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Anisotropy Effects in Atomic-Scale Friction

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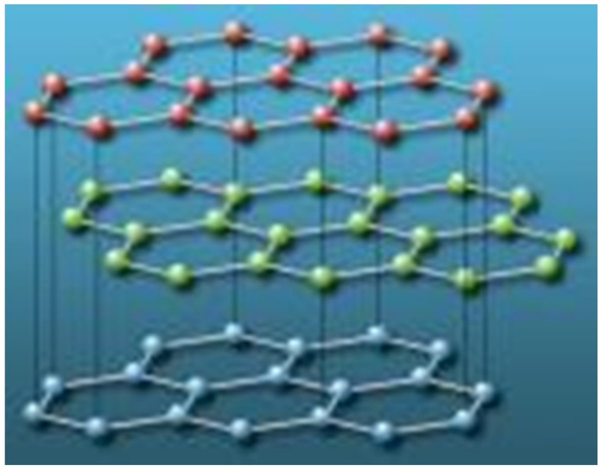
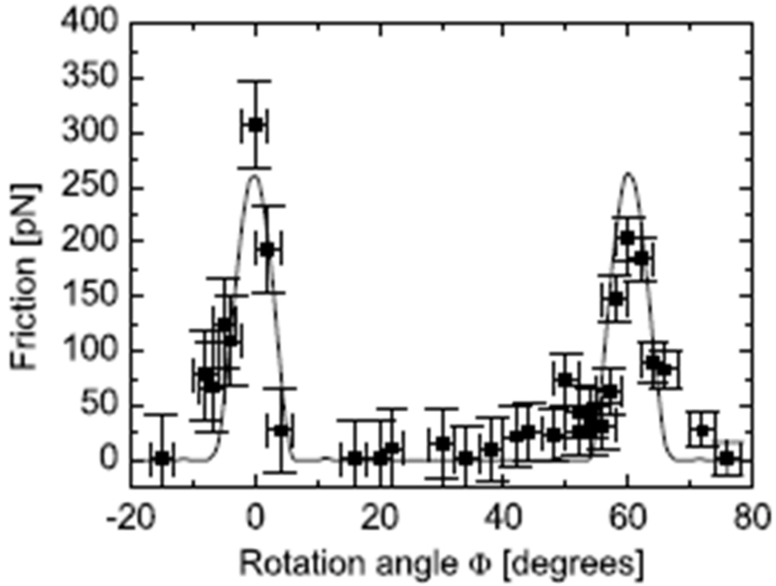
Motivation

• Friction vanishes when two mismatched surface lattices slide past each other

• For instance: Two graphite surfaces with different orientations





M. Dienwiebel et al., Phys. Rev. Lett. 92 (2004) 126101

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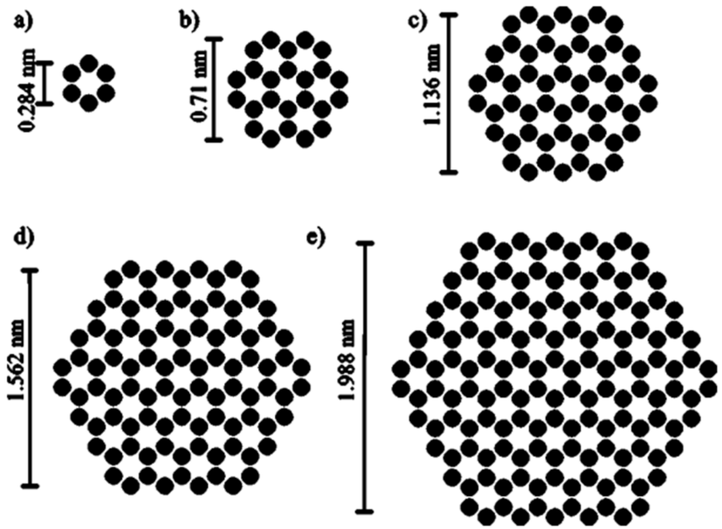
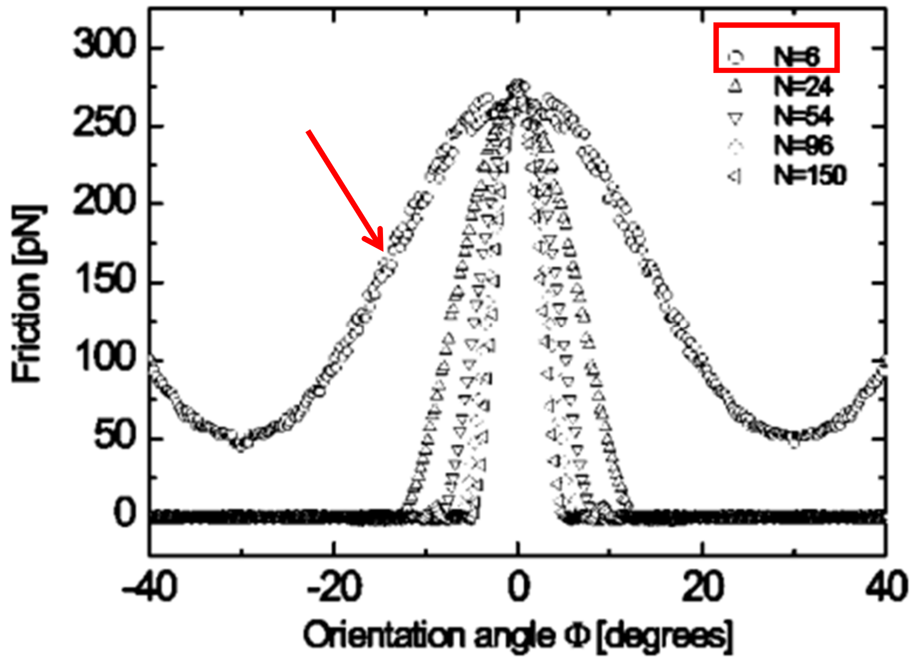
Motivation

