On the Scientific and Technological Importance of Nanotribology

R.W. Carpick

U. Pennsylvania, Dept. of Mechanical Engineering and Applied Mechanics

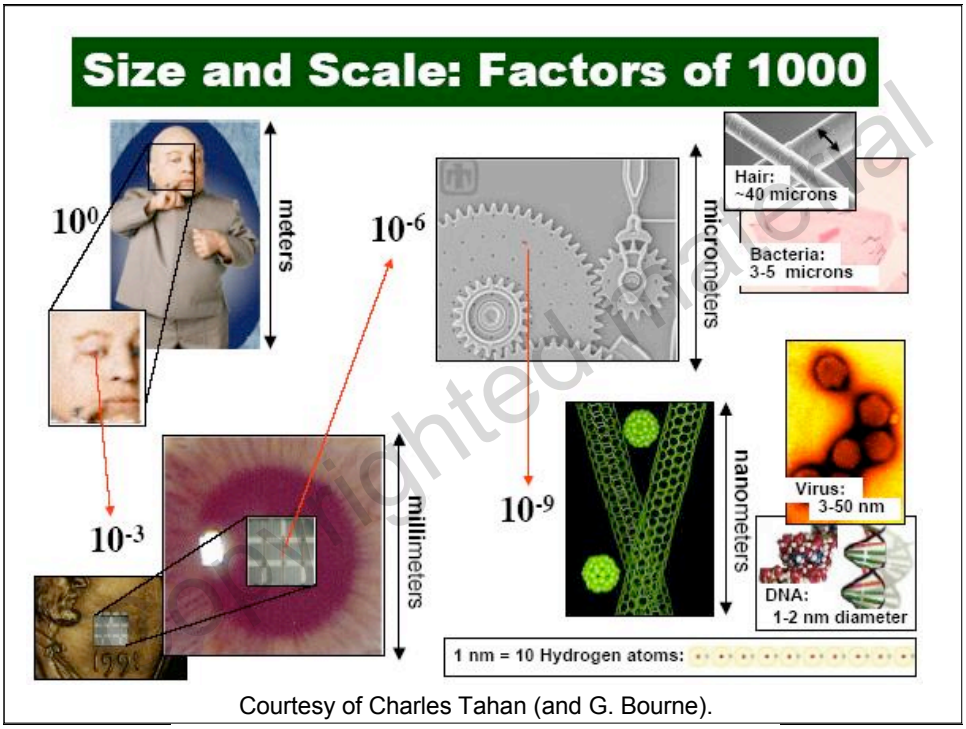
A free resource for you - please join:
http://www.nanoprobenetwork.org

Outline

- Some Nano(tribology) 101
- Examples of applications where nanotribology is critical
- Some scientific challenges, in my view

Shameless plug:

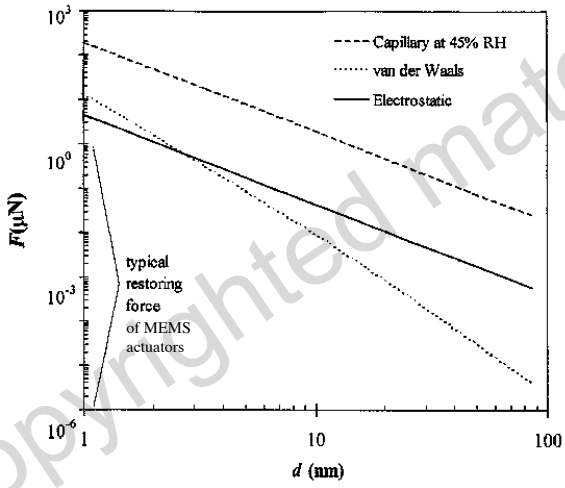
Recent advances in single-asperity nanotribology
Szlufarska, Chandross, & Carpick
J. Phys. D.: Appl. Phys. **41** (2008)



Courtesy of Charles Tahan (and G. Bourne).

