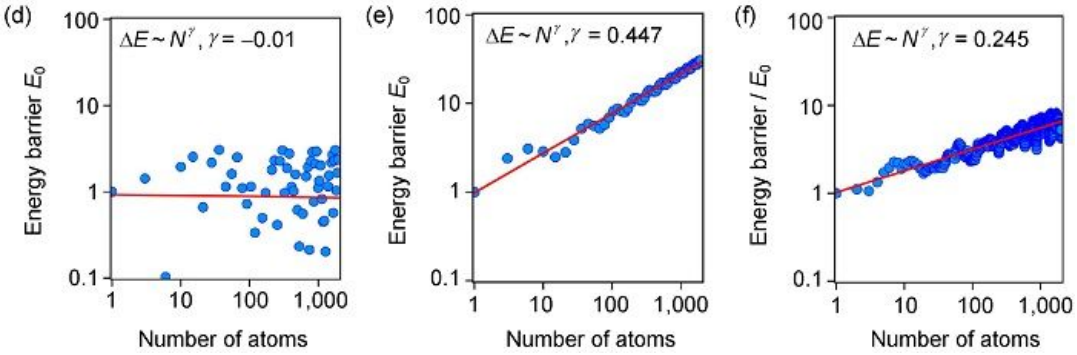


Area scaling?

