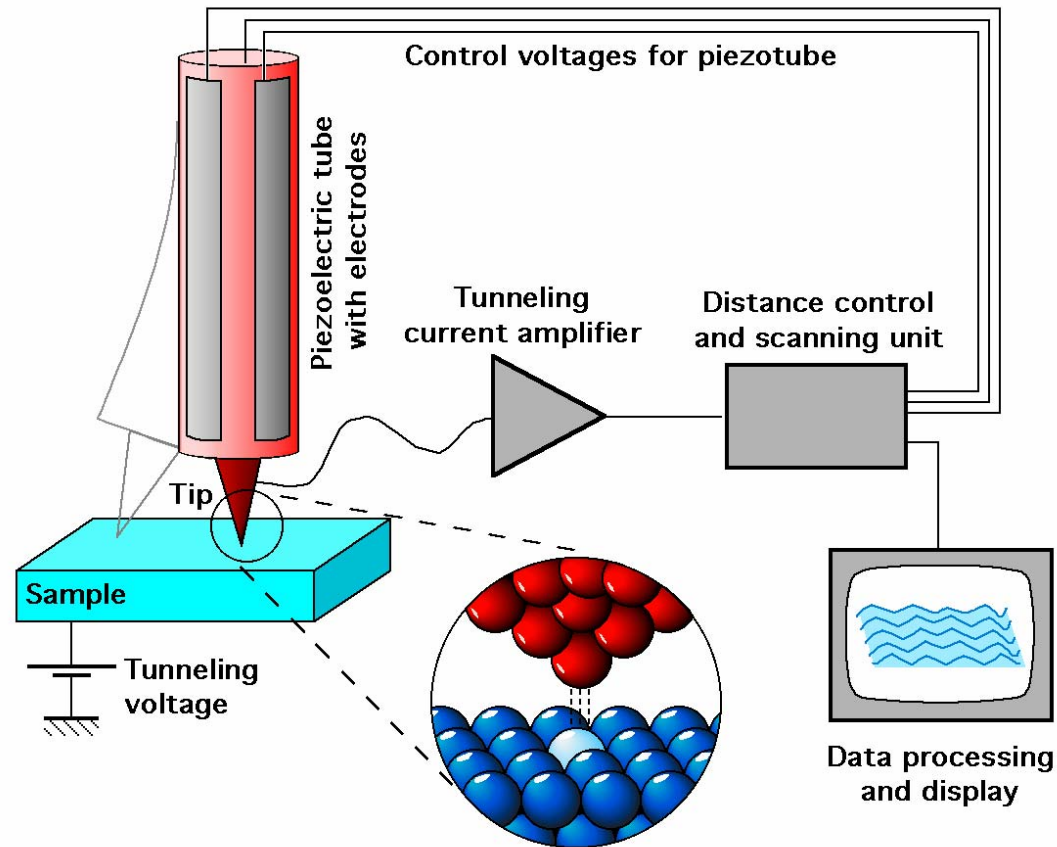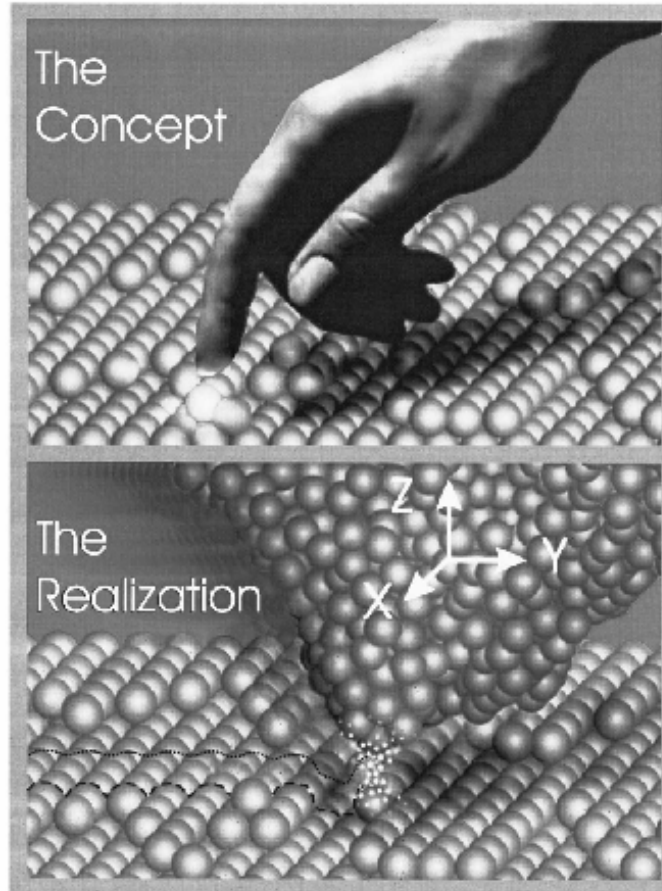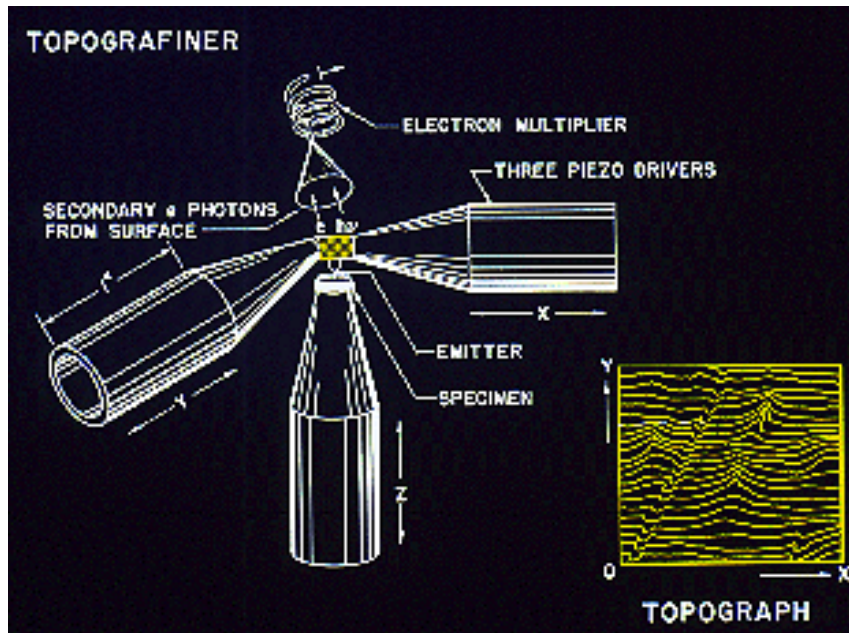# Scanning Tunneling Microscopy

References:

1. G. Binnig, H. Rohrer, C. Gerber, and Weibel, Phys. Rev. Lett. **49**, 57 (1982); and ibid **50**, 120 (1983).

2. J. Chen, *Introduction to Scanning Tunneling Microscopy*, New York, Oxford Univ. Press (1993).
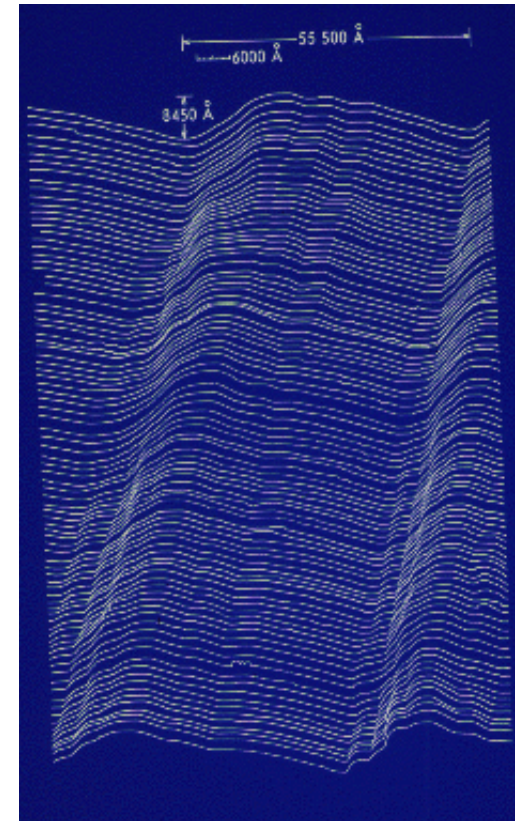
Concept: Eye and Finger