• Model calculations (with rigid lattices):





• Anisotropy is reduced if contact area decreases

• Contact formed by a single chemical bond?

G.S. Verhoeven et al., Phys. Rev. B 92 (2004) 126101

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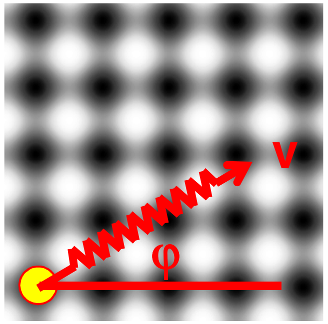
The Prandtl-Tomlinson model in 2D

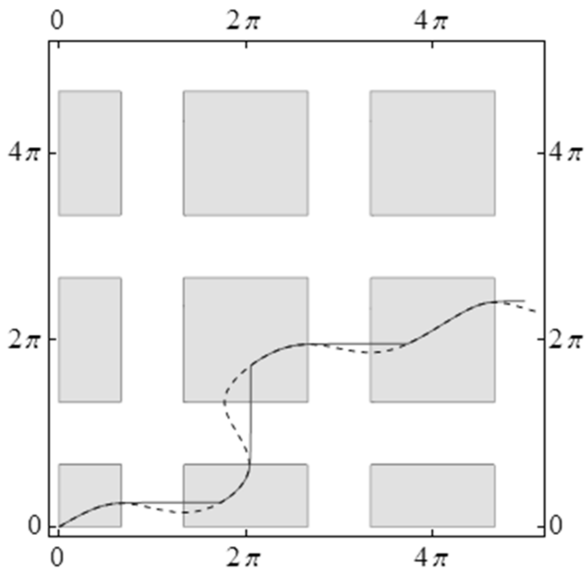


$\boxed{F(\varphi) = ?}$

• Two different approaches:

1) Calculate equilibrium positions for the tip
(OK for static friction)

2) Solve the equations of motion of the tip
(tip mass and damping coefficient appear)



------------------- equilibrium positions of the tip apex

——————— numeric solution of the equation of motion

Stability regions

• On a <u>square lattice</u> jumps are straight and oriented at 0 or 90°
→ The problem is considerably simplified