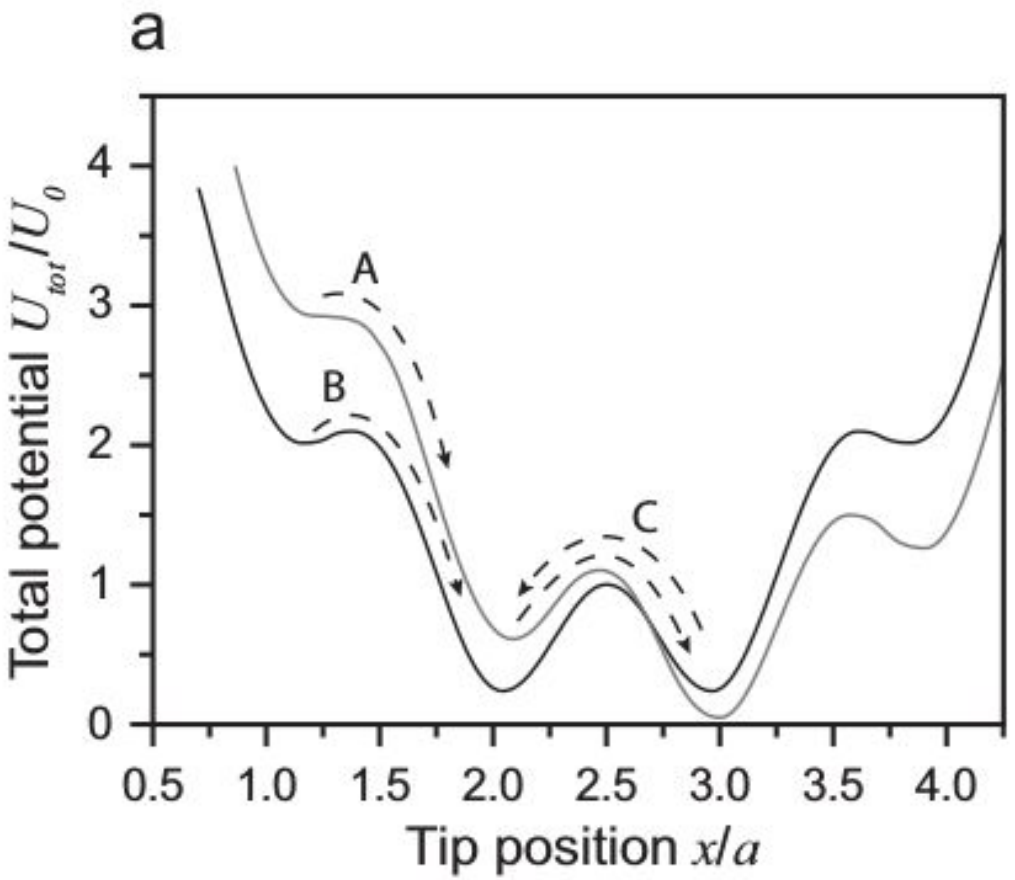




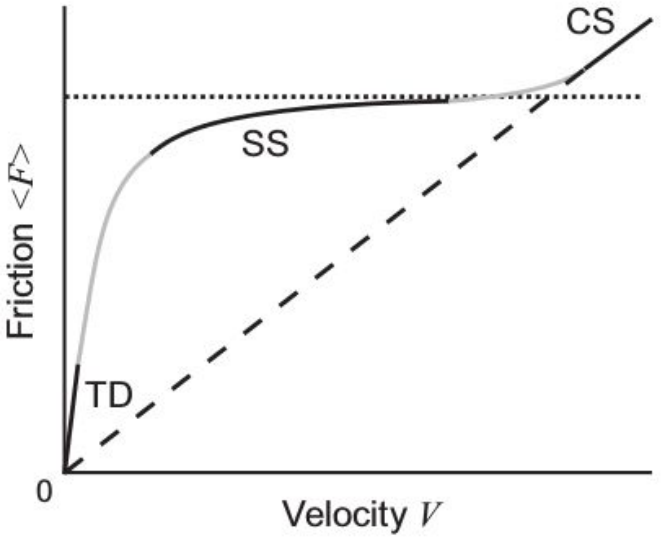




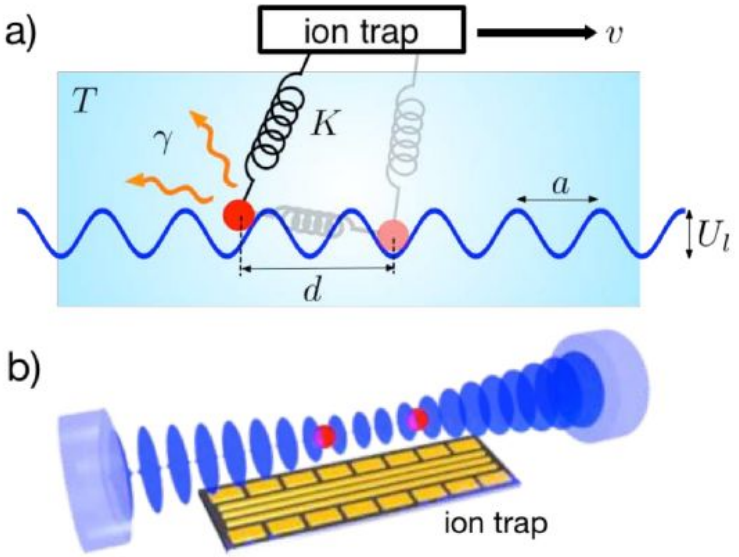