G. Binnig and and H. Rohrer, *Rev. of Mod. Phys.* **71**, S324-S330 (1999).
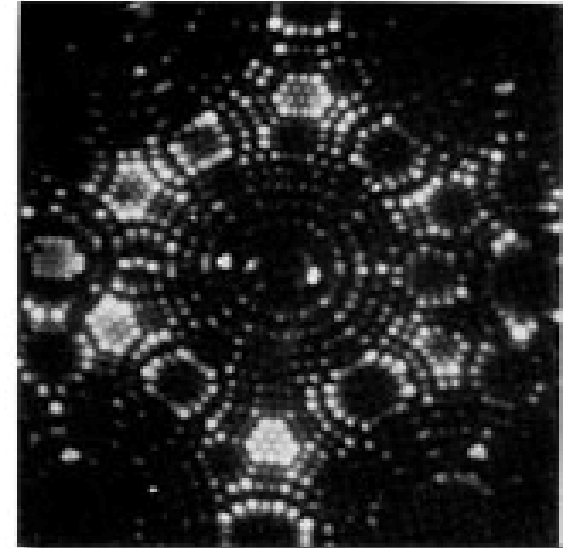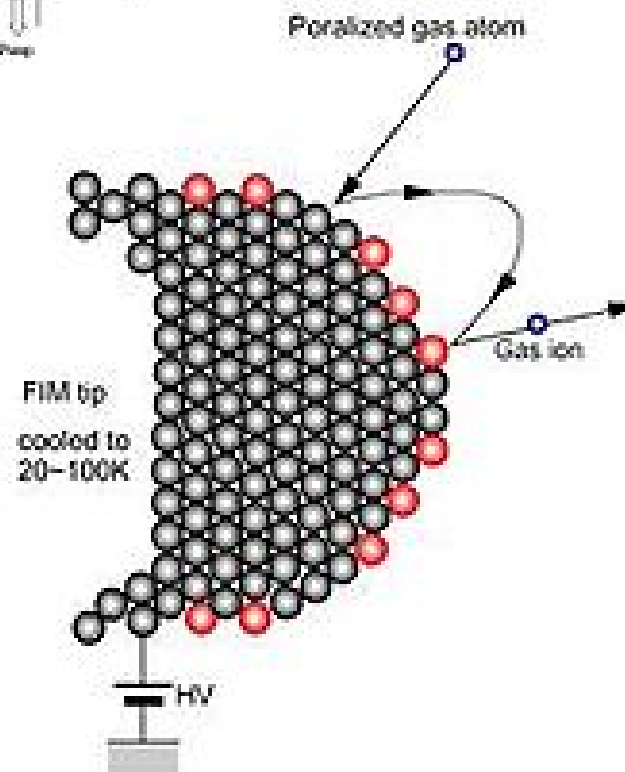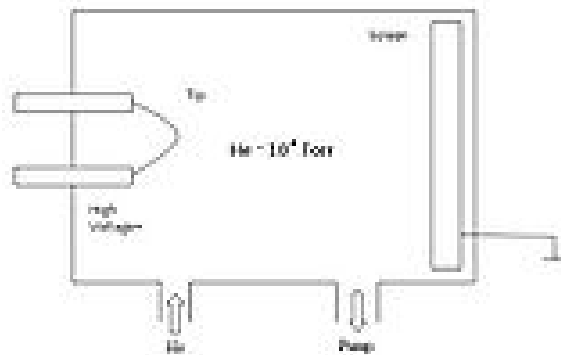
Topografiner

R. Young, J. Ward, and F. Scire, Rev. Sci. Instrum. **43**, 999 (1972).

Topographic map of a 180-line-per-mm diffraction-grating replica

Field Ion Microscopy

Polarized gas atom

Gas ion

FIM tip
cooled to
20–100K

HV

Erwin W. Müller (1951)

Ultra-High Vacuum Scanning Tunneling Microscope

Viewport for observing sample and tip

8-inch UHV mounting flange

Inchworm motor for coarse approach

Spare sample "garage"

Interchangeable sample holder

Suspension spring for low-frequency vibration isolation

Damping and lockdown mechanism

Scanning tube for tip control

Theory of STM

Tip

I

Sample

Constant Current Mode

Tunneling

Tunneling current I_t

$I_t \propto (V/d)\exp(-A\phi^{1/2}d)$

$A = 1.025\ (eV)^{-1/2}\text{Å}^{-1}$

$\phi \sim 4 - 5\ eV$

d decreases by 1 Å,

I_t will be increased by ~10 times.
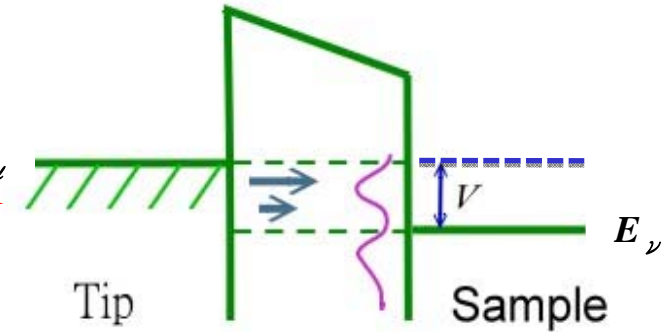
Tunneling current

I_t

I_{t1}

I_{to}

$d_1 d_o$

d

Tunneling current

$$I_{T \to S} = \frac{2\pi e}{\hbar} \sum_{\mu\nu} f(E_\mu)[1 - f(E_\nu + eV)]|M_{\mu\nu}|^2 \delta(E_\mu - E_\nu - eV)$$

where $f(E)$ is Fermi function,

$\quad E_{\mu,\nu}$ is the energy of state, where μ and ν run

$\qquad$ over all the states of the tip and surface,

$\quad M_{\mu\nu}$ is tunneling matrix element.

$$M_{\mu\nu} \equiv \frac{\hbar^2}{2m} \int d\vec{s}(\psi_\mu * \nabla \psi_\nu - \psi_\nu \nabla \psi_\mu *)$$

where ψ_μ is the wave function, and the integral is over any plane in the barrier region.

$$I = I_{T \to S} - I_{S \to T}$$

$$= A' \int_{-\infty}^{\infty} \rho_T(E)\rho_S(E + eV)|M(E)|^2 [f(E) - f(E + eV)]dE$$

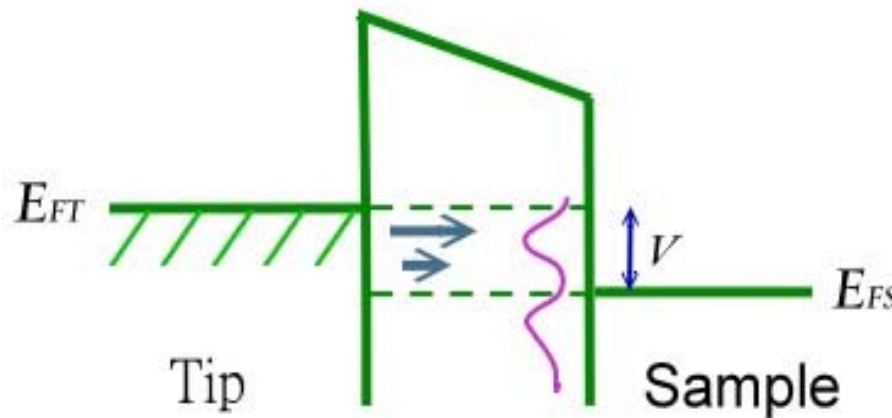where ρ_S and ρ_T are the densities of states in the sample and the tip, respectively.

Tunneling current

$$I \equiv A' \int_{-\infty}^{\infty} \rho_T(E) \rho_S(E+eV) |M(E)|^2 [f(E) - f(E+eV)] dE$$

Transmission probability of the electron

$$M(E) = \exp\left[- A \phi^{\frac{1}{2}} S \right]$$

Usually, we assume ρ_T is featureless (ie. $\rho_T \approx const.$), and the sample electronics states dominate the tunnel spectra.

However, the tips might have effect on the tunnel spectra, if

    1. we have atomically sharp tips ,or

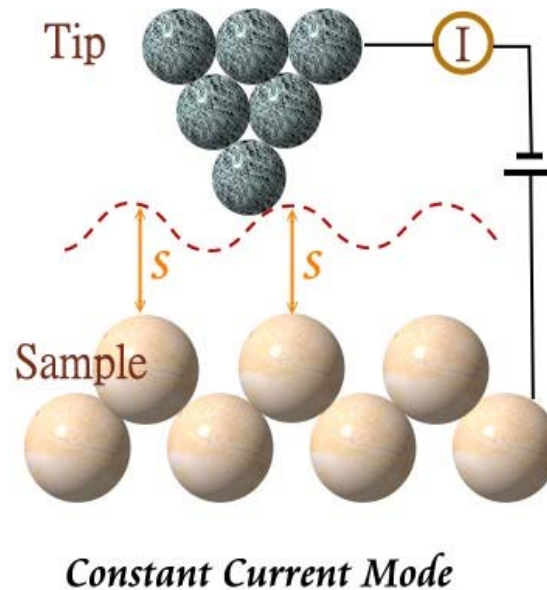   2. the tip has picked up a foreign atom.