Scale effects: Surface-to-volume

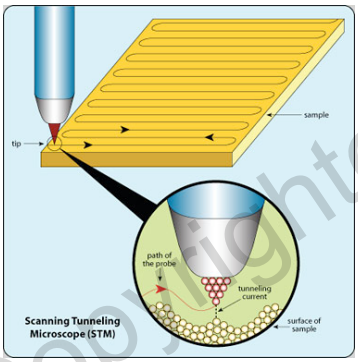
R. Maboudian, Surf. Sci. Rep., **30** (1998) 207-269



Attractive forces per 1 μm² for two perfectly smooth silicon surfaces as a function of separation, *d*.

The laws of mechanics are different at small scales...

- quantum mechanics
  - wave particle duality: electrons can tunnel
    - Scanning tunneling microscope

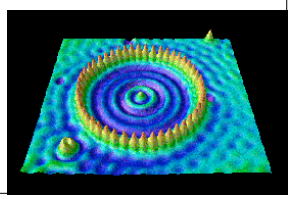


source: http://www.nisenet.org/publicbeta/articles/seeing_atoms/index.html

(SET)

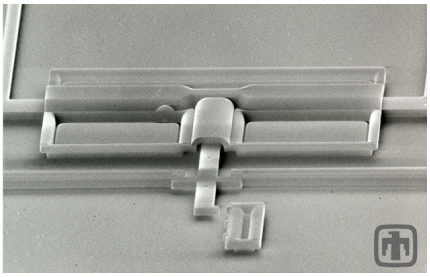
The laws of mechanics are different at small scales...

- quantum mechanics (continued)
  - quantum confinement of electronic states: discrete energy levels for systems
    - discrete energy levels *vs.* the continuum
    - semiconductor nanocrystals, 1- 10 nm wide
      - size quantization effect
      - see - http://www.evidenttech.com/
    - quantum corral



Don Eigler, IBM Research

Problem, or opportunity?



Sandia National Labs

Micro-scale (*not* nano!): Water inside of this micro-compression cylinder is heated by electric current and vaporizes, pushing the piston out. Capillary forces then retract the piston once current is removed.

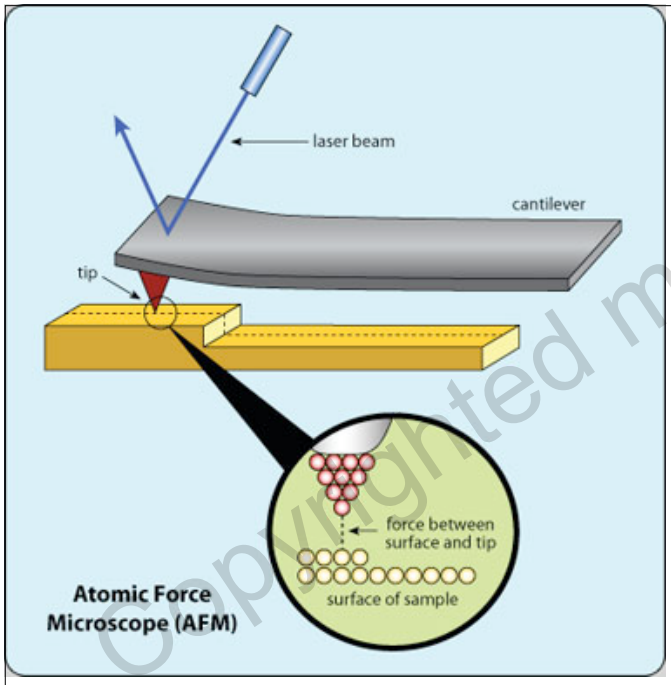
Fig. 2. Tokay gecko (*Gekko gecko*) adhering to molecularly smooth hydrophobic GaAs semiconductor. The strong adhesion between the hydrophobic surface of the gecko's toes and the hydrophobic GaAs surfaces demonstrates that the mechanism of adhesion in geckos is van der Waals force.

