ME597/PHYS57000
Fall Semester 2010
Lecture 03

Some Topics in STM

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Birck Nanotechnology Center

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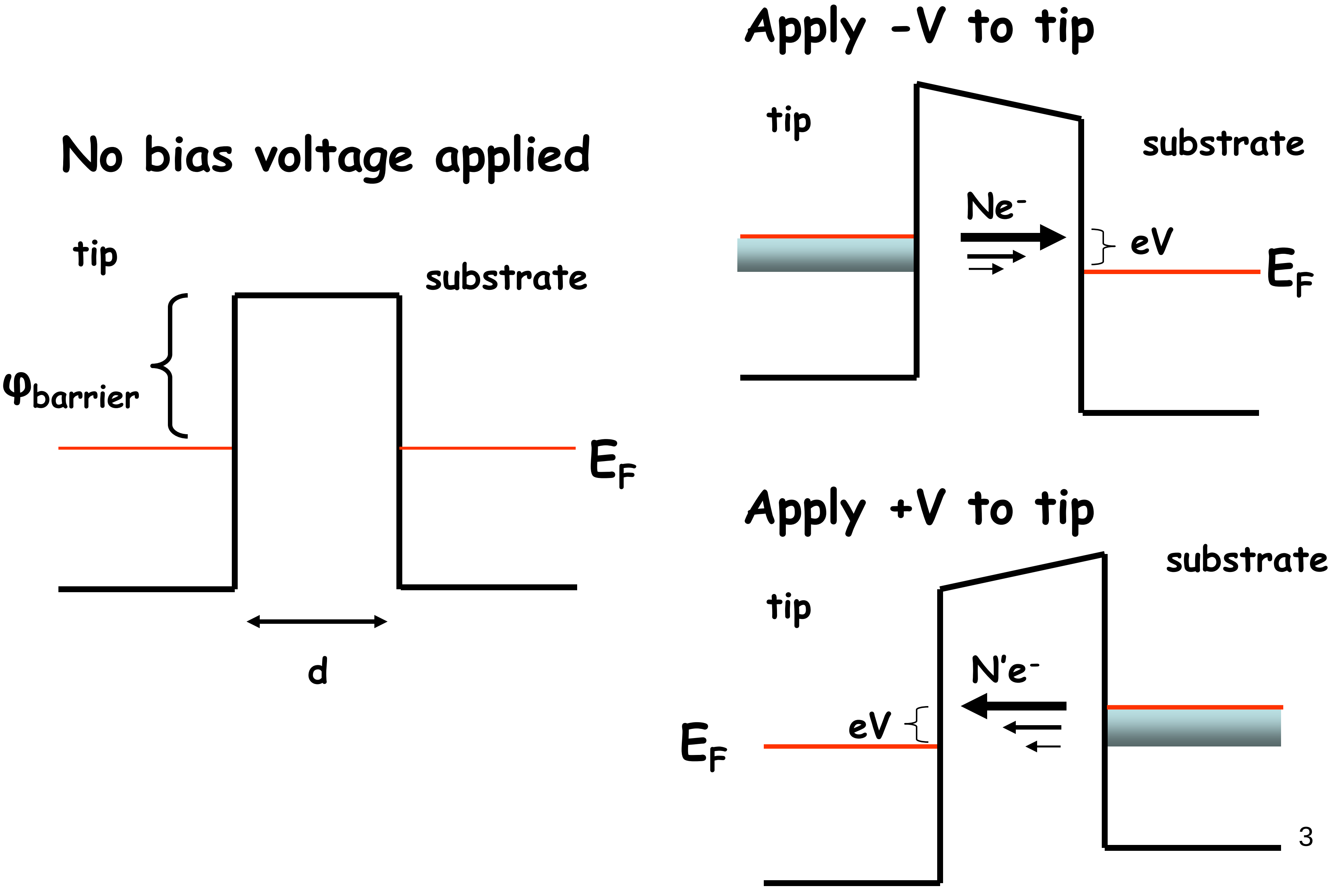
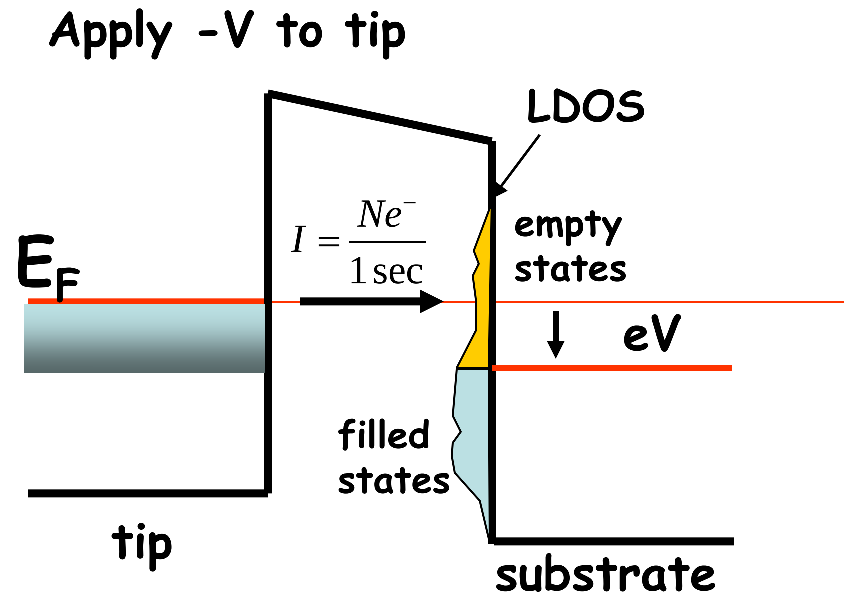
- Scanning Tunneling Spectroscopy (STS)
- Current Imaging Tunneling Spectroscopy (CITS)
- Apparent barrier height
- Force on the tip
- Atomic Corrugation
- Quantum Corrals

Scanning Tunneling Spectroscopy (STS)



What determines number of electrons that flow per unit time for an applied V?



$$I = \frac{4\pi |e^-|}{\hbar} \int_{-\infty}^{\infty} \left[f(E_F + \varepsilon) - f(E_F - eV + \varepsilon) \right] \rho_{tip}(E_F + \varepsilon) \rho_{substrate}(E_F - eV + \varepsilon)\, T(\varepsilon, V)\, d\varepsilon$$