Thermolubricity

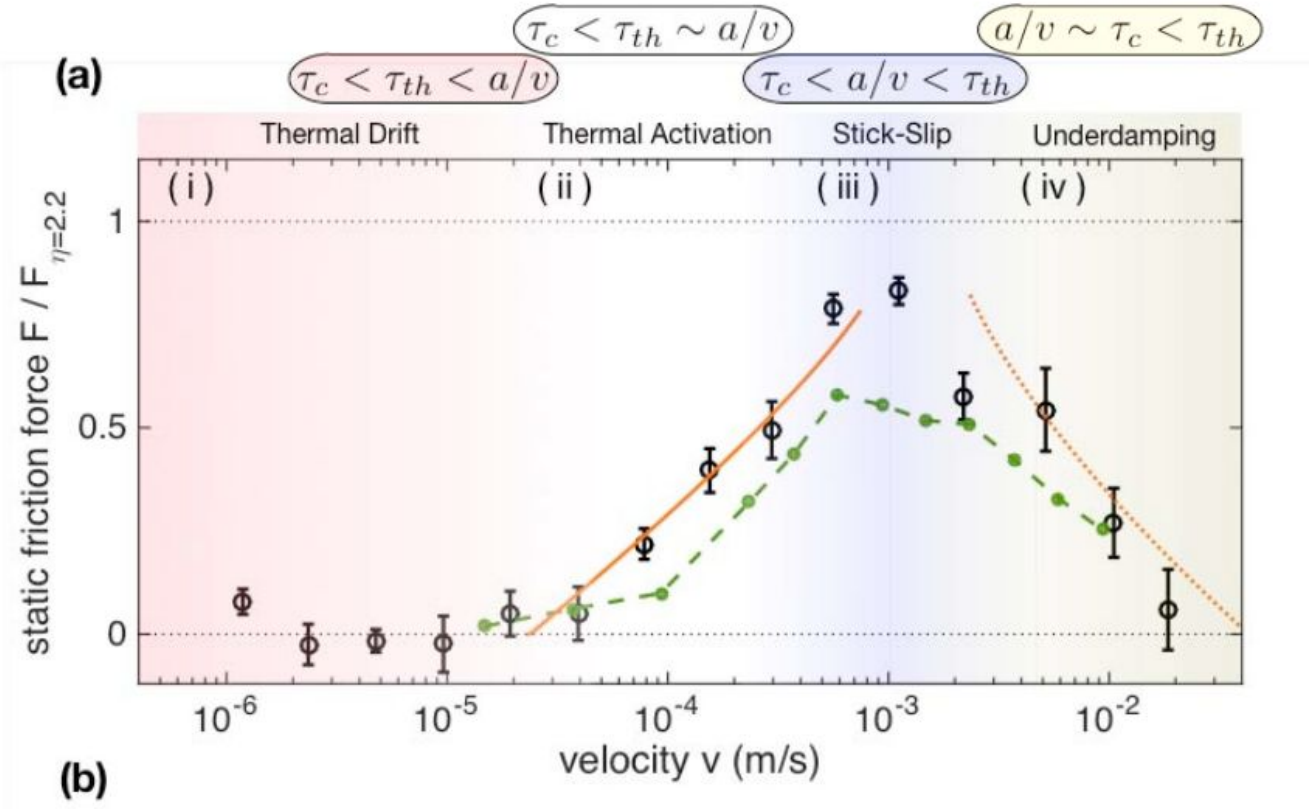


Breakdown of Coulomb's law for small systems at v~exp(-ΔE/KT)