In the low-voltage limit

$$I \propto V \rho_S\left(\tilde{r}_t ; E_F\right) \rho_t\left(E_F\right)$$

where $\rho_S\left(\tilde{r}_t ; E_F\right)$ is the surface density of states of the sample at the center of the

tip($\tilde{r}_t$),

$$\rho_S\left(\tilde{r} ; E\right) \equiv \sum_v \left|\psi_v\left(\tilde{r}\right)\right|^2 \delta\left(E_v - E\right)$$

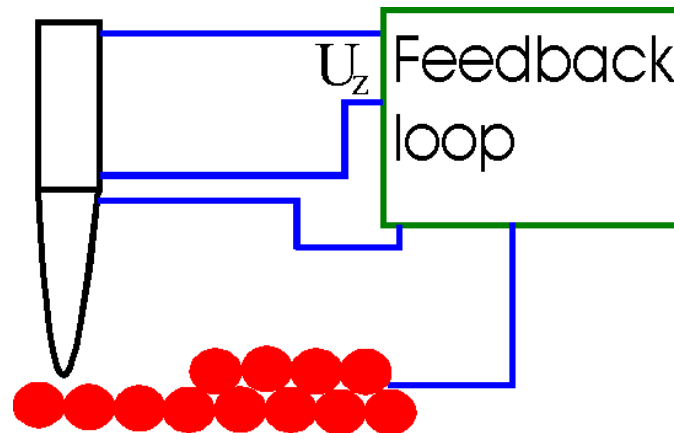$\rho_t\left(E_F\right)$ is the density of states of the tip at the Fermi level and is often

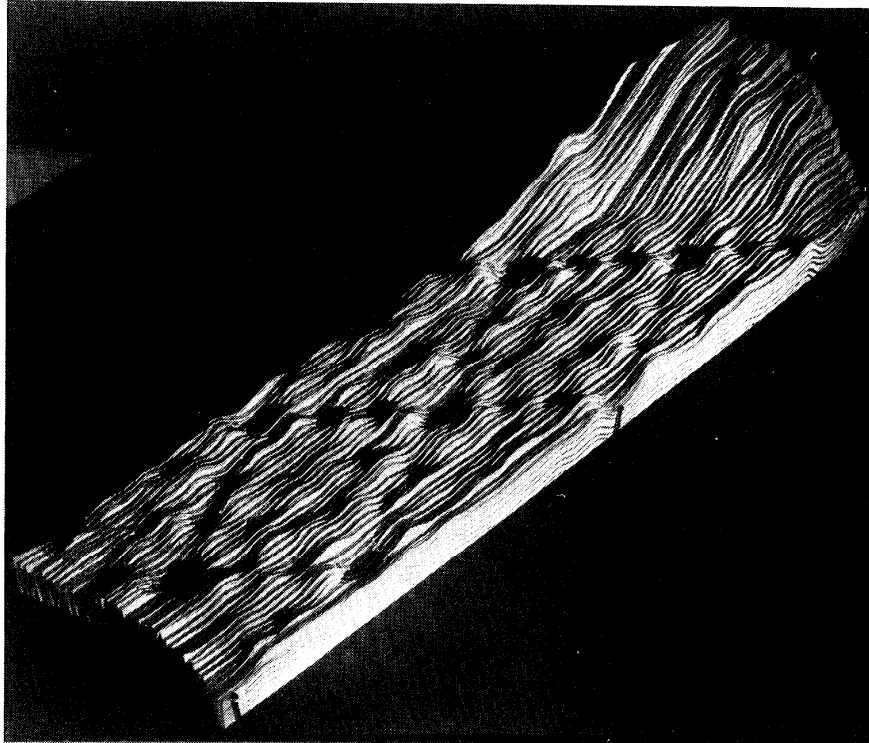regarded as a constant.

Constant Current Mode

Modes of Operation
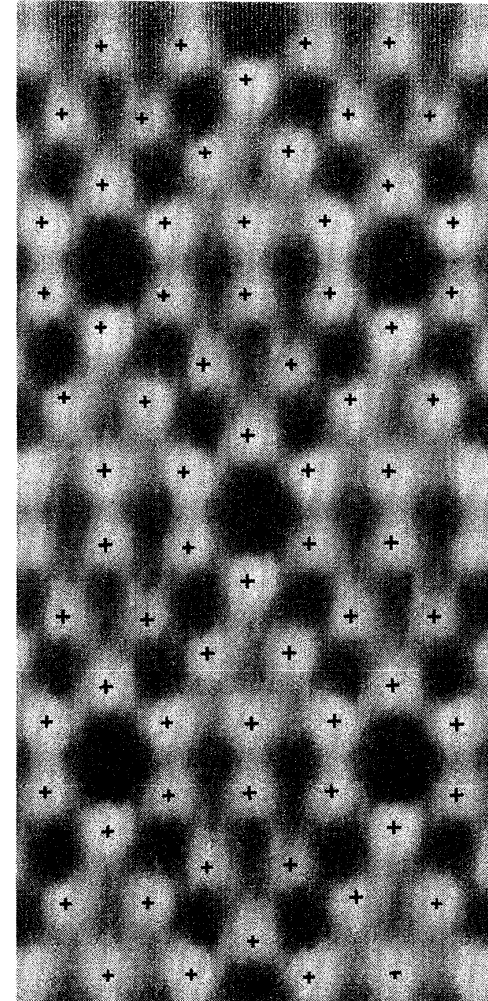
1. **Constant Current Mode**

    By using a feedback loop the tip is vertically adjusted in such a way that the current always stays constant. As the current is proportional to the local density of states, the tip follows a contour of a constant density of states during scanning. A kind of a topographic image of the surface is generated by recording the vertical position of the tip.
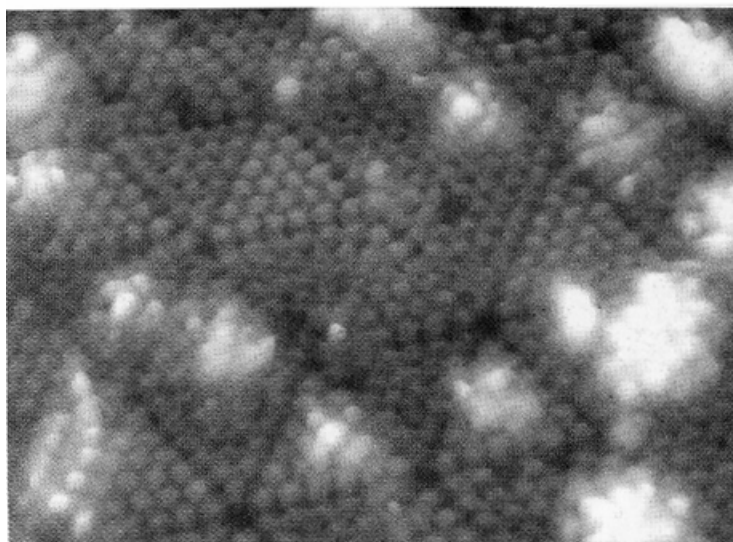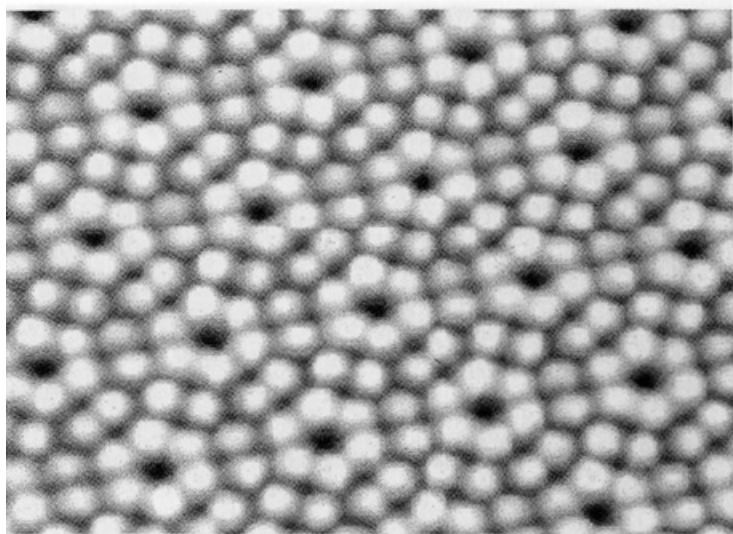
7 × 7 Reconstruction on Si(111) Resolved in Real Space

G. Binnig, H. Rohrer, Ch. Gerber, and E. Weibel
Phys. Rev. Lett. 50, 120 (1983)

Si(111)-(7x7)