$f(E)$ is the Fermi-Dirac distribution function

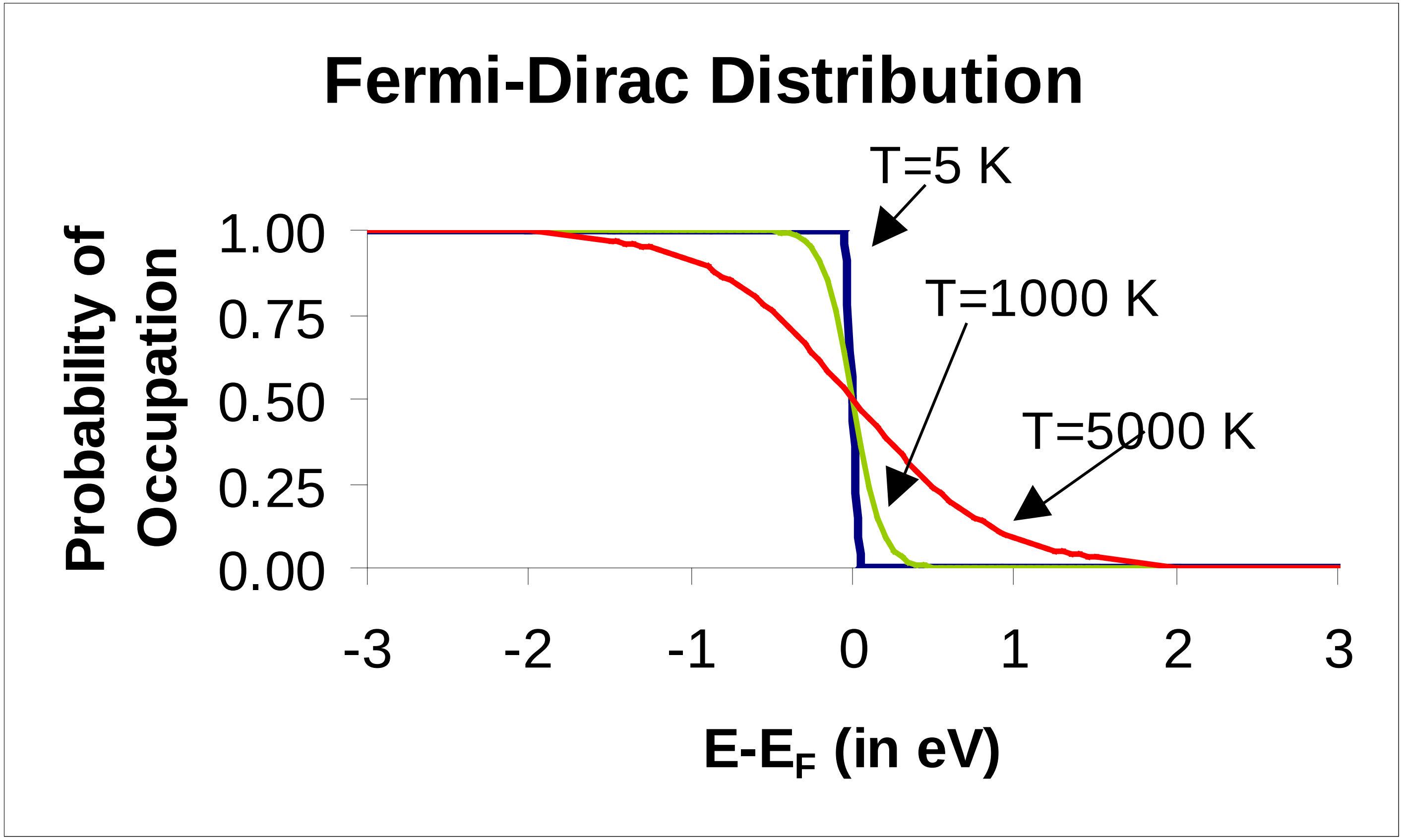
ρ_{tip} is the LDOS of tip

$\rho_{substrate}$ is the LDOS of substrate

$T(E,V)$ is the transmission probability at energy E for an applied voltage V

Fermi-Dirac distribution function

$$f(E) = \frac{1}{1 + e^{[(E - E_F)/k_B T]}}$$



A few reasonable assumptions:

- measurements at room temperature or below; k_BT at room temperature is 0.025 eV
- for voltage increments ΔV > ~2 k_BT/e, f(E) is well approximated by a step function
- assume tip DOS does not change appreciably with energy

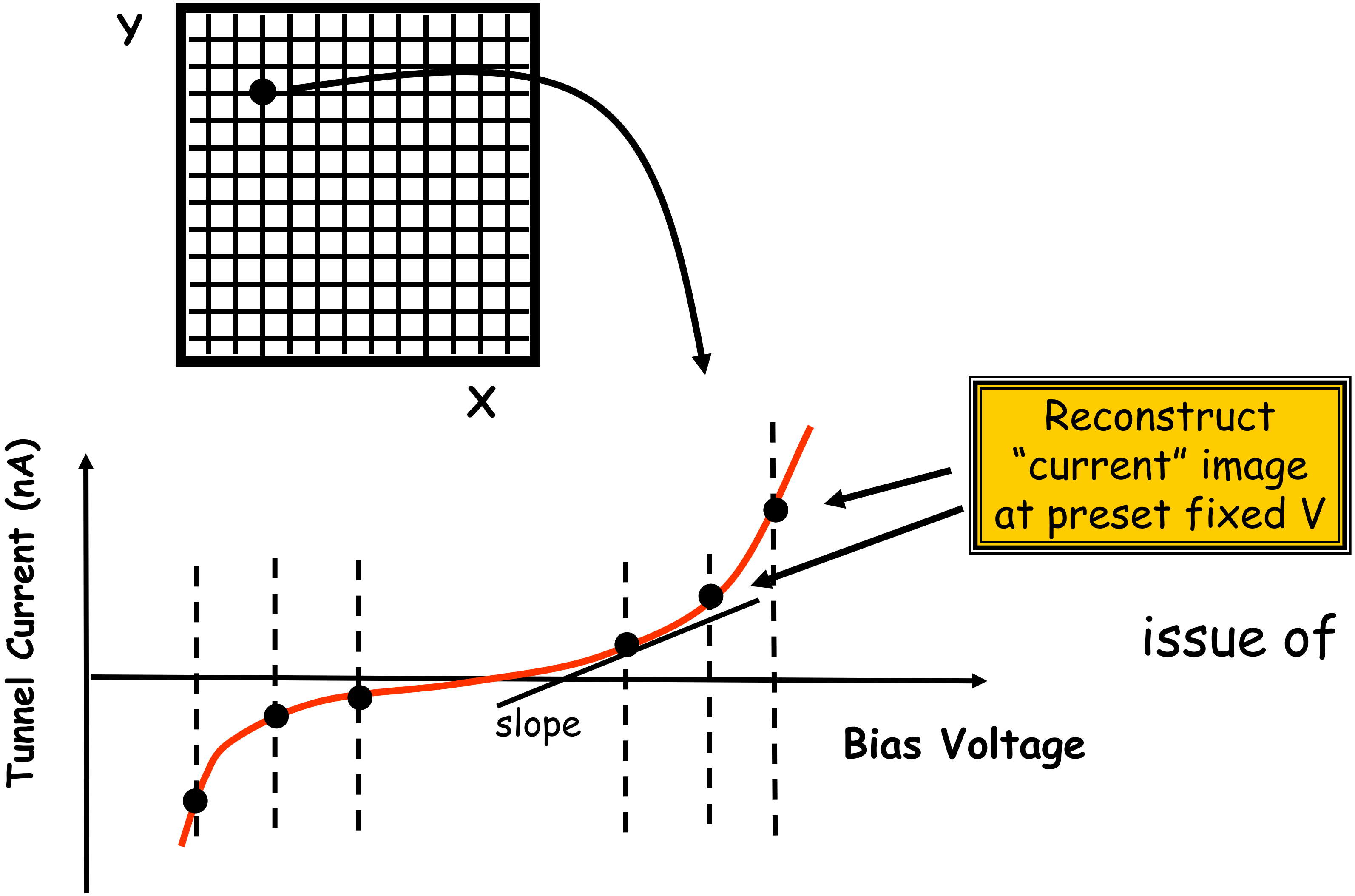
$$I \approx \frac{4\pi e}{\hbar}\rho_{tip}(E_F)\int_{-eV}^{0}\rho_{substrate}(E_F - eV + \varepsilon)\,T(\varepsilon, V)\,d\varepsilon$$

$$\approx \frac{4\pi e}{\hbar}\rho_{tip}(E_F)\langle T\rangle\int_{-eV}^{0}\rho_{substrate}(E_F - eV + \varepsilon)\,d\varepsilon$$

$$\left.\frac{\partial I}{\partial V}\right|_{V} \propto \text{constants}\times\rho_{substrate}(E_F - eV)$$

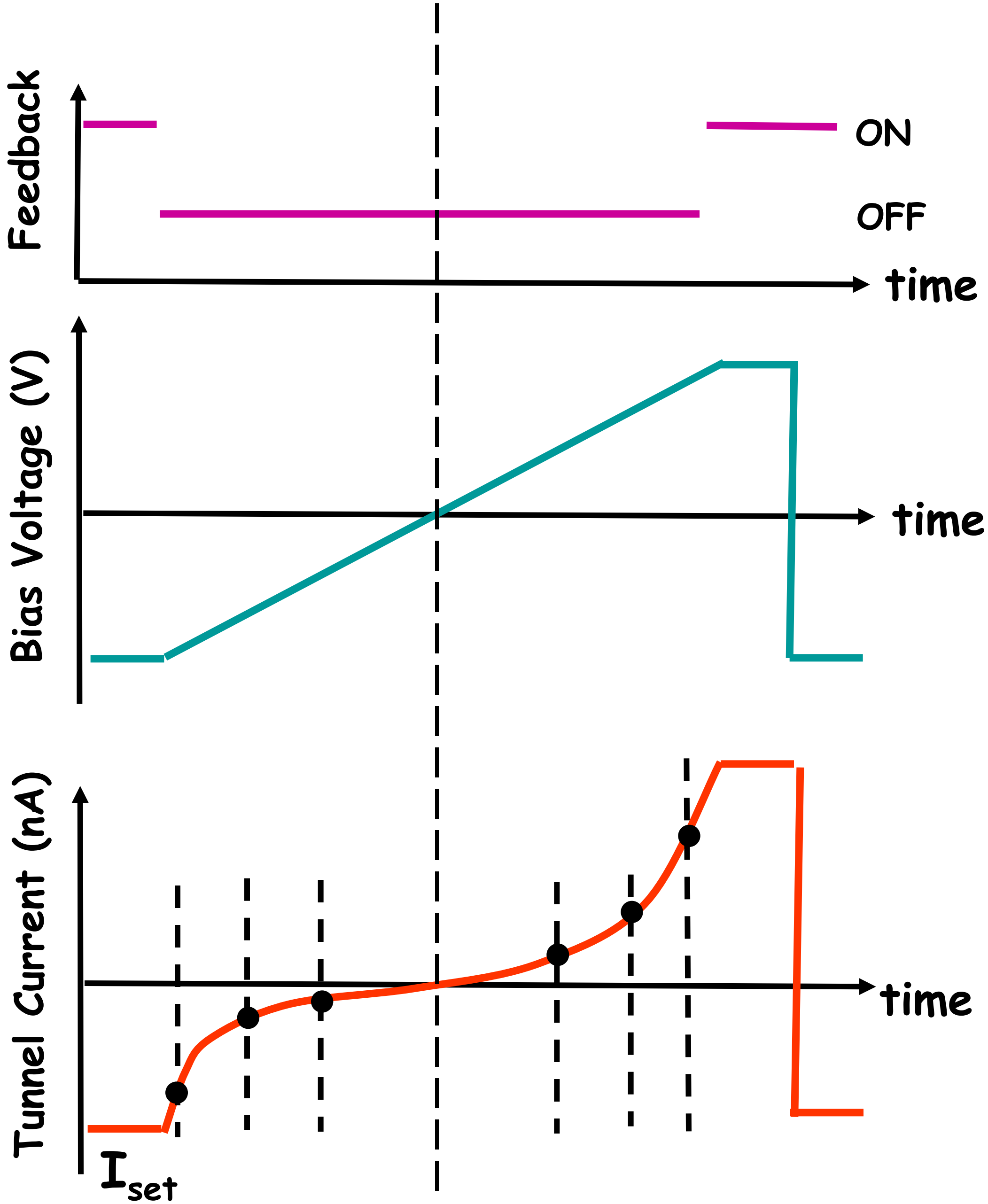
Current Imaging Tunneling Spectroscopy (CITS)