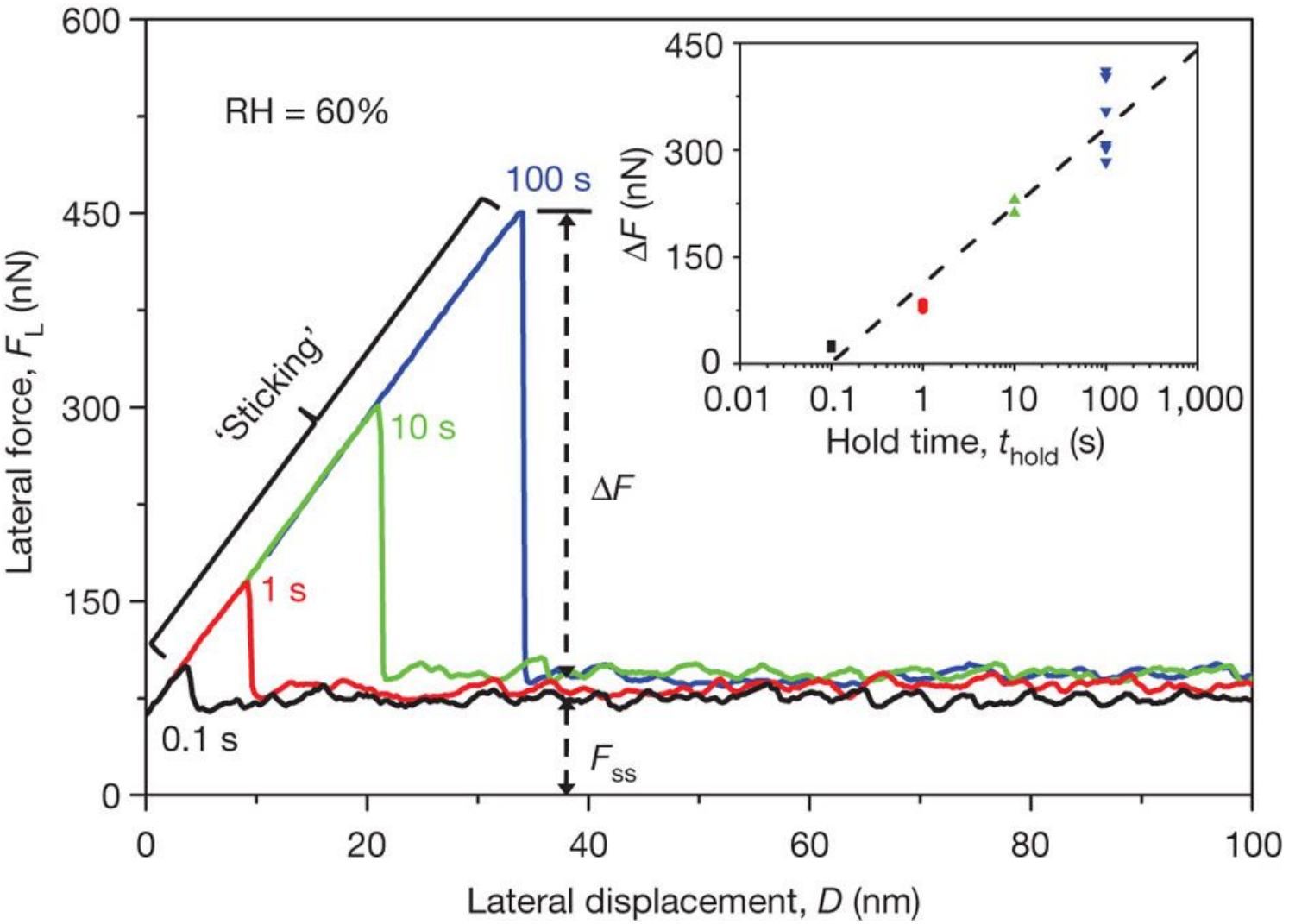


Thermolubricity

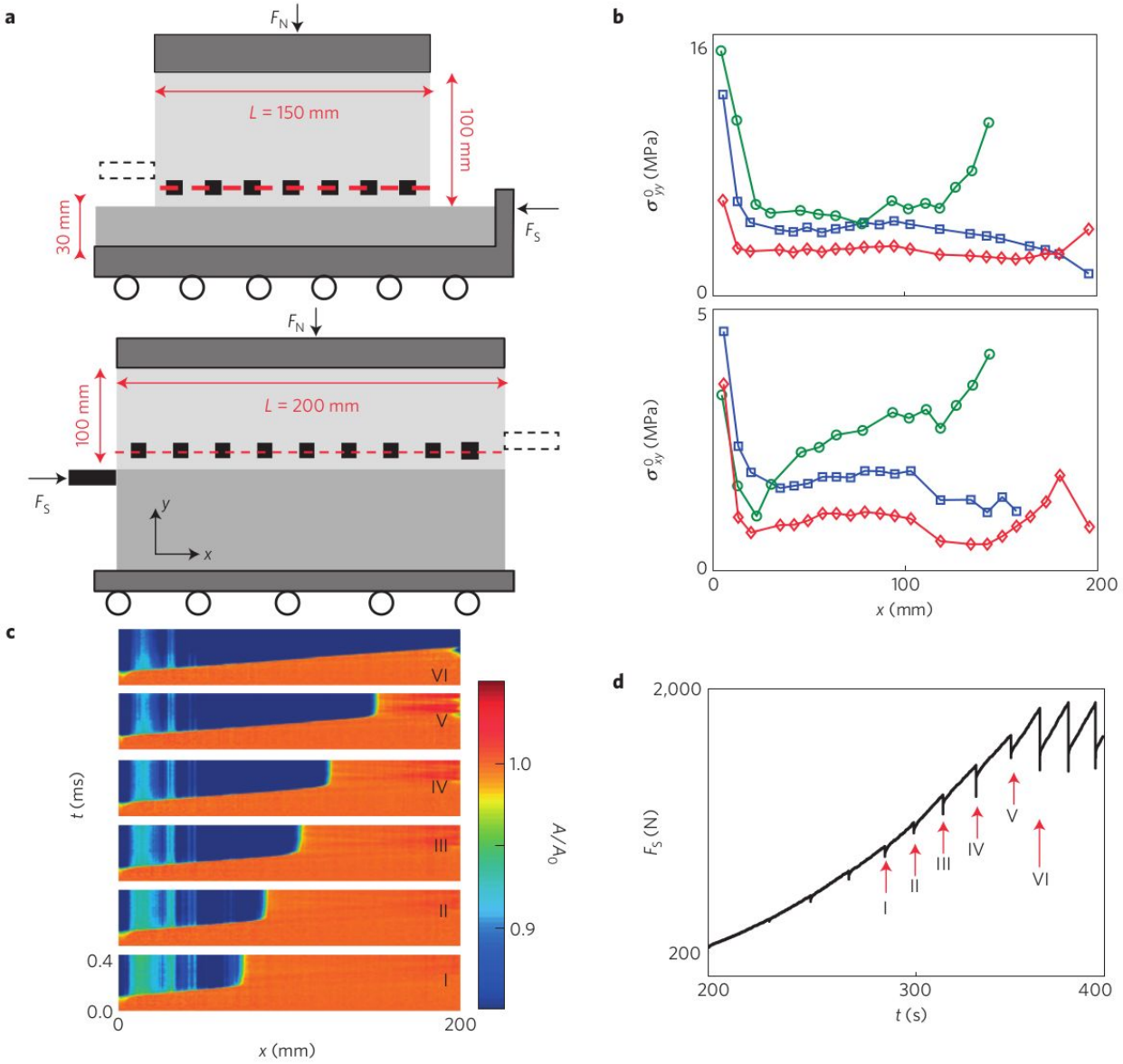




Ageing


RH = 60%
100 s
10 s
1 s
0.1 s
'Sticking'
ΔF
F_ss
Lateral force, F_L (nN)
Lateral displacement, D (nm)
ΔF (nN)
Hold time, t_hold (s)
0
150
300
450
600
0
20
40
60
80
100
0.01
0.1
1
10
100
1,000

Fractures


a
F_N
L = 150 mm
100 mm
30 mm
F_S
F_N
100 mm
L = 200 mm
F_S
y
x
b
16
0
σ^0_{yy} (MPa)
5
0
σ^0_{xy} (MPa)
0
100
200
x (mm)
c
VI
V
IV
III
II
I
t (ms)
0.4
0.0
0
200
x (mm)
1.0
0.9
A/A_0
d
2,000
200
F_S (N)
I
II
III
IV
V
VI
200
300
400
t (s)

Suggested reading

- A. Vanossi, N. Manini, M. Urbakh, S. Zapperi, E. Tosatti, **“Modeling friction: From nanoscale to mesoscale”**, Rev. Mod. Phys. 85, 529 (2013)
- O.M. Braun, Yu.S. Kivshar, **“The Frenkel-Kontorova Model: Concepts, Methods, and Applications”**, Springer (2004)
- B.N.J. Persson, **“Sliding Friction”**, Springer (2000)
- S.Yu. Krylov, J.W.M. Frenken, **“The physics of atomic-scale friction: Basic considerations and open questions”**, Phys. Status Solidi B 251, 711–736 (2014)