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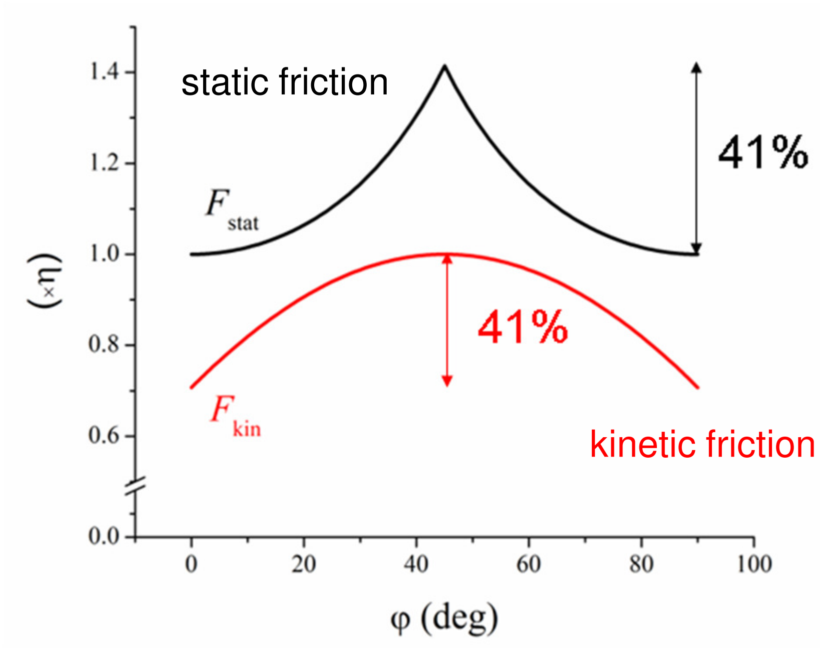
The Prandtl-Tomlinson model in 2D

- If the tip-surface interaction is sufficiently strong (η >>1):

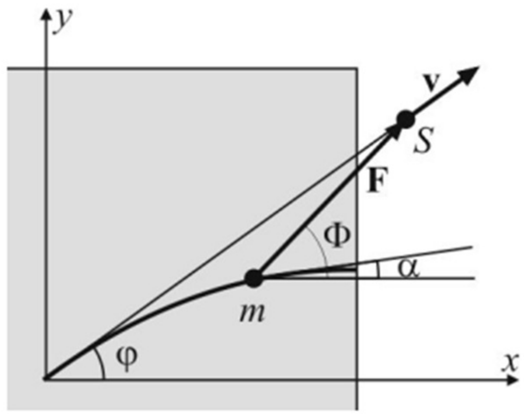


- If η --> static friction is affected by offset

$$F_{stat} = \begin{cases} \dfrac{\eta}{\cos\varphi} & (0° < \varphi < 45°) \\ \dfrac{\eta}{\sin\varphi} & (45° < \varphi < 90°) \end{cases}$$

$$F_{kin} = \eta \cos(45° - \varphi)°$$

In both cases: $\boxed{\dfrac{F_{max}}{F_{min}} = \sqrt{2}}$



Phys. Rev. B 82 (2010) 205417

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Directionality in atomic-scale friction

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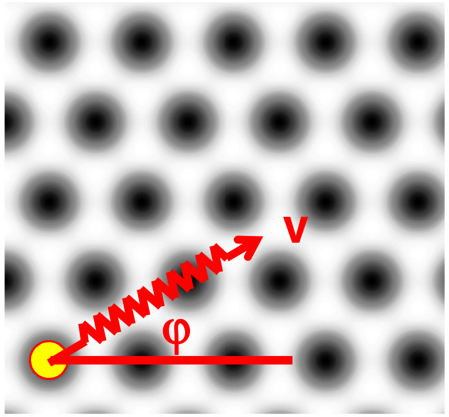
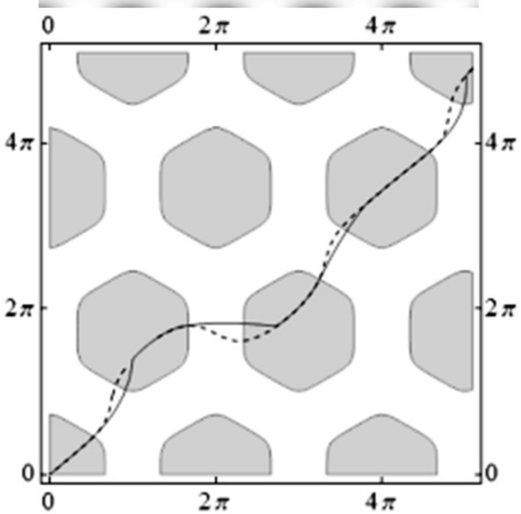
• <u>Hexagonal</u> lattices:





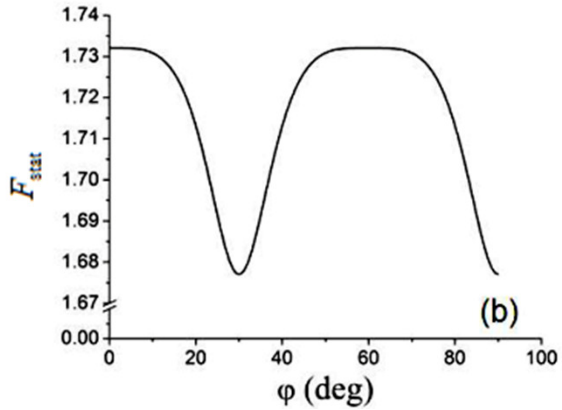
- General solution:

$$\boxed{F_{\text{stat}} = \frac{\eta}{\sqrt{3}}\sqrt{c_x^2 + 4c_x c_y + 7c_y^2 - 4c_x^2 c_y^2 - 4c_x c_y^3 - 4c_y^4}}$$

$$\boxed{c_x = \frac{(\eta-2)c_y - 2\eta c_y^3 \pm \Delta}{\eta}}$$

$$c_x = \cos x, \quad c_y = \cos\frac{y}{\sqrt{3}},$$

$$\Delta = \sqrt{(\eta-1)(\eta+3) - 4(2\eta-1)c_y^2 - 4\eta(\eta-2)c_y^4 + 4\eta^2 c_y^6}$$



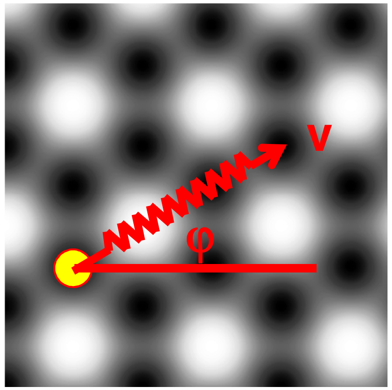
$$\boxed{1.016 < \frac{F_{\max}}{F_{\min}} < 1.033}$$

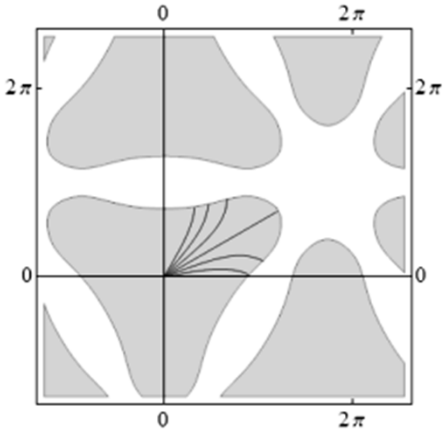
- Static friction is almost independent of the scan direction!

Europhys. Lett. 91 (2010) 66008

Directionality in atomic-scale friction

• "Honeycomb" lattices:





Strong anisotropy of static friction
(~ 75% when η = 2)

- Static friction is strongly influenced by the density of packing of the surface atoms:

6 neighbors: 3% anisotropy
4 neighbors: 41% anisotropy
3 neighbors: 75% anisotropy

- Kinetic friction?
- Experimental results are (almost) missing !

Europhys. Lett. 91 (2010) 66008

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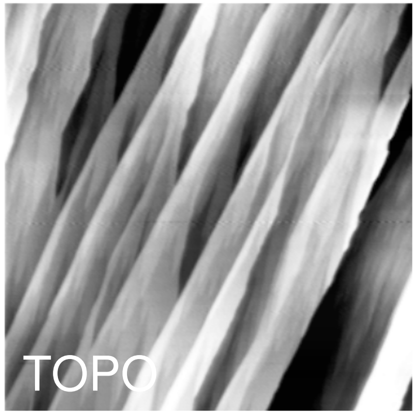
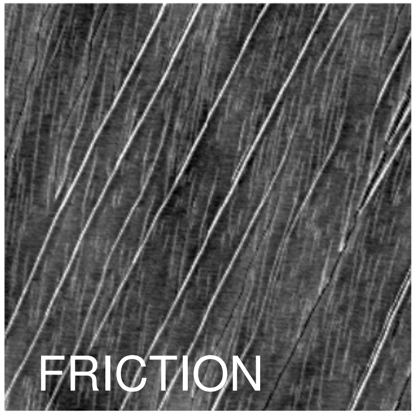
Friction at step edges

- Again dolomite (104) (on a larger scale):





- Friction increases both step-up and step-down
- Effect due to Schwöbel-Ehrlich barrier: see Meyer et al., JVSTB 1996 & Hölscher et al., PRL 2008)
- Experiments performed on KBr(001) in UHV (group of Prof. Ernst Meyer)
- Numeric calculations in collaboration with Prof. Jerzy Konior