Measure topography and I(V) at each point:



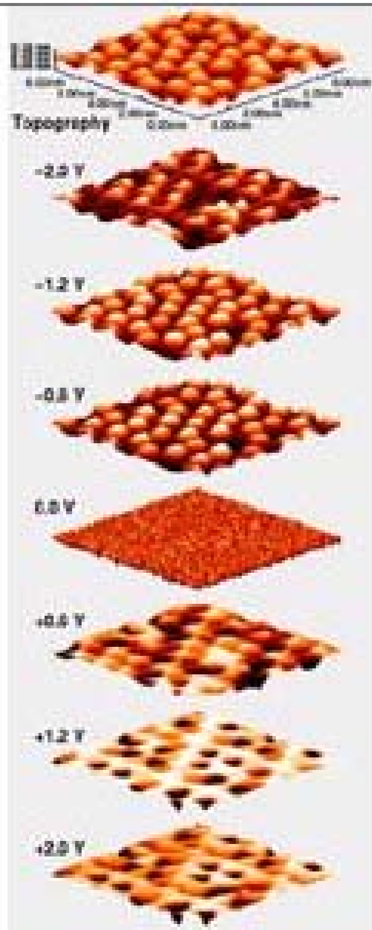
issue of drift

Making it work



Example

Current Imaging (CITS) on a perfect Si(111)7x7 Surface



Current Imaging Tunneling Spectroscopy on Si(111)7x7 at room temperature. The topographic image is shown at the top (I(t) = 0.35 nA, U_{gap} = 1.73 V), followed by several CITS images ranging from -2.0 V to +2.0 V. Spectroscopy data have been taken at every point of the frame for these images.

Key Idea: Acquire an (x,y) image at different voltages. Useful to visualize filled and unfilled states at each (x,y) point

from Omicron web site

Measuring the apparent tunnel barrier height

Recall for a constant tip bias $I = I_o e^{-2\alpha z}$ where $\alpha = \sqrt{\frac{2m\varphi_{barrier}}{\hbar^2}}$

$$\ln(I) = \ln(I_o) - 2\frac{\sqrt{2m\,\varphi_{barrier}(\text{in J})}}{\hbar}\, z(\text{in m})$$

change units: $2\frac{\sqrt{2m}}{\hbar}\left[\sqrt{1.6\times10^{-19}\,\varphi_{barrier}(\text{in eV})}\right]\left[1\times10^{-10}\, z(\text{in } \mathring{\text{A}})\right]$

the constant is now $2\frac{\sqrt{2m}}{\hbar}\left[\sqrt{1.6\times10^{-19}}\right]\left[1\times10^{-10}\right] = 1.029$

$$\ln(I) = \ln(I_o) - 1.029\times\sqrt{\varphi_{barrier}(\text{in eV})}\times z(\text{in } \mathring{\text{A}})$$

$$\left[\frac{\partial[\ln(I)]}{\partial z(\text{in } \mathring{\text{A}})}\right]^2 = (1.029)^2\times\varphi_{barrier}(\text{in eV})$$

$$\therefore\quad \varphi_{barrier}(\text{in eV}) = \frac{1}{(1.029)^2}\times\left[\frac{\partial[\ln(I)]}{\partial z(\text{in } \mathring{\text{A}})}\right]^2 = 0.94\times\left[\frac{\partial[\ln(I)]}{\partial z(\text{in } \mathring{\text{A}})}\right]^2$$

VOLUME 76, NUMBER 9 PHYSICAL REVIEW LETTERS 26 FEBRUARY 1996

Apparent Barrier Height in Scanning Tunneling Microscopy Revisited

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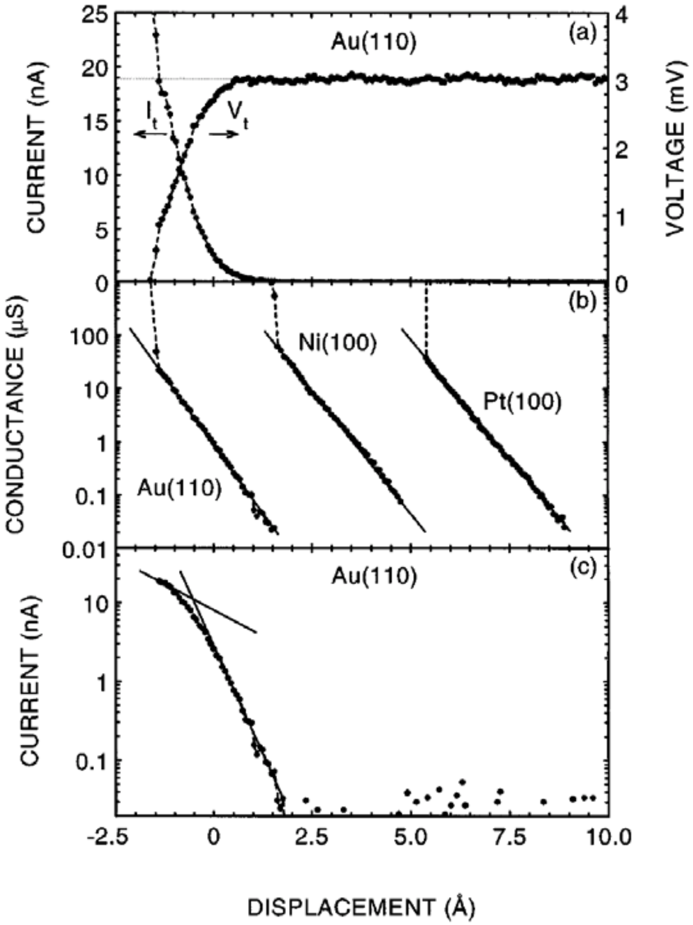
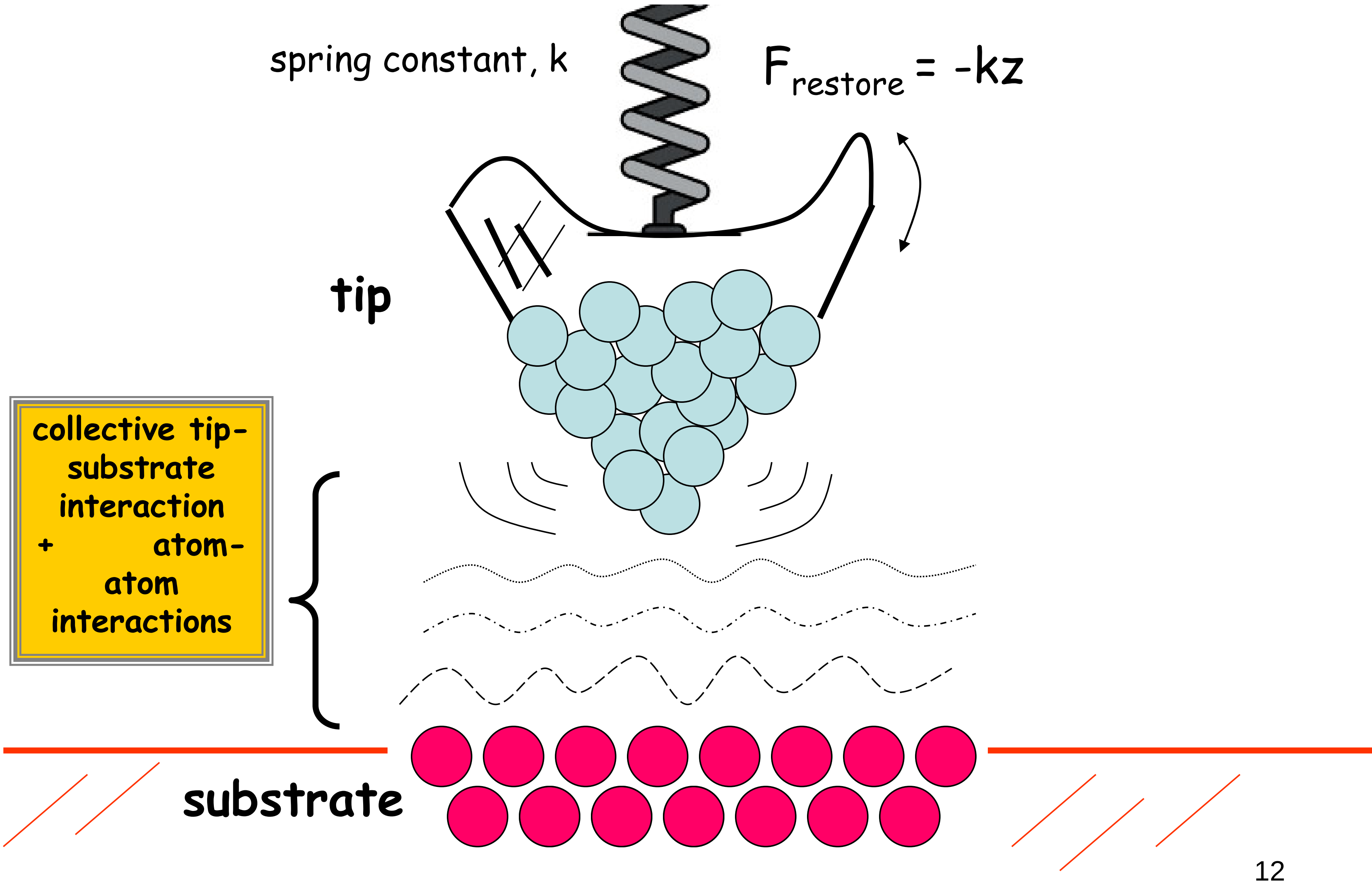
(Received 3 November 1995)