Evidence for van der Waals adhesion in gecko setae, Autumn et al, PNAS, 2003

Scanning Probe Microscopy (SPM)

Definition: Methods for imaging or measuring nanoscale features of surfaces by scanning a sensor (probe) over a surface and measuring a particular type of interaction

- electric current (electrons)
- force
- light (photons)



The atomic force microscope (AFM) senses force in nano-contacts at the nanoNewton level

source: http://www.nisenet.org/publicbeta/articles/seeing_atoms/index.html

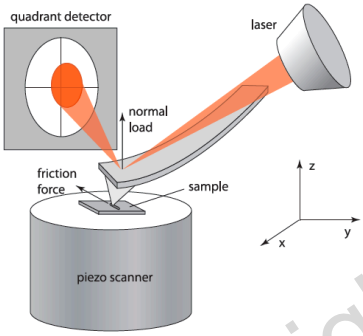
Read this

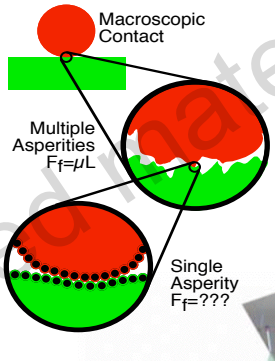
R.P. Feynman, "There's Plenty of Room at the Bottom"

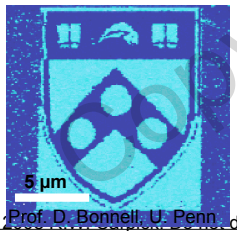
The National Nanotechnology Initiative - Strategic Plan, Dec. 2007

Some applications where nanotribology is critical

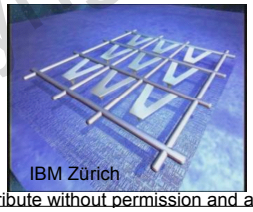
Scanning probe microscopy, and SPM-based applications: Nanolithography, nanomanufacturing, nanomechanical data storage