Si(111)-2x1
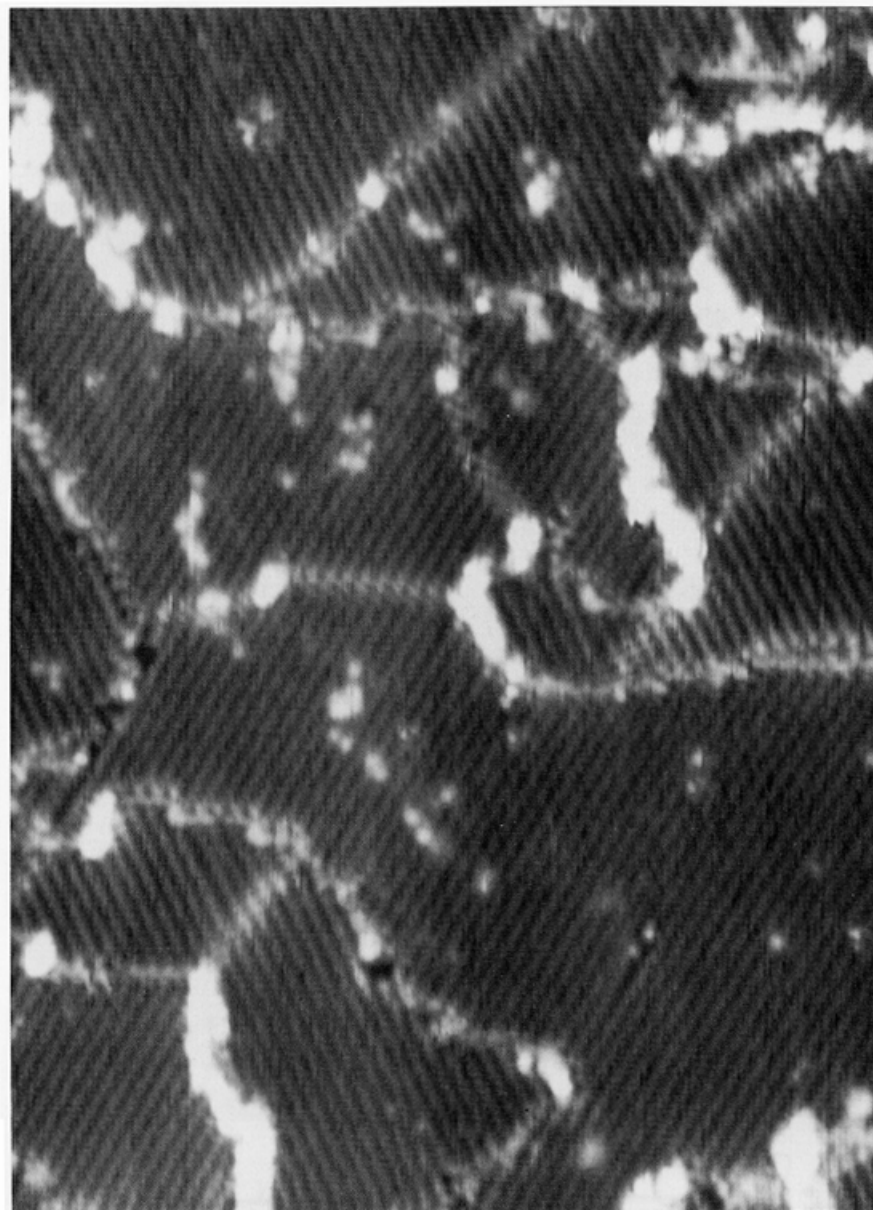

0   50   100 Å

Atomic Model of Si(111)-(7×7)

Top view

26.9 Å

7.7 Å

$\bar{1}\bar{1}2$

⬤ Si adatom

⊕ Si rest atom with a dangling bond

Side view

dangling bond

2nd layer rest atom

faulted half ↔ unfaulted half

Animation about the Si(111)7x7 reconstruction

Please visit Prof. Yan Liang's website at

http://www.tc.umn.edu/~liang050/

or watch the animation directly on Vimeo:
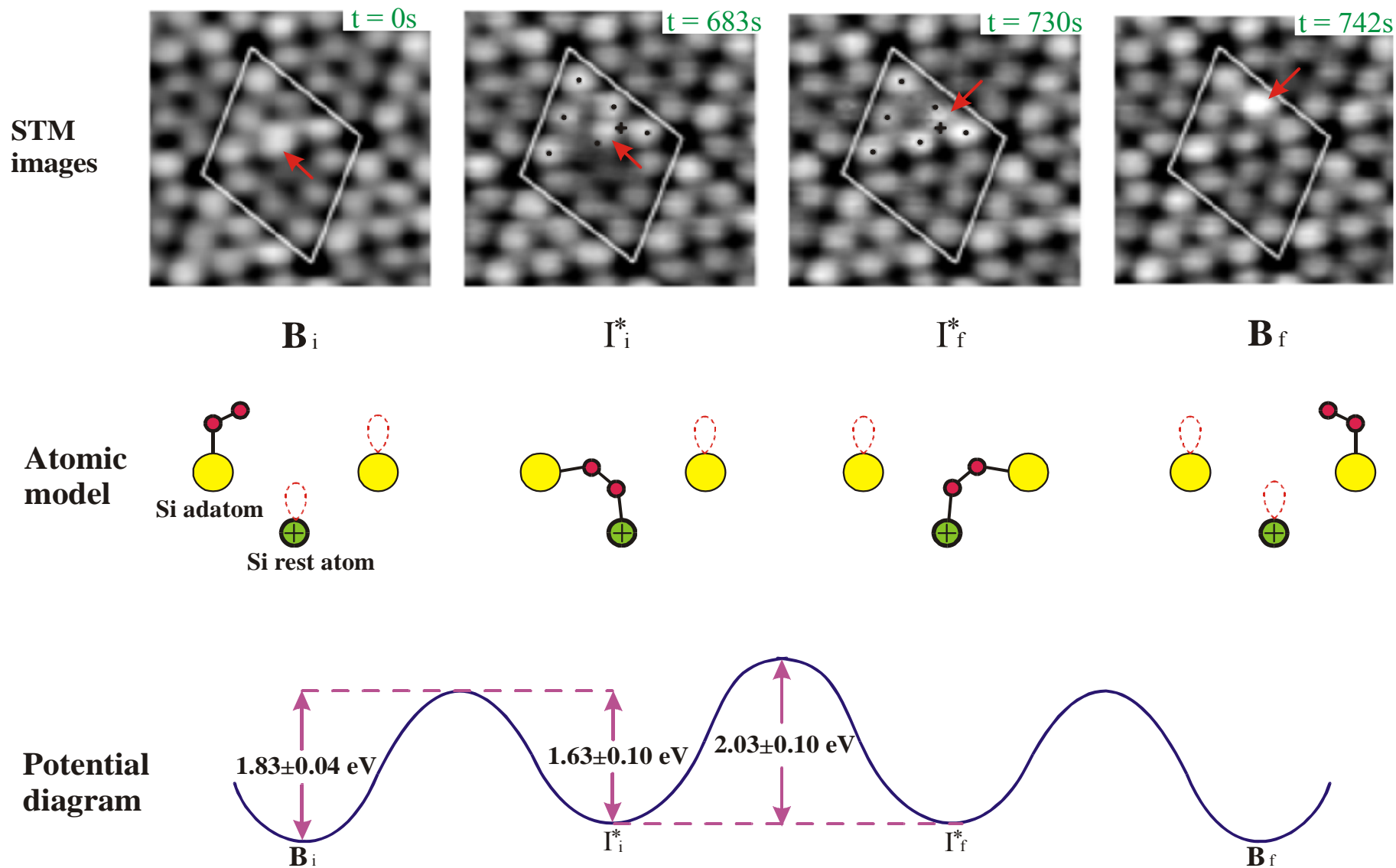
http://www.vimeo.com/1086112

2. Constant Height Mode

In this mode the vertical position of the tip is not changed, equivalent to a slow or disabled feedback. The current as a function of lateral position represents the surface image. This mode is only appropriate for atomically flat surfaces as otherwise a tip crash would be inevitable. One of its advantages is that it can be used at high scanning frequencies (up to 10 kHz). In comparison, the scanning frequency in the constant current mode is about 1 image per second or even per several minutes.