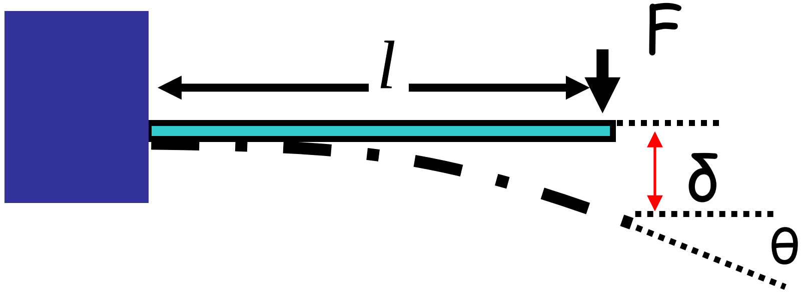
$$\varphi_{barrier}\left[Au(110)\right] = 4.7 \pm 1.0 \text{ eV}$$
$$\varphi_{barrier}\left[Ni(100)\right] = 4.5 \pm 0.7 \text{ eV}$$
$$\varphi_{barrier}\left[Pt(100)\right] = 3.4 \pm 0.8 \text{ eV}$$

The Force on the Tip Atom?



How to measure?

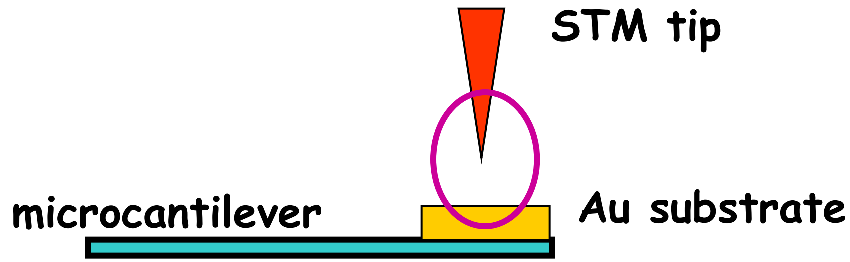
Cantilever Physics - static model

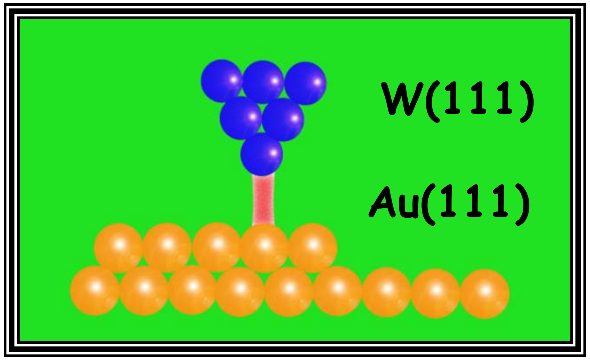


$$\delta = \frac{Fl^3}{3EI} \qquad \theta = \frac{Fl^2}{2EI}$$

$$k = \frac{3EI}{l^3} = \frac{Ewt^3}{4l^3}$$

$$F = k\delta = \frac{2}{3} k\, l \Theta$$





see Cross et al., Phys. Rev. Lett. **80**, 4685 (1998).

Adhesion Interaction between Atomically Defined Tip and Sample

G. Cross, A. Schirmeisen, A. Stalder, and P. Grütter*
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(Received 24 November 1997)

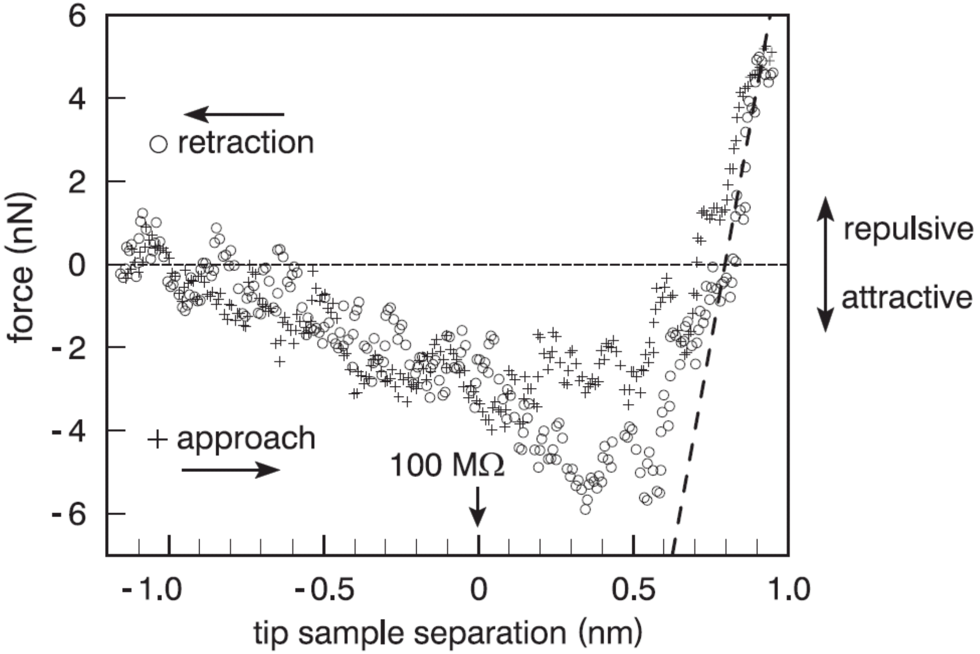

FIG. 3. Force versus tip-sample separation measured on a flat terrace using a W-trimer tip (tip-sample separation is defined as the relative motion of the tip with respect to the substrate using a tunnel resistance of 100 MΩ as the reference point). Note the hysteresis of 7 eV between the approach and retraction curve, indicating that dissipative processes take place in the range of the adhesion maximum. Also note that no spontaneous jump to contact followed by the formation of an adhesion neck occurs. The attractive interaction has a length scale of 1 nm, 1 order of magnitude larger than expected from universal scaling laws. The repulsive branch of the force curve is essentially linear (corresponding to a contact stiffness of 40 ± 20 N/m, indicated by the dashed line) and reversible. Surprisingly, the tip-sample junction can support a repulsive load of at least 5 nN corresponding to a contact pressure of 25 GPa. The compounded errors in determining the force scale correspond to ±35%; the compounded errors in the tip-sample separation s are ±20%.