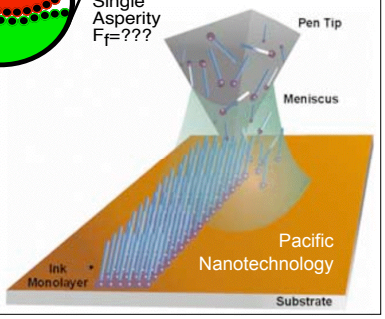




Prof. D. Bonnell, U. Penn

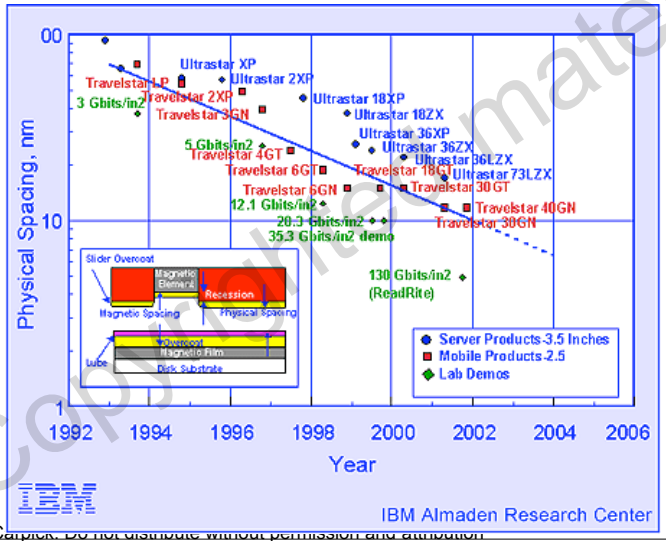


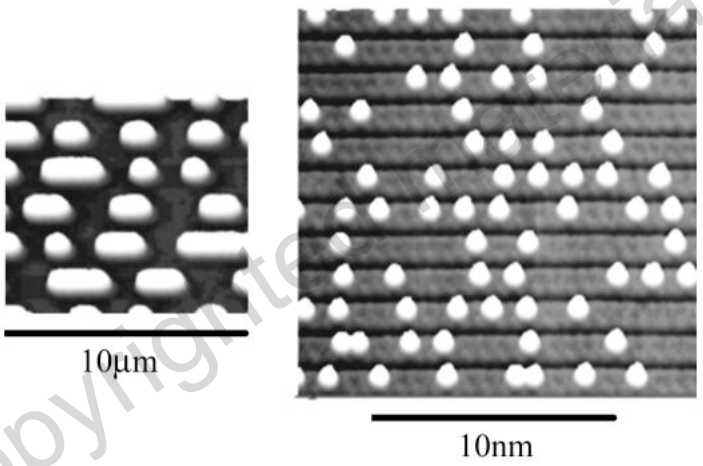
IBM Zürich



New technologies can be enabled by understanding how to apply "traditional" and "nano" mechanics approaches

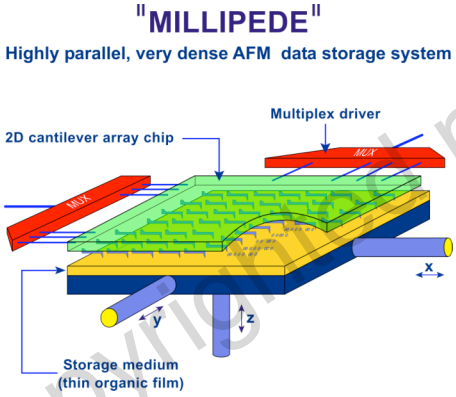
– Data storage

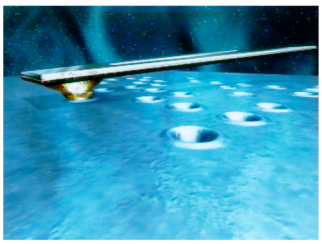




F. Himpsel, UW-Madison

IBM's "Millipede" project





Vettiger, IBM Research journal (1999)

We have already achieved several key micro- and nano-mechanical capabilities

- Working MEMS devices
- Computer hard disks
- AFM/scanning probes
  - imaging of atomic structure, manipulation of individual atoms and molecules, measurement of molecular interactions, high-resolution mechanical properties measurements
- Nanomanipulation

Key point

Widespread commercial/societal success of nanotechnology relies critically on scientific and technological advances in nanomechanics and nanotribology

Some scientific challenges

History: First observation of atomic-scale stick-slip behavior

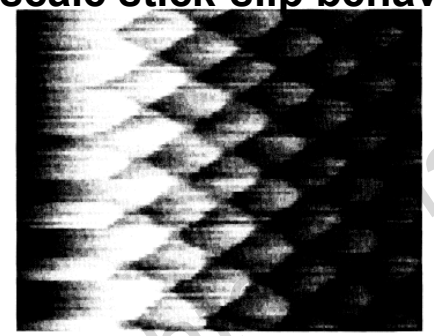
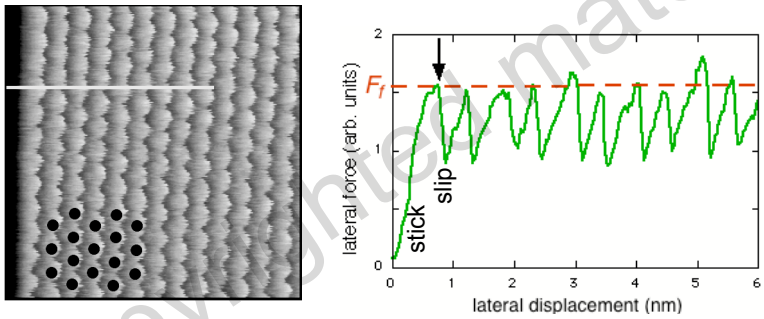


FIG. 3. The frictional force in the x direction as a function of x and y. The intensity of the image is scaled to the frictional force with the bright areas corresponding to a high force. The full-scale change from dark to bright corresponds to 1.8×10^{-6} N. Only scans in left-to-right direction are shown. The size of the image is 20 by 20 Å.^{2} with no correction for distortion from the piezoelectric scanners. The load on the tip is 5.6×10^{-5} N, and the wire spring constant is 2500 N/m.