I

Site Hopping of O$_2$ Molecule on Si(111)-(7x7)

STM images

t = 0s   t = 683s   t = 730s   t = 742s

B$_i$ I$_i^*$ I$_f^*$ B$_f$

Atomic model

Si adatom

Si rest atom

Potential diagram

1.83±0.04 eV   1.63±0.10 eV   2.03±0.10 eV
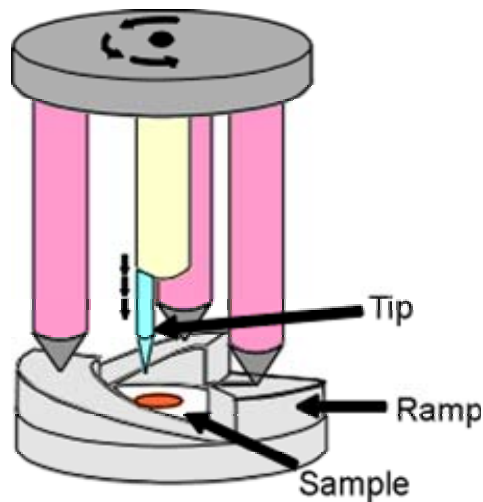
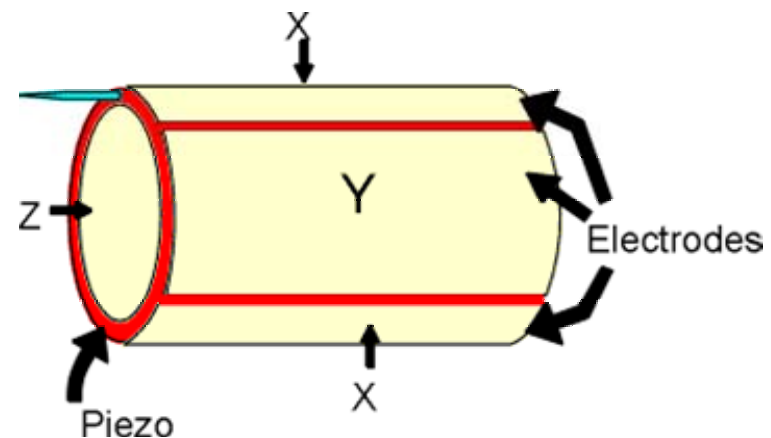B$_i$ I$_i^*$ I$_f^*$ B$_f$

Technical Aspects

Demands:

1. Controlling the tip-sample distance from a few mm down to 0.01Å
2. Exact lateral positioning
3. Stabilized tip-sample distance
4. Sharp tip
5. Measuring a current in the range of 0.01nA-50nA

Positioning

The large distance range the tip has to be controlled on makes it necessary to use two positioners: a coarse and a fine positioner. The fine positioner is also used as a scanner. Every fine positioner/scanner is made out of a piezocrystal or piezoceramic material.
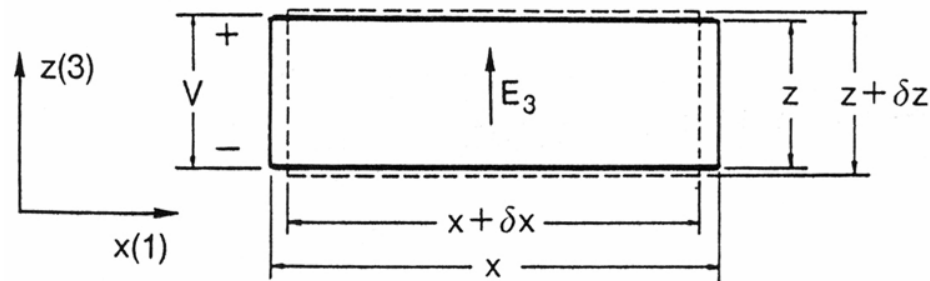
coarse positioner (beetle)

fine positioner/scanner
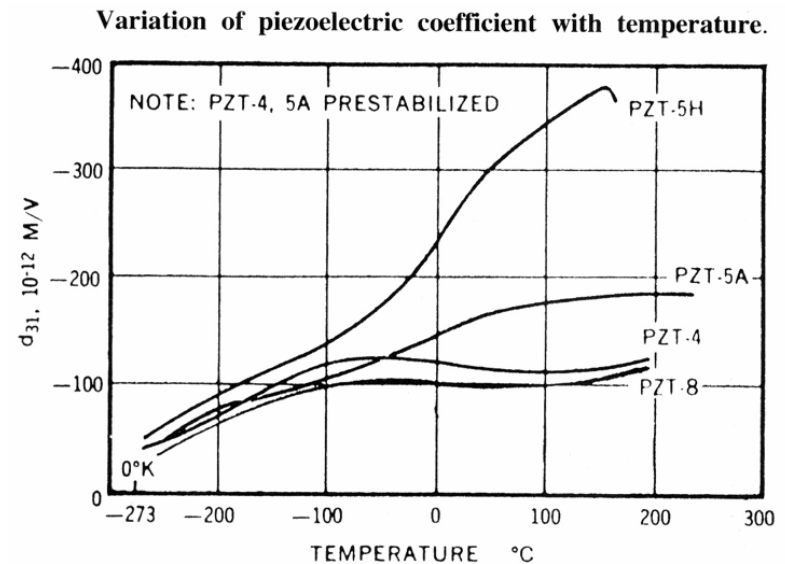
Piezoelectric Response

Variation of piezoelectric coefficient with temperature.

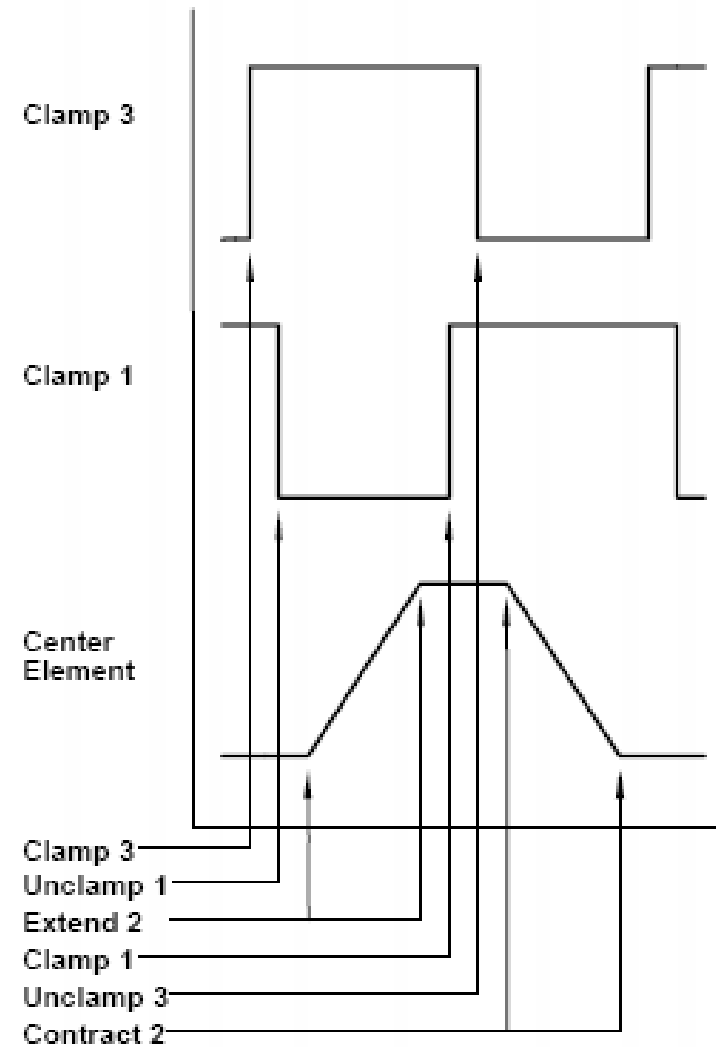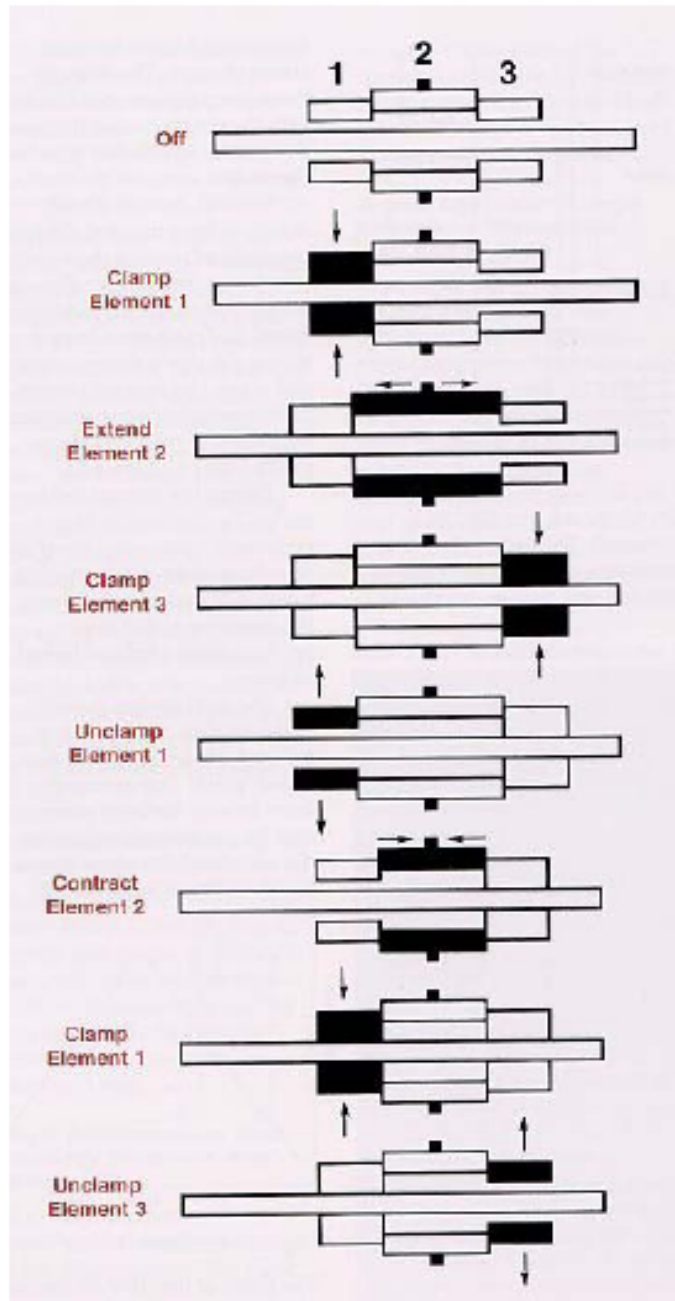**Strain:** $S_1 = \delta x/x$, $S_3 = \delta z/z$