$$\frac{V_{bias}}{I} = 100 M\Omega$$

PHYSICAL REVIEW B 71, 193407 (2005)

From tunneling to point contact: Correlation between forces and current

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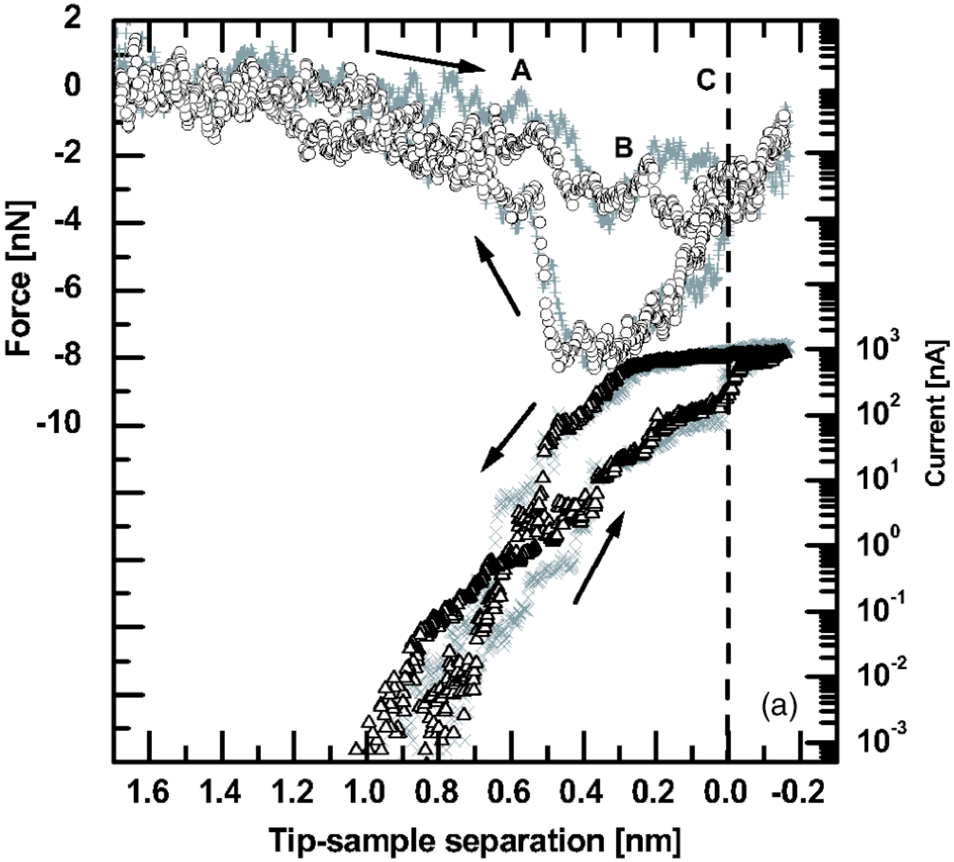
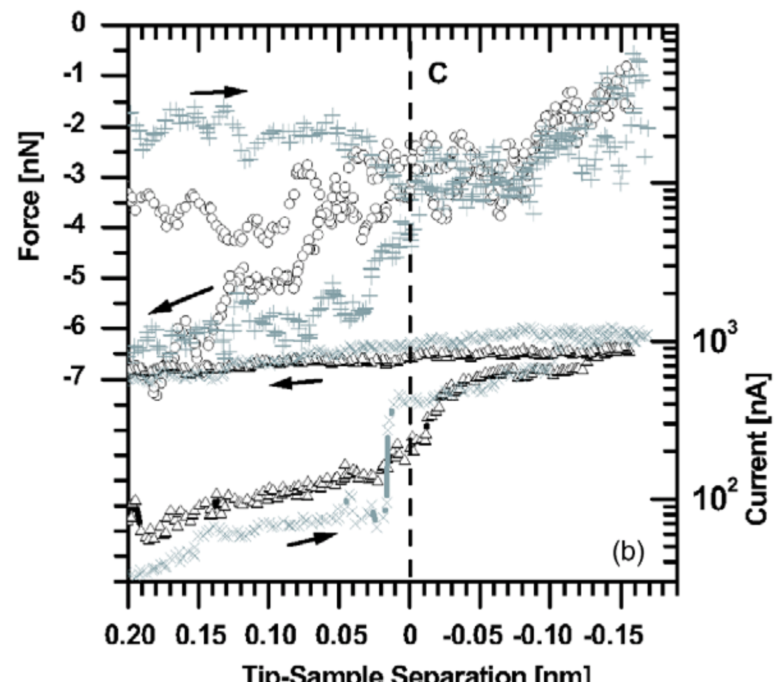
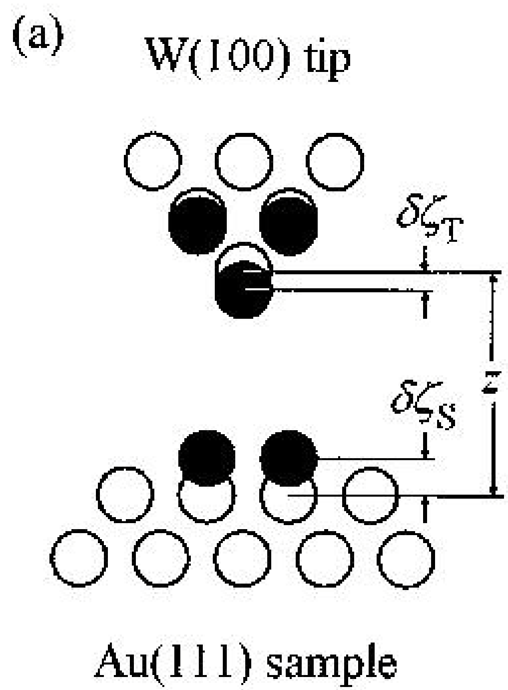
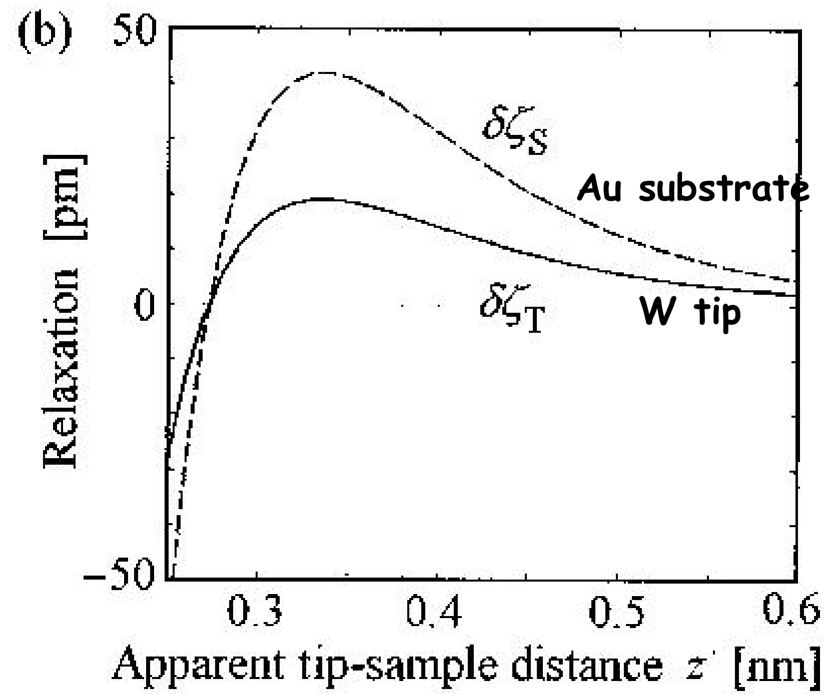
(Received 7 February 2005; published 25 May 2005)





Junction Stability
Nanomechanical Effects





from *Intro to Scanning Tunneling Microscopy*, C. Julian Chen (Oxford Press, Oxford - 2003), pg. 228

Atomic Corrugation – How High is an Atom?