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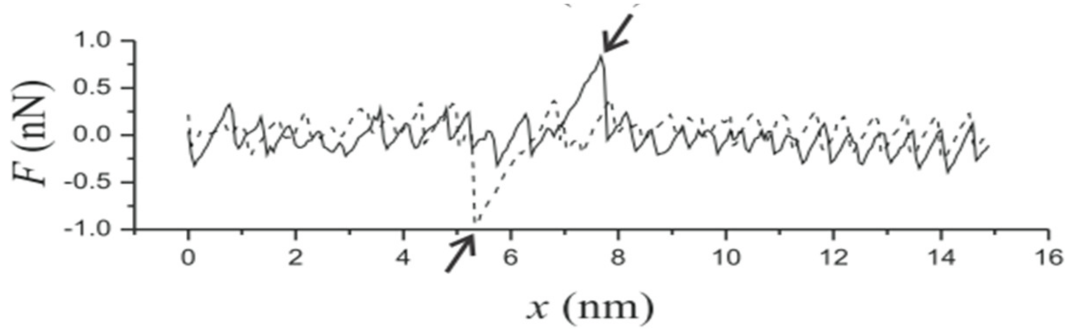
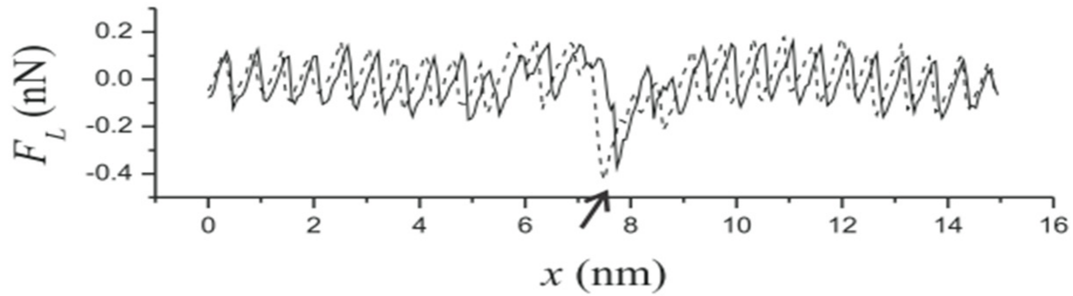
Friction at step edges

- Case 1) Friction increases both step-up AND step-down (most common, see PRL Hölscher 2008):



- Case 2) Friction increases step-up BUT decreases step-down:



Phys. Rev. Lett. 106 (2011) 186104

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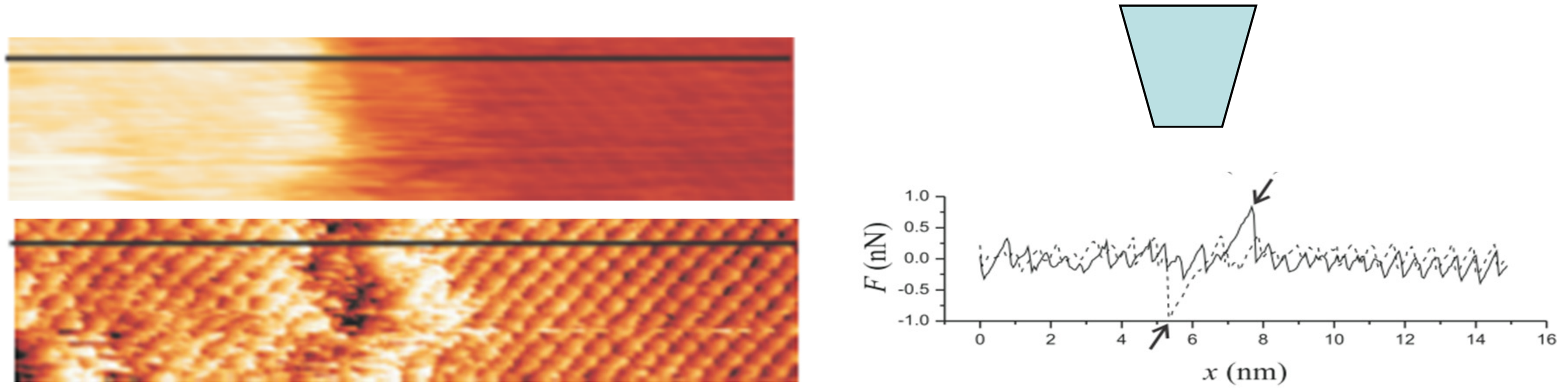
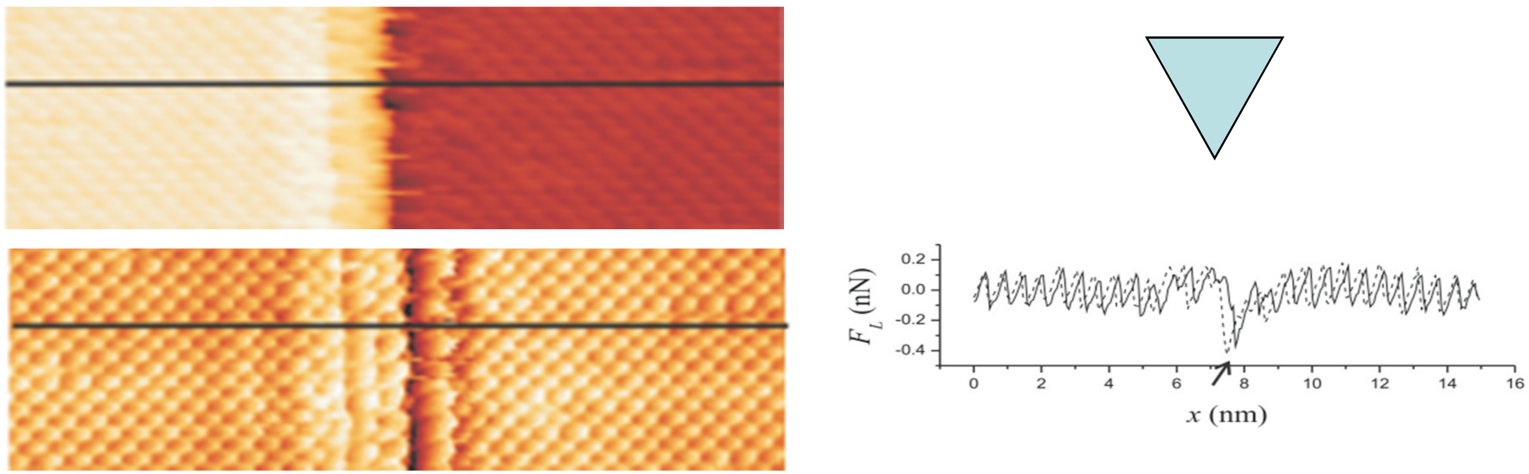
Friction at step edges

- Blunt tips → Friction increases step-up and step-down:



- Sharp tip → Friction increases step-up BUT decreases step-down:



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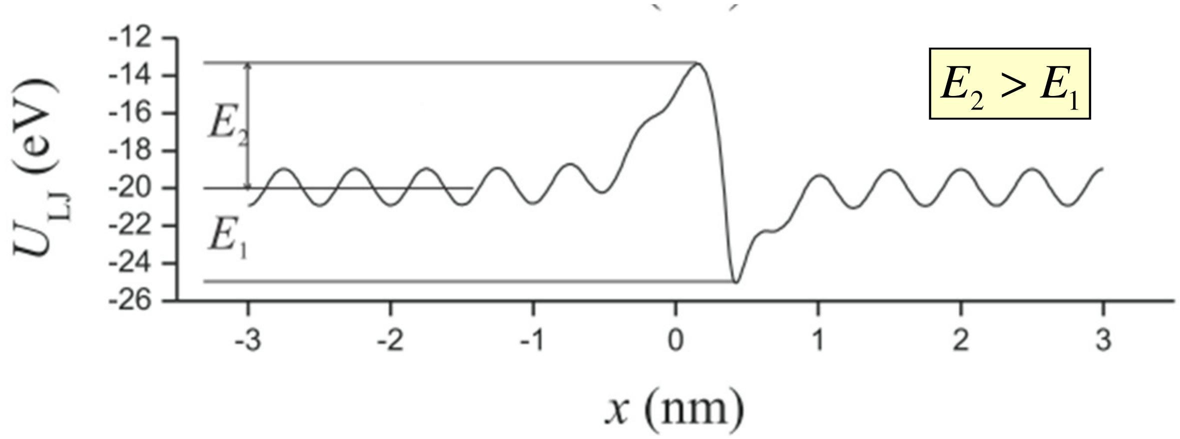
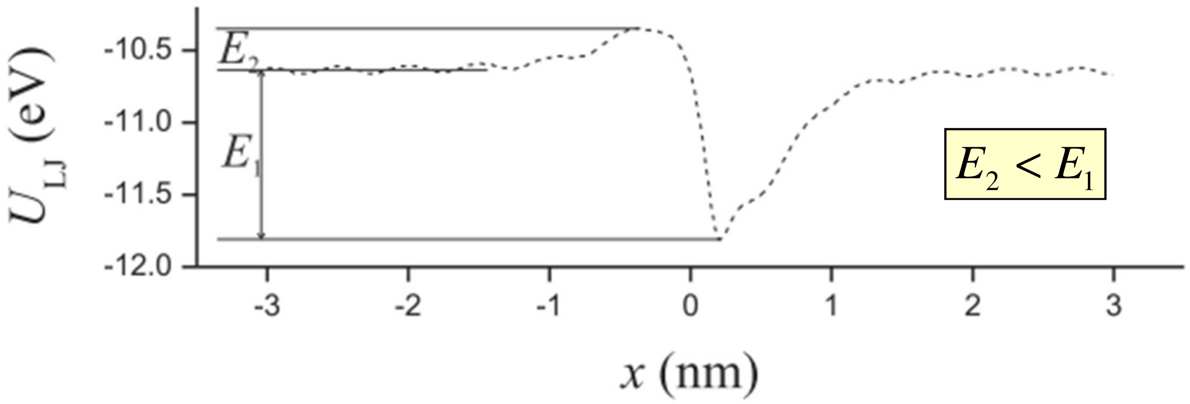
Friction at step edges