C. M. Mate, G. M. McClelland, R. Erlandsson, and S. Chiang, "Atomic-Scale Friction of a Tungsten Tip on a Graphite Surface," Phys. Rev. Lett. 59, 1942 (1987)

Atomic-scale stick-slip motion with a well-defined friction force is frequently observed

Muscovite mica
7.5 x 7.5 nm²



Tomlinson Model

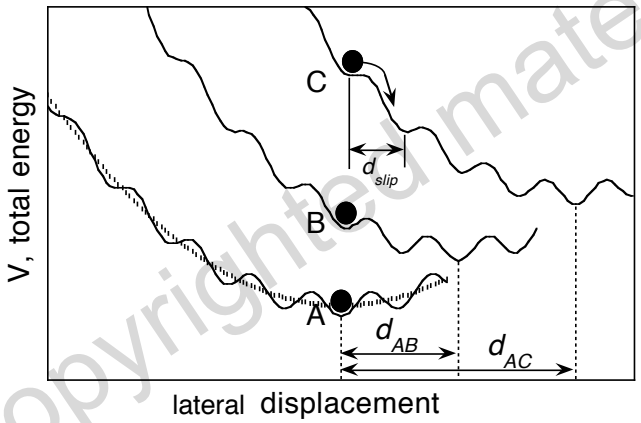
$$U = U_{\text{elastic}} + U_{\text{interface}}$$
$$= \tfrac{1}{2}k\left(x - x_{tip}\right)^2 + U_0 \sin\left(kx\right)$$

Stable equilibrium: $\partial U/dx = 0,\ \partial^2 U/\partial x^2 > 0$.

Metastable equilibrium: $\partial U/dx = \partial^2 U/\partial x^2 = 0$

Unstable equilibrium: $\partial U/dx = 0,\ \partial^2 U/\partial x^2 < 0$.

Energy *vs.* lateral displacement



http://www.nano-world.org/frictionmodule/content/

"Superlubricity"

VOLUME 92, NUMBER 13 PHYSICAL REVIEW LETTERS week ending 2 APRIL 2004

Transition from Stick-Slip to Continuous Sliding in Atomic Friction: Entering a New Regime of Ultralow Friction