PHYSICAL REVIEW B VOLUME 58, NUMBER 24 15 DECEMBER 1998-II

Prediction of bias-voltage-dependent corrugation reversal for STM images of bcc (110) surfaces: W(110), Ta(110), and Fe(110)

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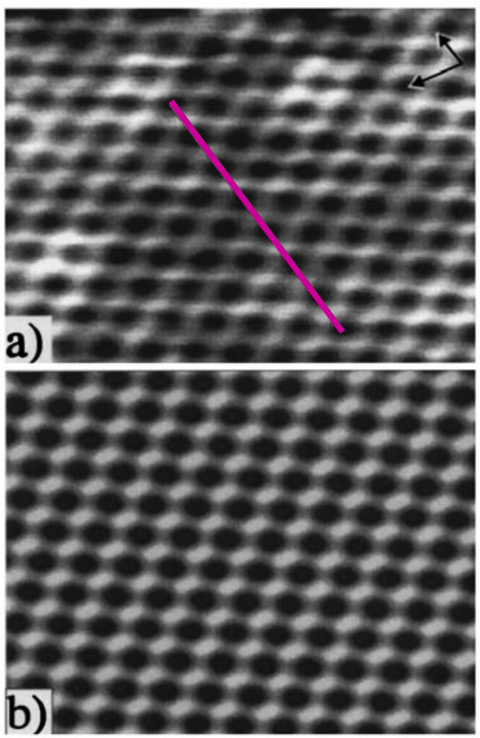
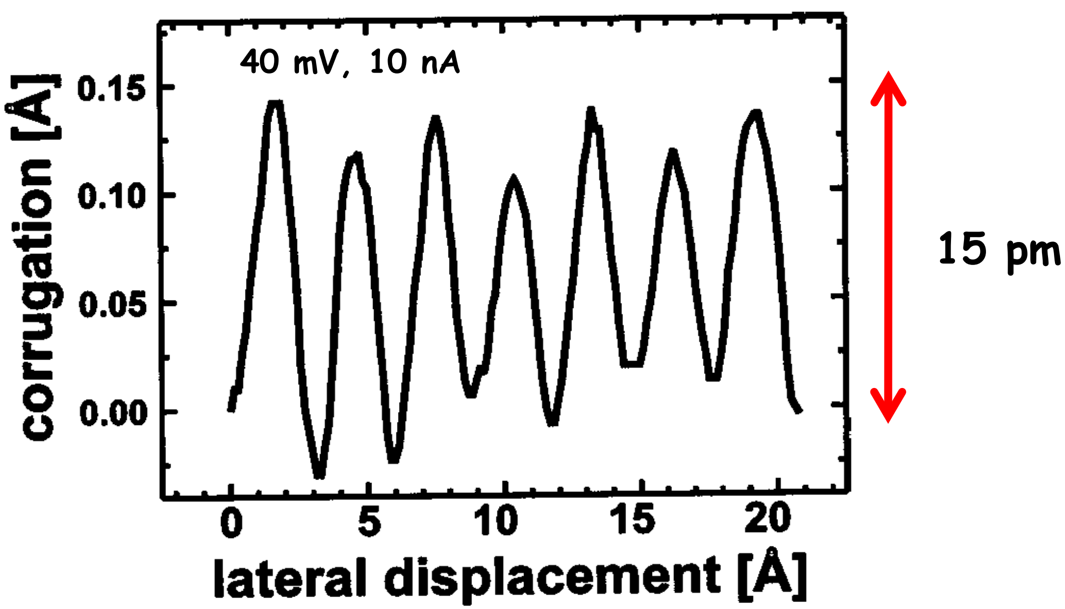
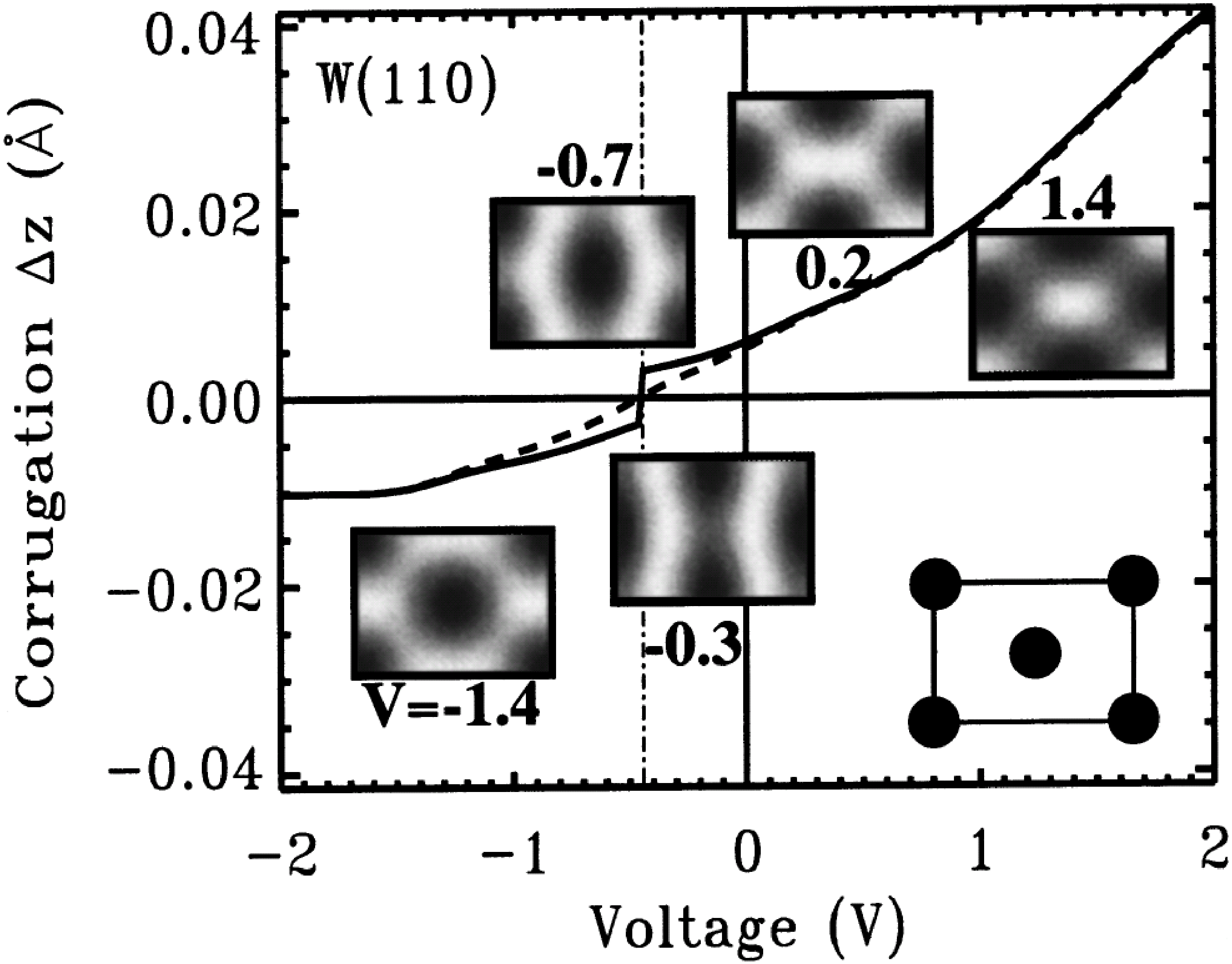
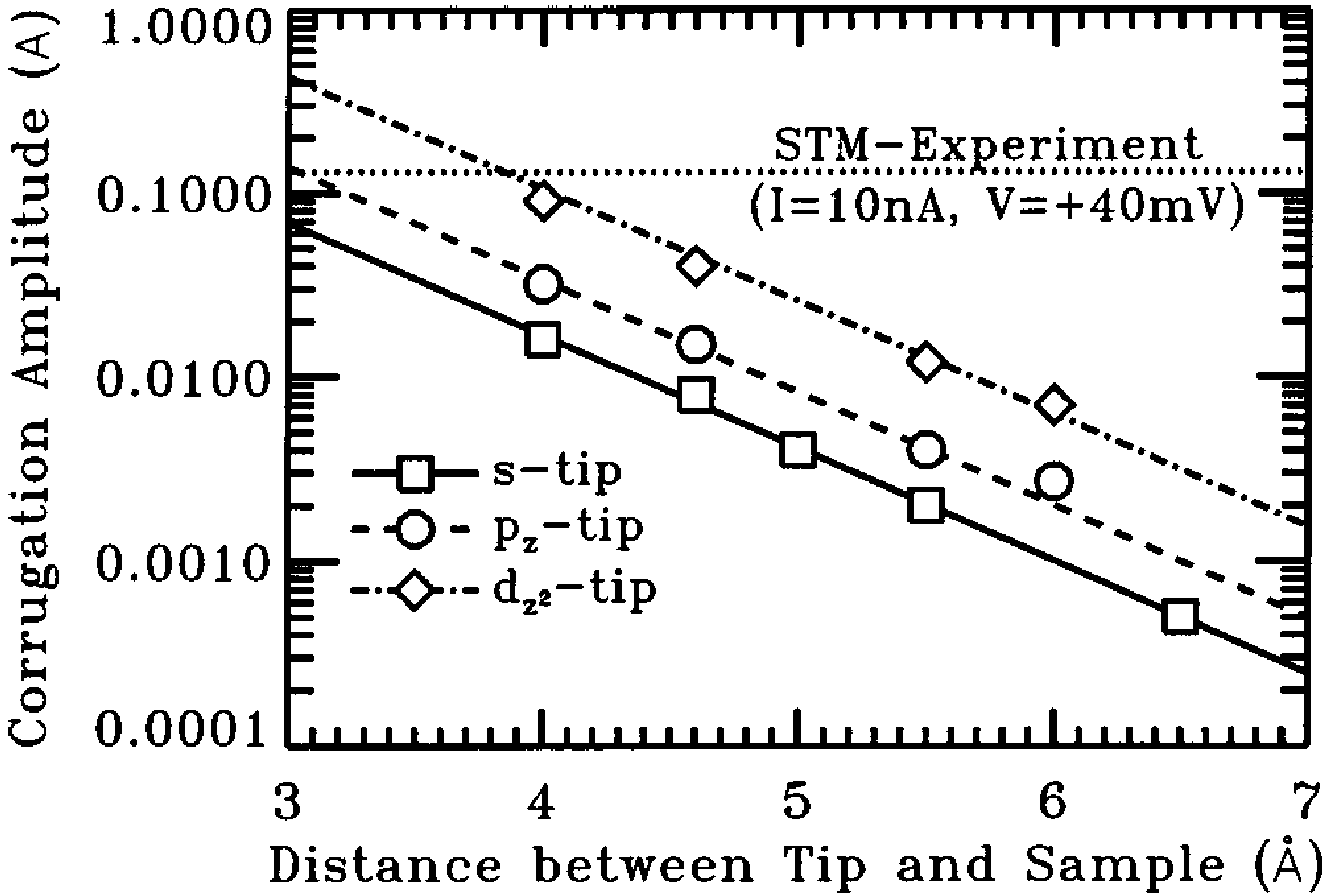
(Received 15 July 1998)