Electric field: $E_3 = V/z$

Piezoelectric Coeff.: $d_{33} = S_3/E_3$, $d_{31} = S_1/E_3$

Typical values for $d_{31} \sim -1$ Å/V, $d_{33} \sim 3$ Å/V.

Inchworm Motor

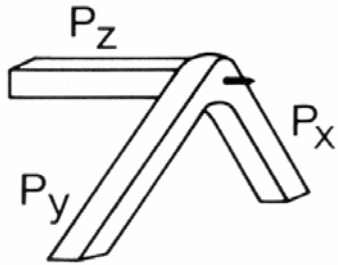# Piezoelectric Scanner

Tripod scanner

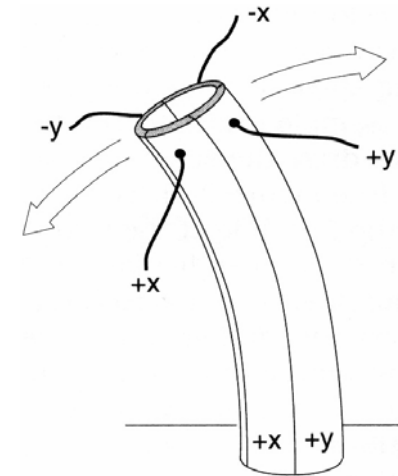

Tube scanner

$S_1 = \delta x/x = d_{31}E_3 = d_{31}V/z$

Piezoelectric Constant:

$K = dx/dV = d_{31}L/h$

Resonance Freq. for bending:

$f = 0.56\ \kappa C/L^2\ ,\quad \kappa = h/\sqrt{12}$

Piezoelectric Constant:

$K = dx/dV = 2\sqrt{2}d_{31}L^2/\pi Dh$
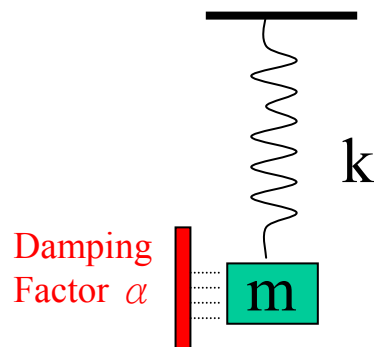
Resonance Freq. for bending:

$f = 0.56\ \kappa C/L2\ ,\quad \kappa = (D^2 + d^2)^{1/2}/8$

Vibration Isolation

The tip-sample distance must be kept constant within 0.01Å to get good atomic resolution. Therefore it is absolutely necessary to reduce inner vibrations and to isolate the system from external vibrations.
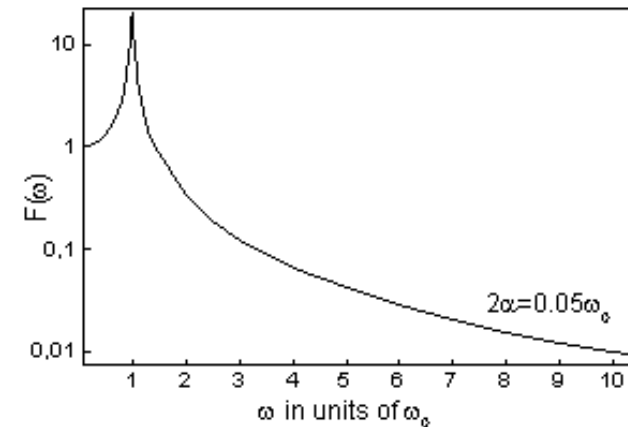Environmental vibrations are caused by:
• Vibration of the building 15 - 20 Hz
• Running people 2 - 4 Hz
• Vacuum pumps
• Sound

$$\omega_0 = \sqrt{k/m}$$

$$Q = \omega_0/2\alpha$$

k

Damping Factor α

m

Damping can be done by
• Suspension with springs (including additional eddy current dampers)
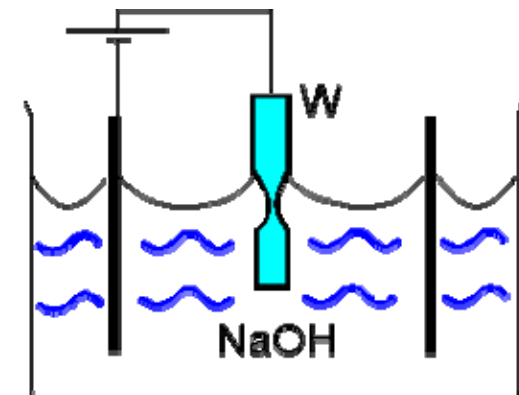• Stacked plate systems
• Pneumatic systems

Tip

The tip is the trickiest part in the STM experiment. It needs a small curvature to resolve coarse structures. For atomic resolution a minitip with a one atomic end is necessary. Tips typically are made out of tungsten, platinum or a Pt-Ir wire.
A sharp tip can be produced by:
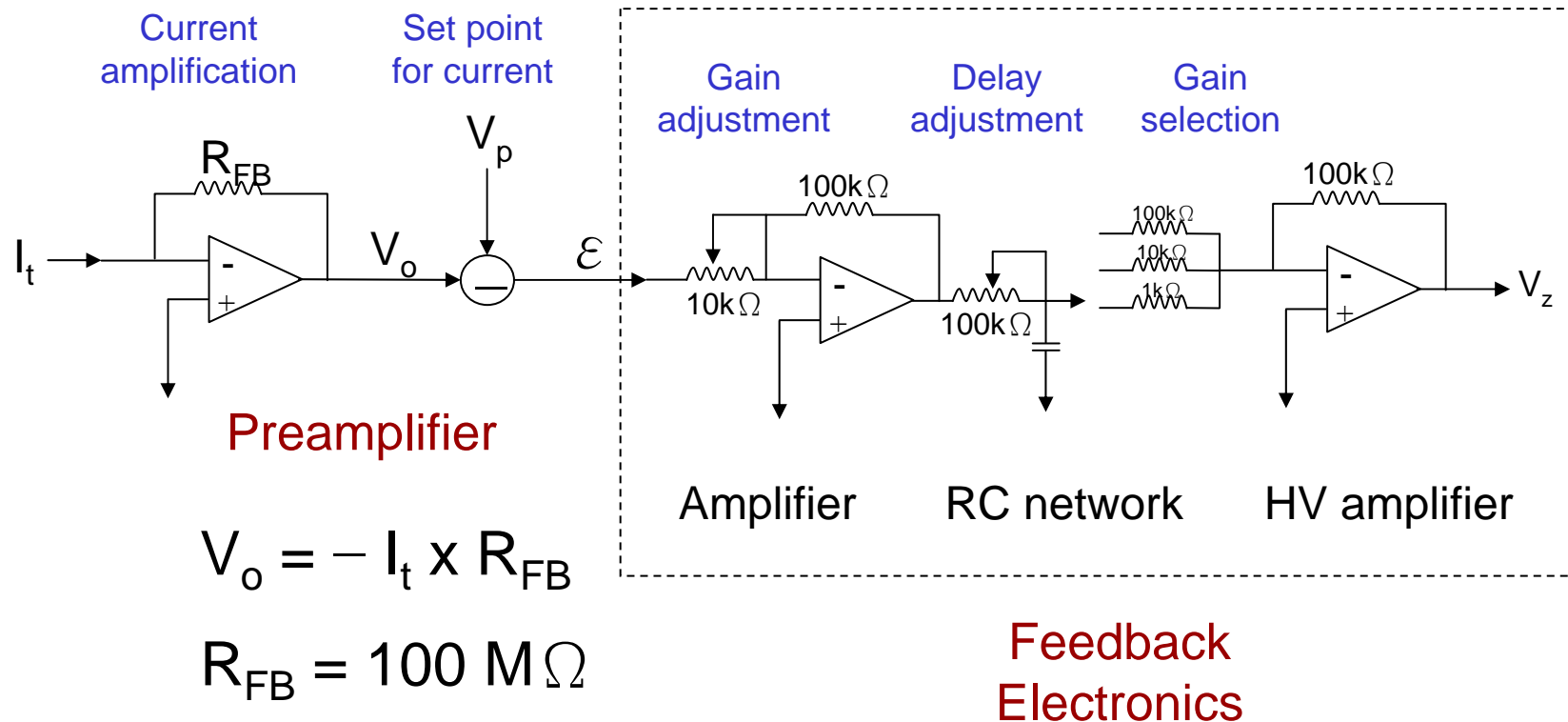• Cutting and grinding
• Electrochemical etching