A. Socoliuc, R. Bennewitz,* E. Gnecco, and E. Meyer

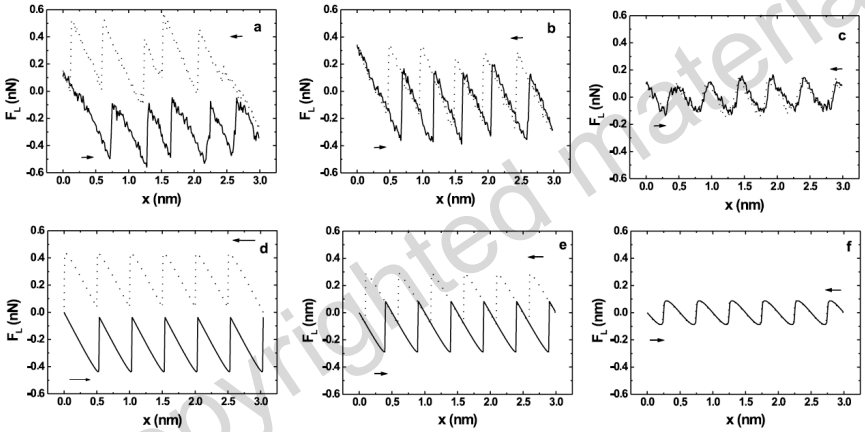


FIG. 1. (a)–(c) Measurements of the lateral force acting on the tip sliding forward and backward in (100) direction over the NaCl(001) surface. The lines are typical cross sections through a two-dimensional scan along the strongest force amplitude. The externally applied load was (a) $F_N = 4.7$ nN, (b) $F_N = 3.3$ nN, and (c) $F_N = -0.47$ nN. (d)–(f) Corresponding numerical results from the Tomlinson model for (d) $\eta = 5$, (e) $\eta = 3$, and (f) $\eta = 1$. The stiffness was chosen as $k = 1$ N/m and the lattice constant as $a = 0.5$ nm. Note that for values of $\eta \leq 1$ the hysteresis loop enclosed between the forward and the backward scan vanishes; i.e., there is no more dissipation within this model.

What is happening at the interface?

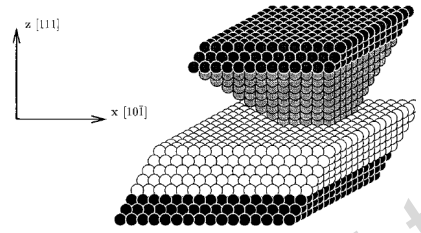


FIG. 1. A flat Cu(111) tip in matching contact with a Cu(111 substrate. There are 5×5 atoms in the bottom layer of the tip.

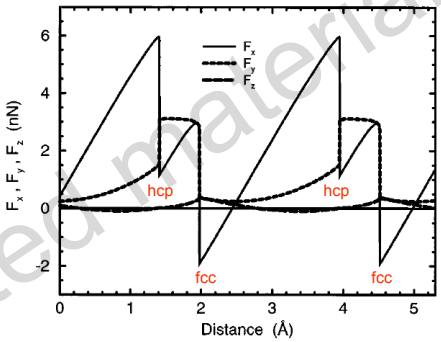


FIG. 2. The three components of the force on the tip as a function of the sliding distance. The contacting Cu(111) surfaces have identical orientation. $T = 0$ K.

PHYSICAL REVIEW B VOLUME 53, NUMBER 4 15 JANUARY 1996-II

Simulations of atomic-scale sliding friction

M. R. Sørensen, K. W. Jacobsen, and P. Stoltze

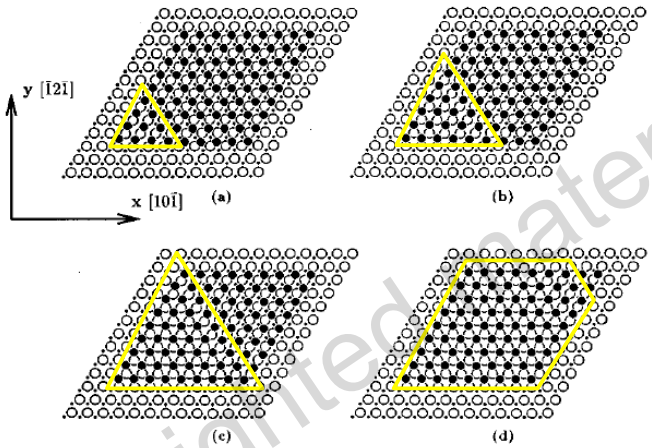
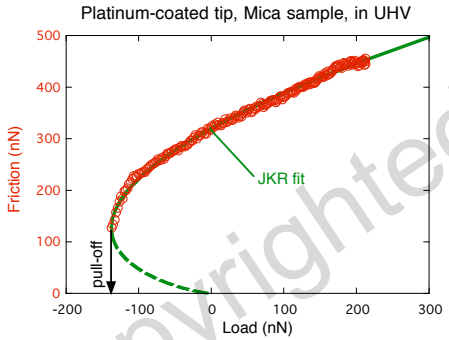