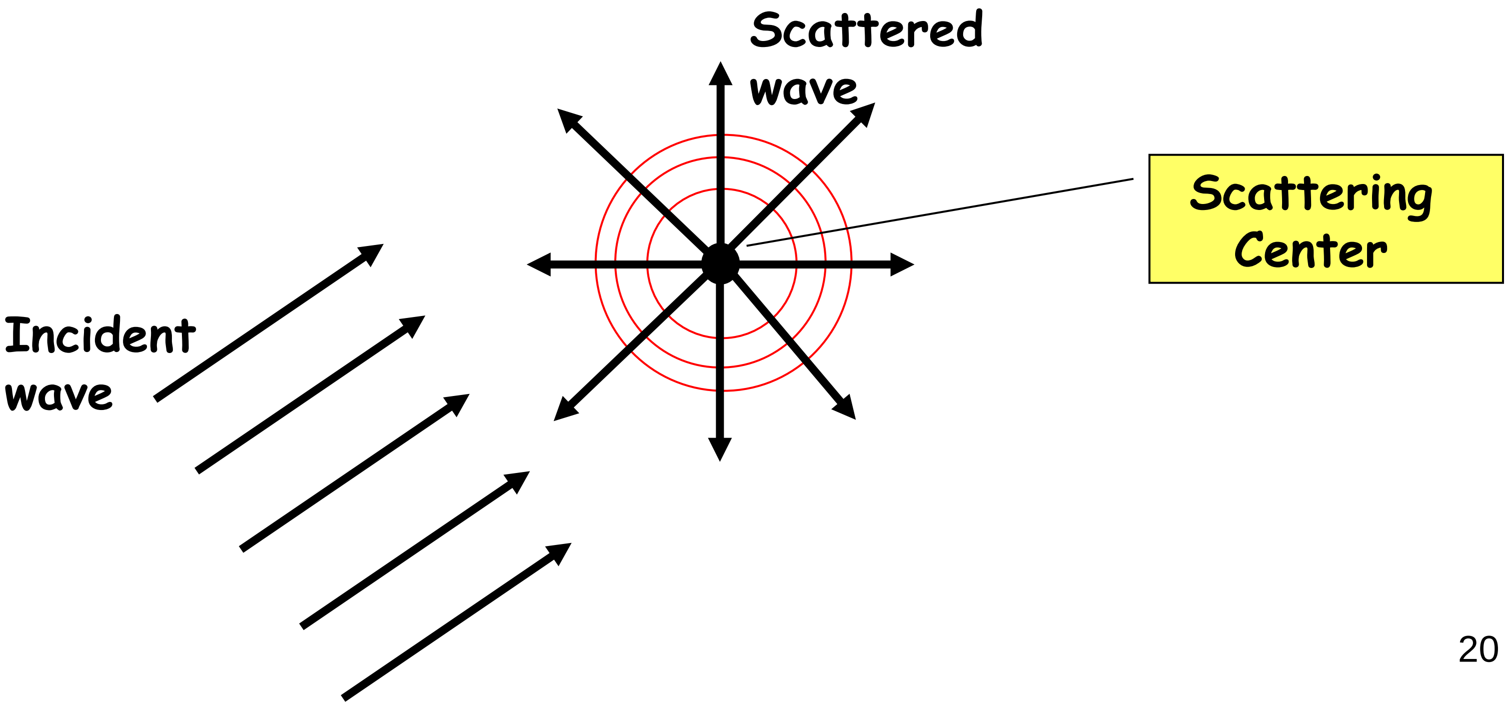
Heinze et al., Phys. Rev. **B58**, 16432 (1998).



Heinze et al., Phys. Rev. **B58**, 16432 (1998).

Quantum Corrals

- Confine electrons inside artificial structures
- Requires atomically flat metallic substrates
- Requires the presence of surface electron states
- Construct 2D atomic "fence" of electron scattering centers
- New way of guiding information through a solid