Most often the tip is covered with an oxide layer and contaminations from the etchant and is also not sharp enough. Thus other treatments to the tip, like annealing or field evaporation are necessary.
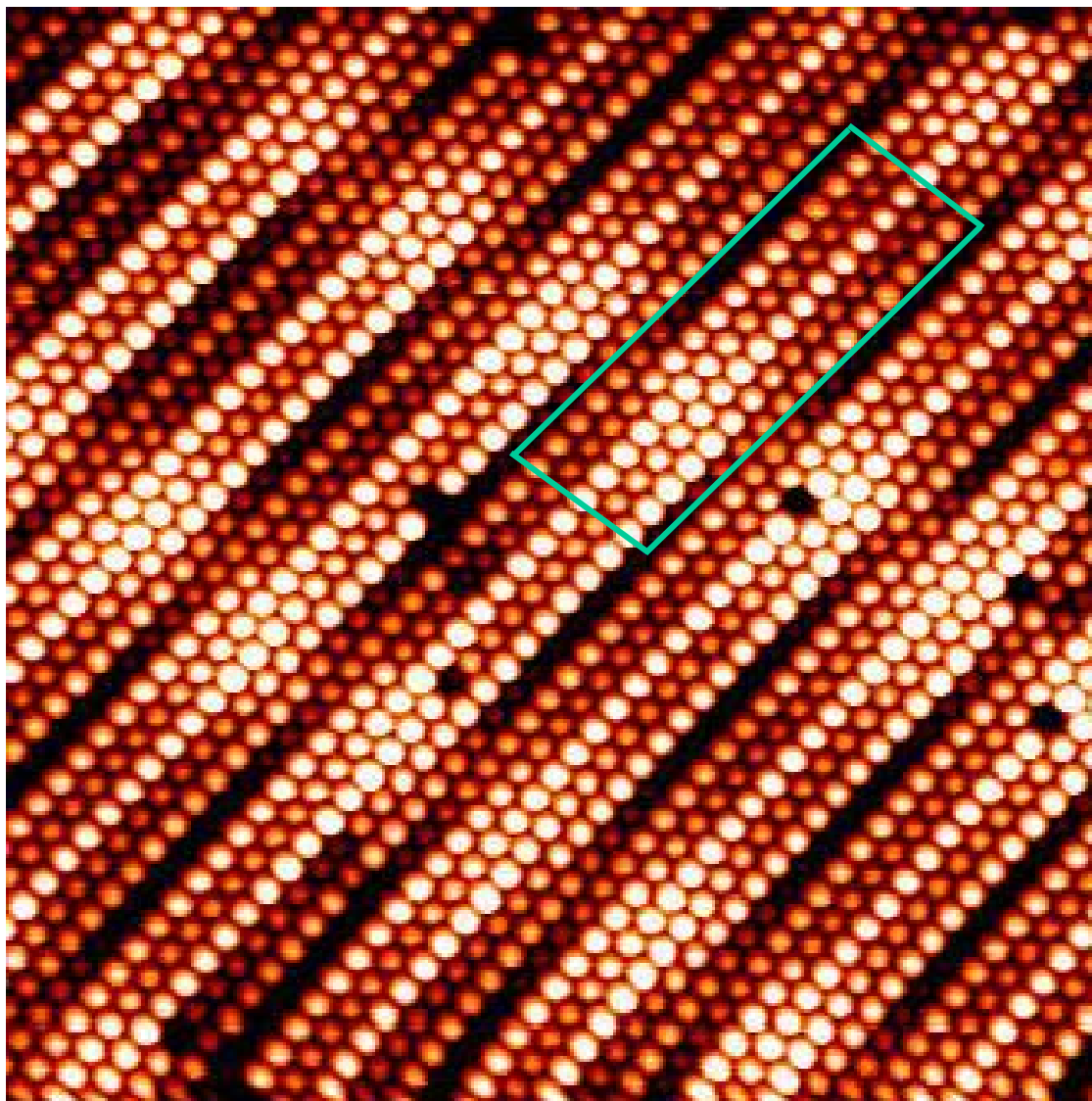
It is also possible to do tip-sharpening during tunneling.
• Sudden rise of the bias voltage to about -7V (at the sample) for 2-4 scan lines. By this treatment some W atoms may walk to the tip apex due to the nonuniform electric field and form a nanotip.
• Controlled collision on Si surface.
  The tip may pick up a Si-cluster which forms a monoatomic apex with a p_z like dangling bond.

STM electronics and control

Current amplification   **Set point for current**   **Gain adjustment**   **Delay adjustment**   **Gain selection**

R_{FB}

V_p

I_t

V_o

ε

100kΩ

100kΩ

10kΩ

100kΩ

100kΩ
10kΩ
1kΩ

V_z

Preamplifier

Amplifier   **RC network**   **HV amplifier**

$$V_o = - I_t \times R_{FB}$$

$$R_{FB} = 100 \text{ M}\Omega$$

Feedback Electronics

The tunneling current (0.01nA-50nA) is converted into a voltage by a current amplifier. To get a linear response with respect to the tunneling gap (the current is exponentially dependant on the tip-sample distance) the signal is processed by a logarithmic amplifier. The output of the logarithmic amplifier is compared with a predetermined voltage which is used as a reference current. The error signal is passed to feedback electronics, which applies a voltage to the z piezo to keep the difference between the current set point and the tunneling current small. Care has to be taken to keep the noise signal ratio on a low level. Also the response time of the feedback has to be minimized without loosing accuracy.