FIG. 7. Snapshots showing the 9×9 atoms in the bottom Cu(111) layer of the tip (black circles) and the atoms in the top Cu(111) layer of the substrate (white circles), during a slip event. The atoms in the second-topmost layer of the substrate are shown as black dots. These indicate the hcp positions on the surface of the substrate. The sliding direction is to the left.

from MD, at 12K

Single asperity contact results: Friction is proportional to the true contact area; continuum mechanics 'works' at nm scale



$F_f = \tau \cdot A$

friction | contact area

shear strength

Carpick et al., J. Vac. Sci. Technol. B **14** 1289 (1996)
Carpick et al., Langmuir **12** 3334 (1996)

τ ~ GPa, approaches ideal strength

but... Robbins' model

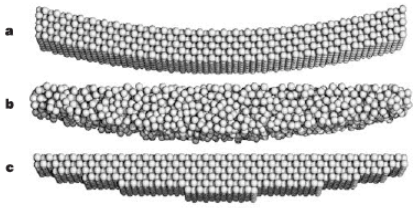
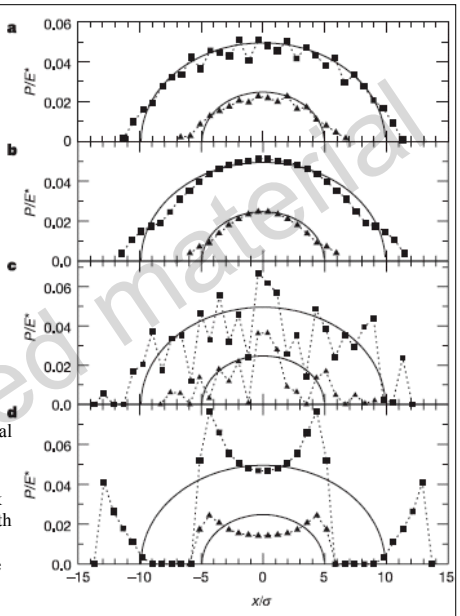


Figure 1 | Cylindrical surfaces with different atomic-scale roughness.

RIGHT: Local pressure distributions for cylinders with different atomic scale roughness. Pressure P is plotted as a function of lateral distance x from the cylinder axis for bent incommensurate crystal (a), bent commensurate crystal (b), amorphous cylinder (c), and stepped crystal (d). Results for two loads, $N/lRE^* = 0.0019$ (black triangles) and 0.0077 (black squares), are averaged along the length l of the cylinder axis and over bins of width σ along x. Solid lines show continuum predictions for the two loads, which are the same for all panels.



The breakdown of continuum models for mechanical contacts

nature

Binquan Luan[1] & Mark O. Robbins[1]