Elliptical Shapes are Special

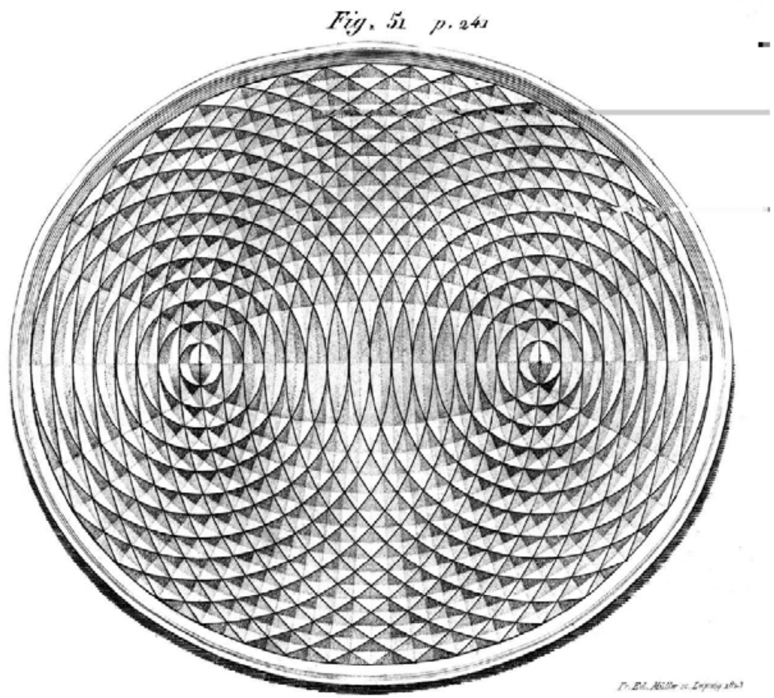
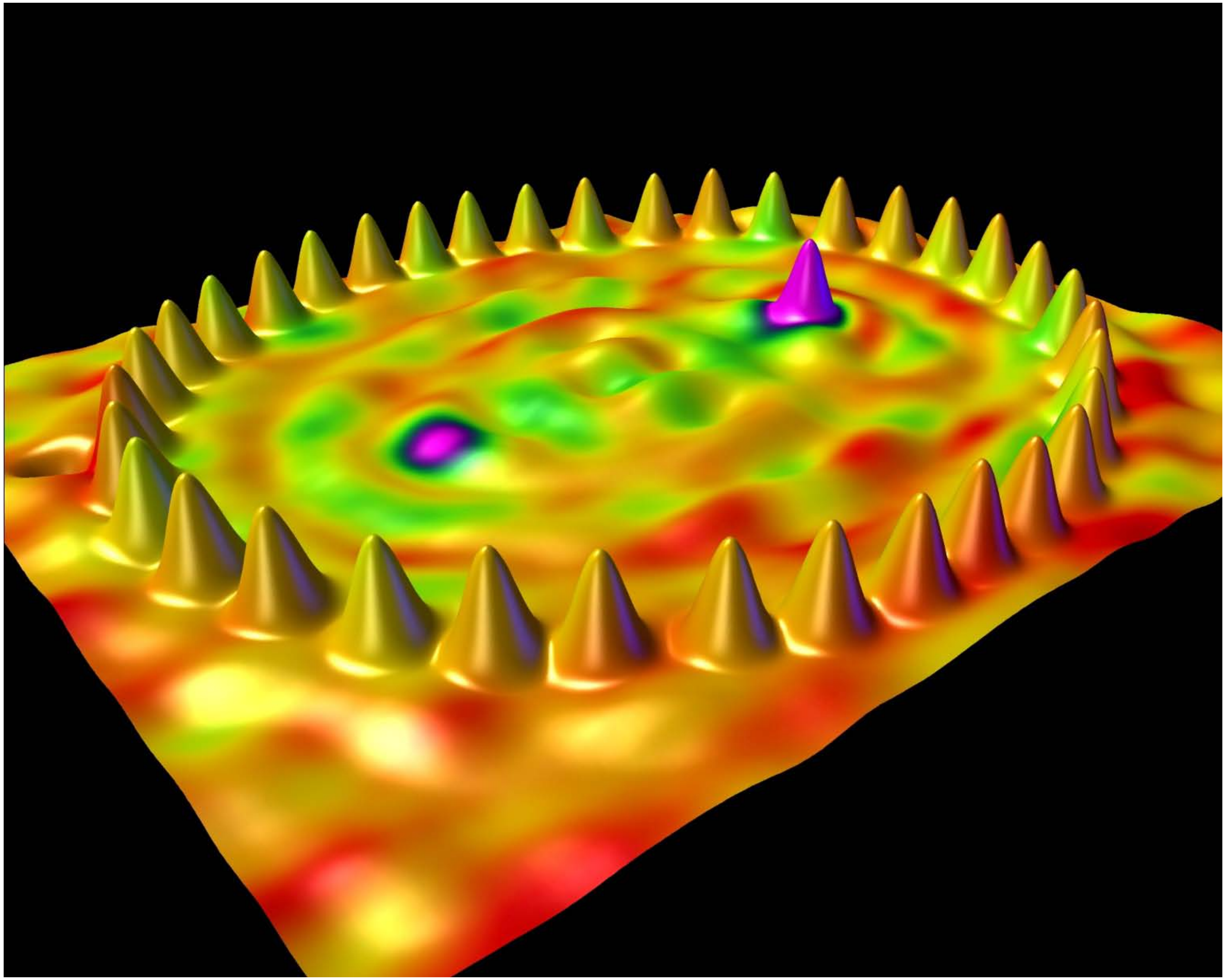


FIG. 10 A sketch from “Wellenlehre” (“Wave Teachings”), an 1825 book published in Leipzig on wave theory by two of the three Weber brothers scientists from Saxony, Ernst and Wilhelm, showing the wave pattern of mercury waves when small amounts of mercury are dropped in at one focus. Notice how the other, opposite focus looks identical, indicating that from the point-of-view of the wave, the two foci are excited equally.

from Fiete and Heller, Rev. Mod. Phys. **75**, 933 (2003)

36 cobalt atoms forming an elliptical structure on Cu(111) substrate

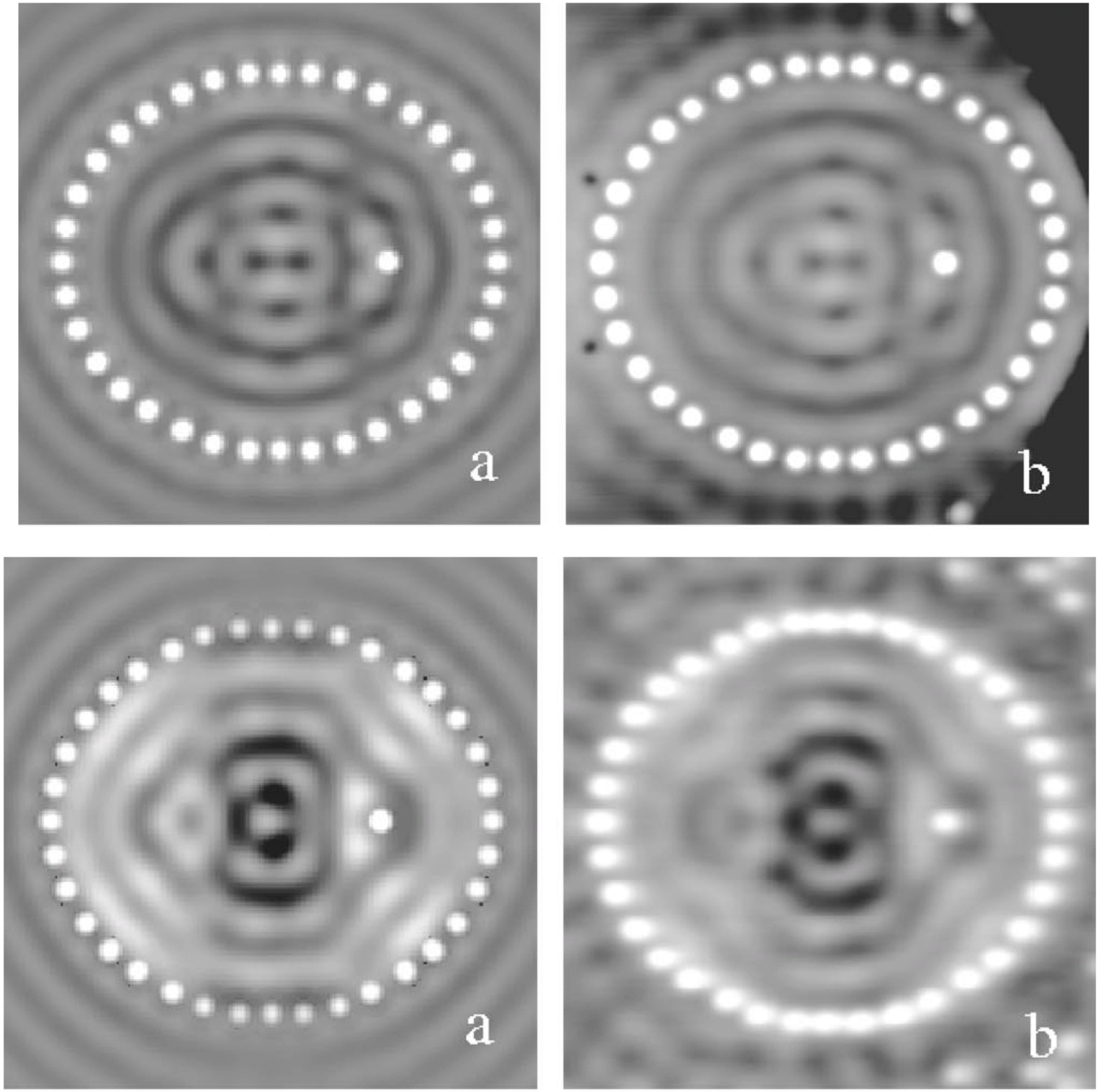


Manoharan, Lutz and Eigler, *Nature*, 3 February 2000

Theory **Experiment**

Topography

DOS (dI/dV)



Fiete and Heller, Rev. Mod. Phys. **75**, 933 (2003)

Quantum Corral Simulation

http://mw.concord.org/modeler1.3/mirror/quantum/corral.html

See also Prof. E.J. Heller's lecture at
https://nanohub.org/resources/3253/

SUMMARY

To do STM well, you need

i) high quality, FLAT, well characterized, electrically conducting substrates;

ii) UHV and Low Temperature equipment;

iii) lots of time and money;

iv) infrastructure, infrastructure, infrastructure;

and

v) good theoretical support.