



Single-asperity mechanics: Nanoscale plasticity and friction

*T. Filleter*¹, *Ph. Egberts*^{1,4}, *J. McChesney*², *A. Bostwick*², *E. Rotenberg*², *K. Emtsev*³, *Th. Seyller*³, *K. Horn*⁴, <u>*R. Bennewitz*^{1,5}</u>

¹McGill University, Montreal ²Lawrence Berkeley National Laboratory ³Universität Erlangen-Nürnberg ⁴Fritz-Haber-Insitute, Berlin ⁵INM – Leibniz Institute for New Materials, Saarbrücken

Outline: Force Microscopy in Nanomechanics

- Forces required
- Dissipation encountered

- Moving into the surface Plasticity and Wear
- Moving on the surface Friction on the Atomic Scale
- Moving close to the surface –
 Dissipation Force Microscopy

- Incipient plasticity
- Friction on thin films I: KBr on Cu(100)
- Atomic friction: Questions coming with the Tomlinson model
- Friction on thin films II: Graphene on SiC(0001)

Force and Dissipation in Nanomechanics



- Chemist
 - Force: 1 eV/1A = 1.6 nN
 - Dissipation: 1 eV

- Surface Scientist
 - Force: $2\pi 0.2 \text{eV}/0.33 \text{ nm} = 0.6 \text{ nN}$
 - Dissipation: 0 eV

Indentation experiment

Oxidized silicon AFM tip



Force vs. displacment curve in KBr(100)



• Force 2.5 µN to observe onset of plasticity

- Tip jumps by 0.33 nm (one atomic layer) into the surface
- Four jumps in this indentation experiment
 - Work per event 2.5 μN ×0.33 nm = 5000 eV

Phys. Rev. B 73 (2006) 155433

Dislocation structure and shear strength

KBr(100) after indentation



Detail including a preexisting square hole.

Phys. Rev. B 73 (2006) 155433



- Screw dislocation penetrate the surface around the indentation.
- Dislocation motion leaves steps edge trace behind.
- Force can be converted into a Yield stress 4.8 GPa, 14% of Young's modulus.
- Shear stress acting on {110} glide planes is 2.5 GPa, in agreement with DFT calculations.
- Plastic energy is stored along dislocation lines (15 eV / nm).
 5000 / 12 = 400 nm upper bound for dislocation line length through the bulk.

Power of resolution

KBr(100) about 100 nm from an indentation.



Atomic resolution of hilliocks reveals two edge dislocations with opposite Burgers vectors.



Reversibility of plasticity



KBr(100)

- Annihilation of two dislocation about 1 hour after indentation.
- Screw dislocations move, cross-slip, curve, and meet.
- How much work went into strain energy?

Friction on KBr/Cu(100) films



Friction on islands and substrate steps



Friction Force Microscopy



- Ultimate goal: Understanding the friction vs. load curve.
- Ingredients: contact mechanics, surface interactions, dissipaton

 Actual measurement: friction vs. time for varying paramters, averaged over time





How can the lateral force become negative?

Tomlinson model for small lateral potential corrugation



$$E(t) = E_0 \left(\frac{1}{2} - \frac{1}{2} \cos\left(\frac{2\pi x}{a}\right) \right) + \frac{1}{2} k_{eff} (x - vt)^2$$



- For small lateral potentials and stiff (=larger) contacts the can jump to a minimum which corresponds to a negative lateral force.
- Simplest idea: Energy of jump is dissipated (i.e. dissipation channels are irrelevant) Reality:

Forces related to thermal effects are too large to be neglected.

 Most interesting things happen in the slip phase. Temporal detail of slip phase





$$\langle \xi(t)\xi(t')\rangle = 2m_{tip}\gamma_{tip}k_BT\delta(t-t')$$

includes thermal noise

Cantilever:
$$m_{cl}\ddot{x}_{cl} + m_{cl}\gamma_{cl}\dot{x}_{cl} - k_{cl}(\upsilon t - x_{cl}) + \sum_{i} k_{tip}(x_{tip,i,0} - x_{tip,i}) = 0$$

Newtons Equation

Experiment



Simulation

Duration of slip events



Relevant time scales



The relevant time scales

- 1) The mechanical resonance of the cantilever about 200 kHz = $1 / 5\mu$ sec
- 2) The oscillation of the contact in the molecular potential MHz
- 3) The time constant of internal damping of the cantilever Q/f = 3.5 msec
- 4) The time constant of coupling tip motion to phonons ????

Thermally activated Tomlinson model

- No thermal activation: Dissipation is determined by lateral potential and contact stiffness.
- Simple thermal activation of slip: Dissipation is reduced by thermal activation of jump to lower minimum.
- Complex thermal activation os slip I: Tip is jumping forth and back around the slip event, cantilever can not follow fast jumps.
- Complex thermal activation of slip II: Tips are jumping forth and back around the slip event, cantilever can not follow fast jumps.
- Contact delocalisation: Tip continously moved between adjacent minima, time average of cantilever appears as stick-slip.

Epitaxial graphene on SiC(0001)

Single and bilayer graphene on SiC(0001) grown by thermal decomposition in ambient pressure argon. (Erlangen group)





- Complex topography of epitaxial graphene.
- Islands and terraces.
- Only few edges with obvious crystallographic orientation.
- Clear identification of layers in Kelvin probe force microscopy.

Friction on graphene films



Atomic friction on single and bilayer



- Stick-slip occurs on both layers.
- Lateral stiffness is the same.
- Symmetry is the same.
- No contrast in interfacial interactions.
- But: Contrast in dissipation.
- Interface layer (6x6) visible.



- Factor of two in friction between single and bilayer graphene.
- No significant contribution of adhesion.
- No load dependence of 6x6 modulation observed.

Materials considerations



- Huge decrease of friction compared to (contaminated) interface layer.
- Bilayer outperforms graphite as solid lubricant due to lower adhesion.



Friction and electron-phonon coupling

- Hypothesis: Friction on single layer graphene is higher due to stronger electron-phonon coupling.
- Mechanism: Can act only in the slip phase of atomic stick-slip. Load dependence is classical contact mechanics.
- Energy is more effectively dissipated, therefore there is less thermolubrication.
- Question: Are we in one of Krylov's averaging regimes?



Current team