• Lennard-Jones potential at different loads (atomically sharp tip, Coulomb interaction is neglected):



d = 0.55 nm



d = 0.65 nm

- Depending on the distance, either the Schwöbel barrier or the potential well prevails

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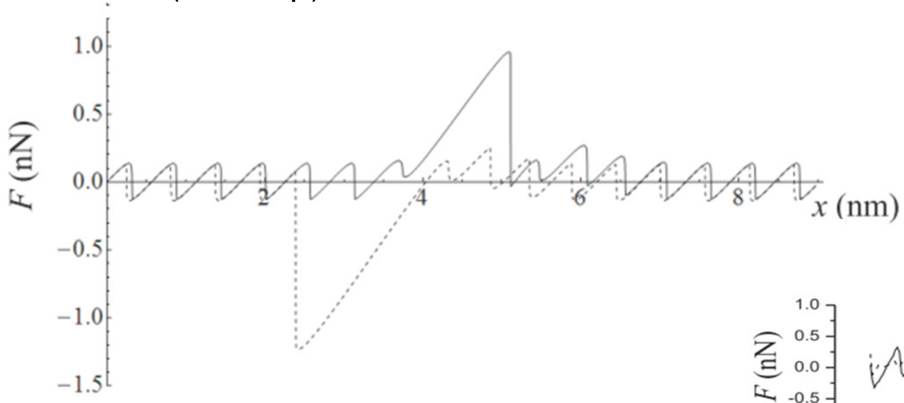
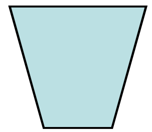
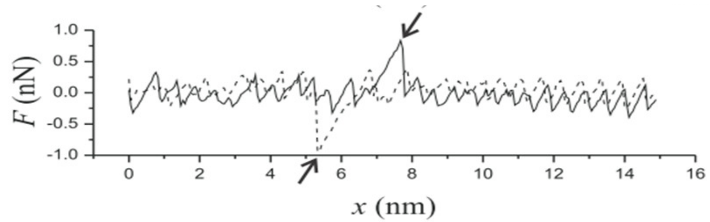
Friction at step edges

• Experimental results are reproduced using empirical potentials based on previous calculations:

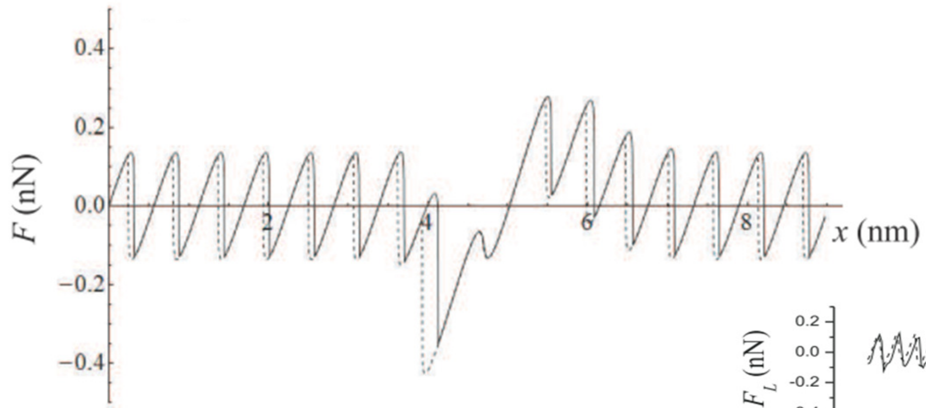
- Case 1 (blunt tip):