Vol 435|16 June 2005|doi:10.1038/nature03700

sphere radius R=100σ=30nm
σ^3=volume per atom

ribution

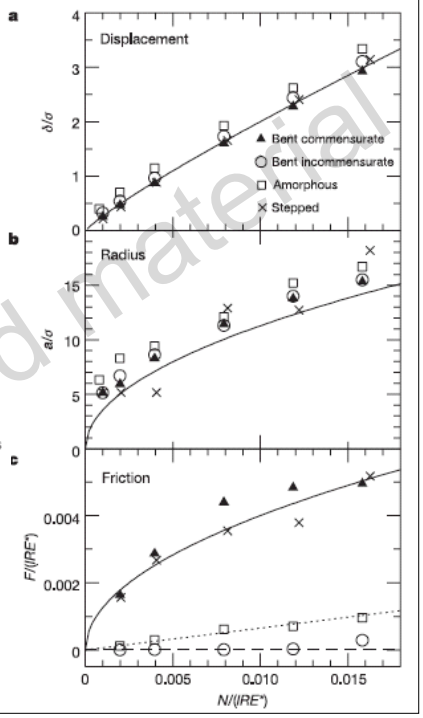
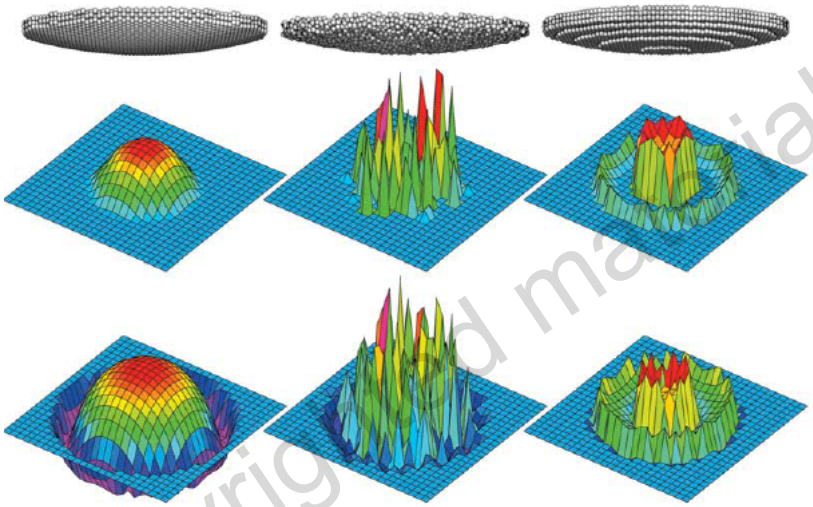


Figure 2 | Variation of normal displacement, contact radius and friction with normal load. Dimensionless plots of normal displacement δ (**a**), contact radius a (**b**) and static friction F (**c**) versus normal force N for the given cylinder surfaces (symbols). For stepped surfaces, a increases in discrete jumps. Here $R = 100\sigma$, the zero of δ corresponds to the first non-zero force, and a is half the range over which the force on substrate atoms is non-zero (Fig. 3). Solid lines show continuum predictions, with the assumption that F is proportional to area in **c**. The broken lines in **c** are linear fits.



Geometry and stress for spherical tips with and without adhesion. The top row shows the central regions (diameter 50σ) of bent, amorphous and stepped spherical tips, from left to right. The second and third rows show the pressure distributions for these tips with non-adhesive and adhesive interactions, respectively. In the adhesive case, the interaction potential between surfaces is about half as strong as interactions within the substrate (Supplementary Information). In all cases $N/E^*R^2 = 0.0013$ and $R = 100\sigma$. The pressure is plotted over a central square region of edge 42.9σ, with a constant vertical scale. Almost 107 atoms are included in the substrate to include subsurface deformations.

Nanoscale mechanics theories are rapidly emerging

- First-principles (ab-initio) techniques
  - Every atom is treated quantum-mechanically
- Molecular dynamics (MD)
  - Classical/semi-classical trajectories of atoms are calculated
- Hybrid atomistic-continuum approaches
  - e.g. finite element modeling+MD

At small scales, disciplinary boundaries disappear. Mechanics becomes integral to all of nanotechnology.

- Materials science, mechanics, chemistry, physics, electrical engineering, biology
- optics, electronics, sensors & actuators, power generation, information storage, environmental safety, security

Larger questions raised

- How do you measure and quantify wear of a tip at the nanometer scale?
- How do nanoscale wear rates compare to macroscopic wear rates?
- What are the mechanisms of wear of nanoscale tips?
  - catastrophic fracture events?
  - progressive removal of atoms?
  - tribochemistry?
- Does studying nanoscale wear shed any light on wear mechanisms for larger scale contacts?

Summary

- Mechanics and tribology are different at the nanoscale
  - Surfaces, defects, scale effects, atomic structure, quantum effects
- New theories and experimental techniques are needed, but existing approaches retain substantial utility
- Consideration of other disciplines (chemistry, physics, materials science…) becomes critical
- Similarly, other fields must consider tribology and mechanics in order to implement functioning devices, applications, techniques *etc.*