Atomic Structure of the Pt(001) Surface

50 Å

500 Å

Dislocation lines
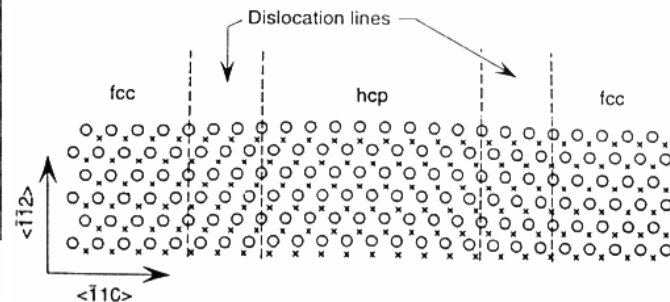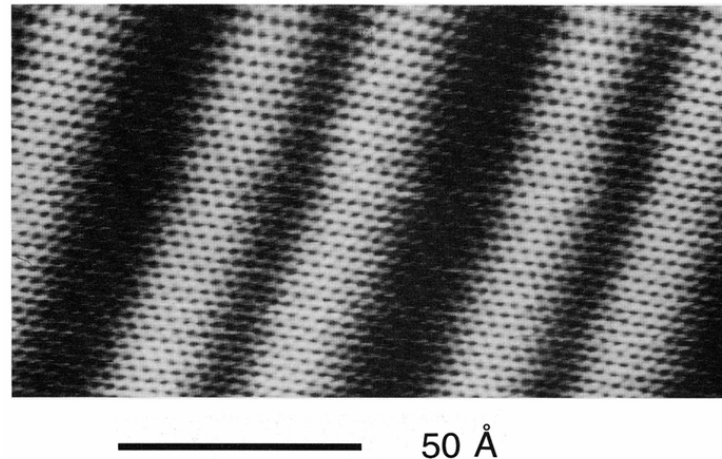
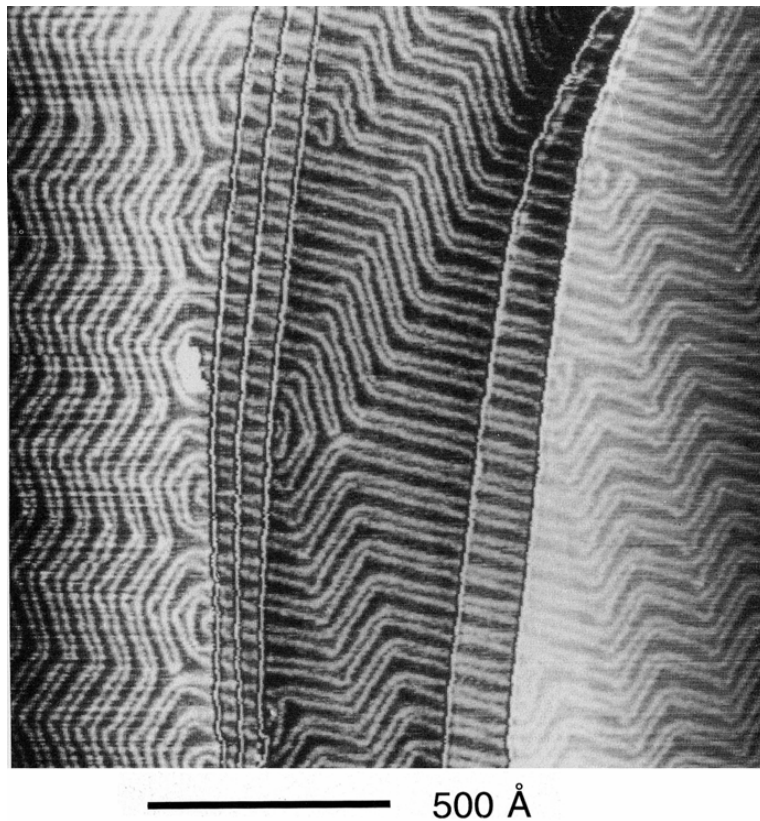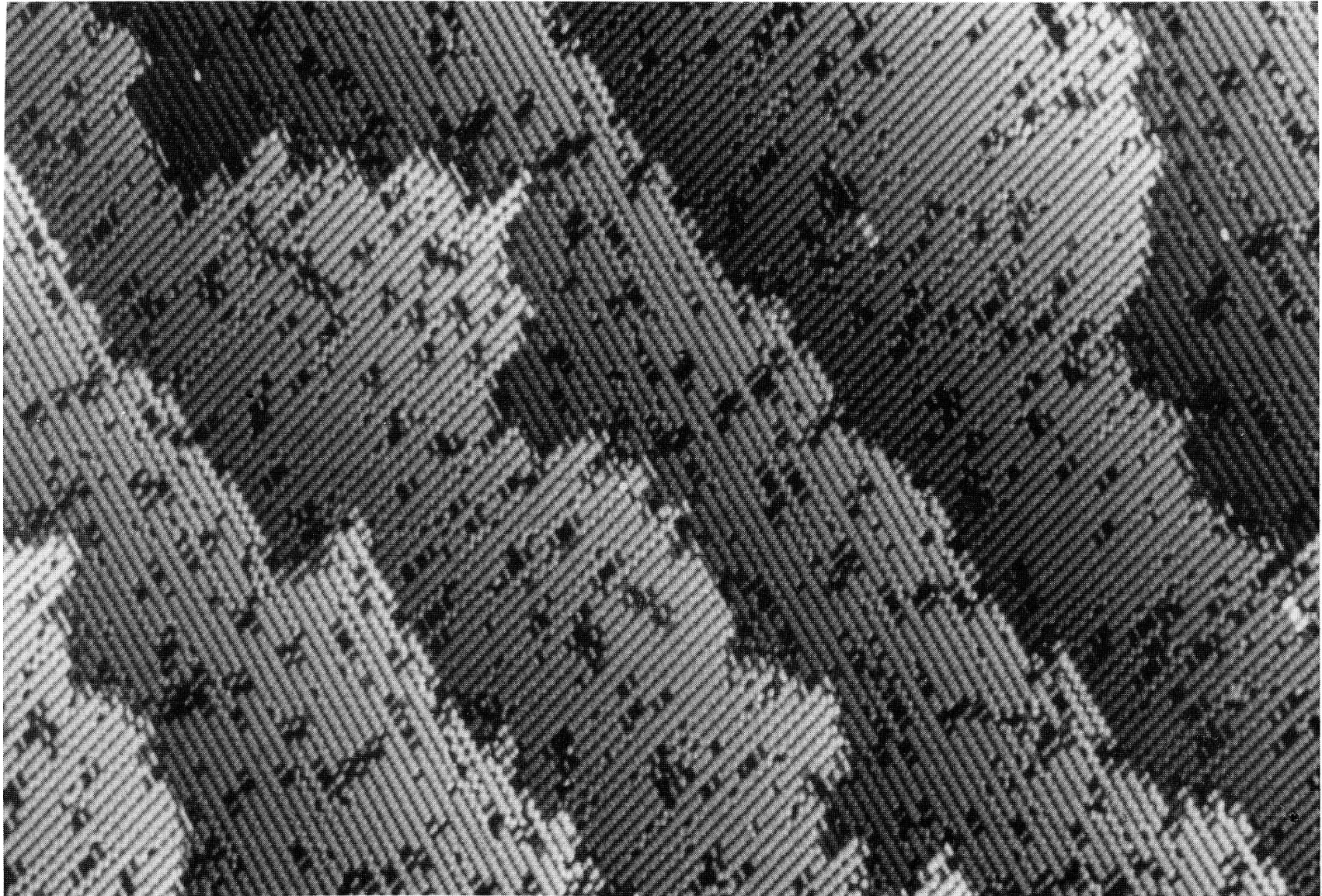fcc   hcp   fcc

⟨1̄1̄2⟩

⟨11̄0⟩

Fig. 1. In-plane structure of the Au(111) surface with a $22 \times \sqrt{3}$ reconstruction. The circles and crosses correspond to atoms in the first and second surface layers, respectively. Surface atoms in both sides of the figure lie on fcc sites, whereas atoms in the center of the figure lie on hcp sites. The domain walls (dislocation lines) involve atoms in bridge sites.
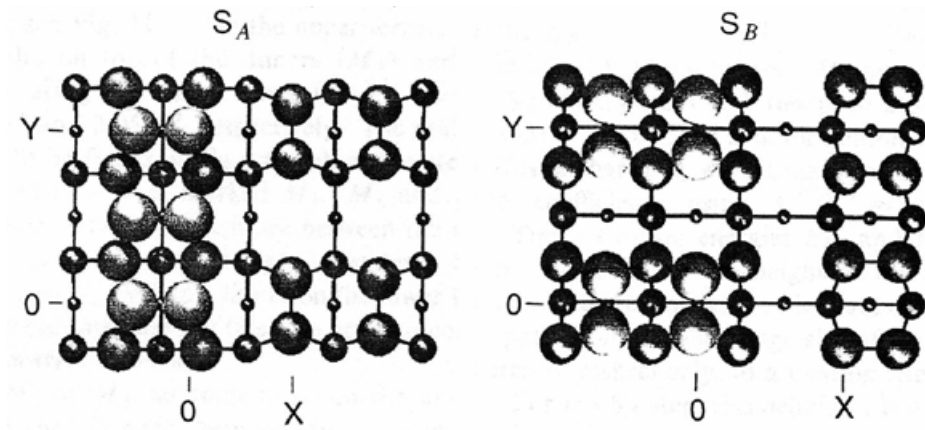
Large-scale image of the Au(111)-$22 \times \sqrt{3}$ reconstruction. The Au(111) surface reconstructs at room temperature to form a $22 \times \sqrt{3}$ structure, which has a two-fold symmetry. On a large scale, three equivalent orientations for this reconstruction coexist on the surface. Furthermore, on an intermediate scale, a herring-bone pattern is formed.
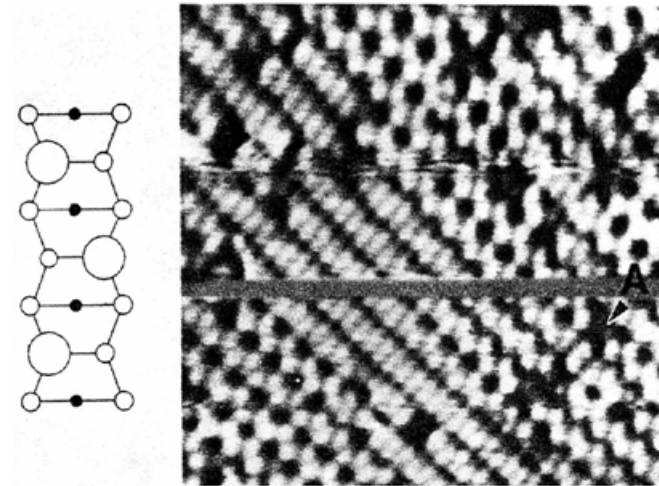
Science 258, 1763 (1992).

Atomic Structure of the Si(001) Surface

Si(001)-2x1 and 1x2

Si(001)-c(4x2)

Si(111)-(2x1)