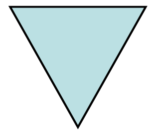


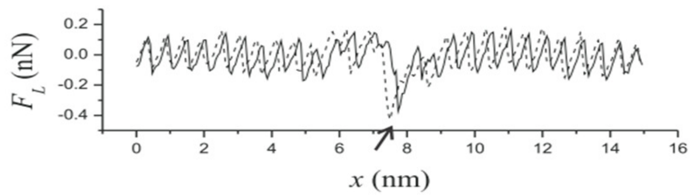




- Case 2 (sharp tip):







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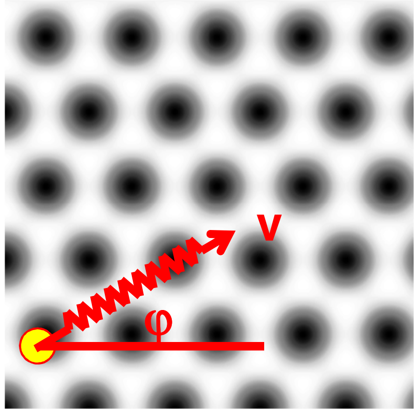
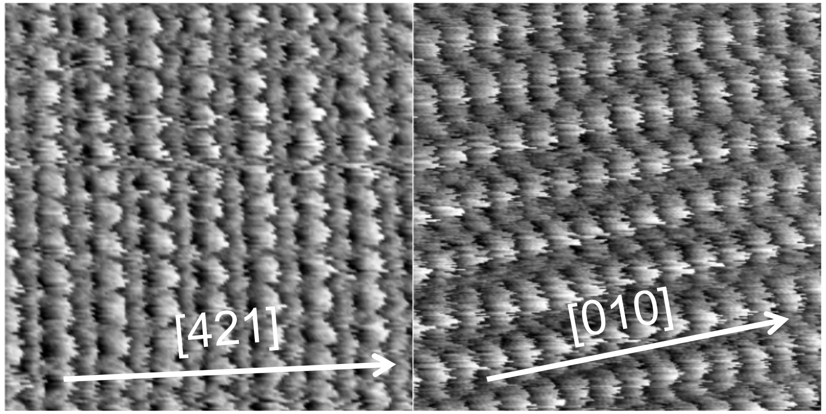
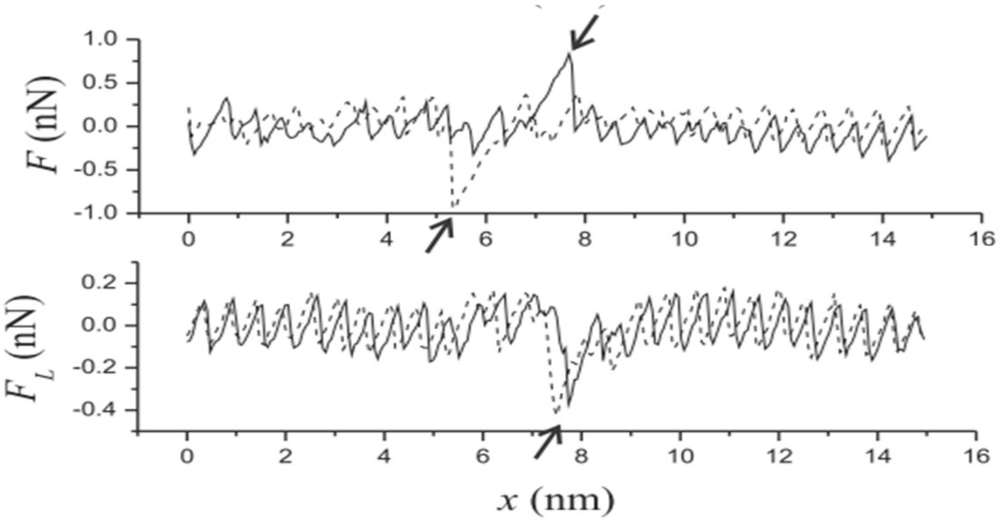
Conclusions

1) Prandtl-Tomlinson applied to predict static and kinetic friction in 2D systems
2) Selective formation of chemical bonds while sliding
3) Anisotropy of friction at step edges (also explained by the PT model)







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