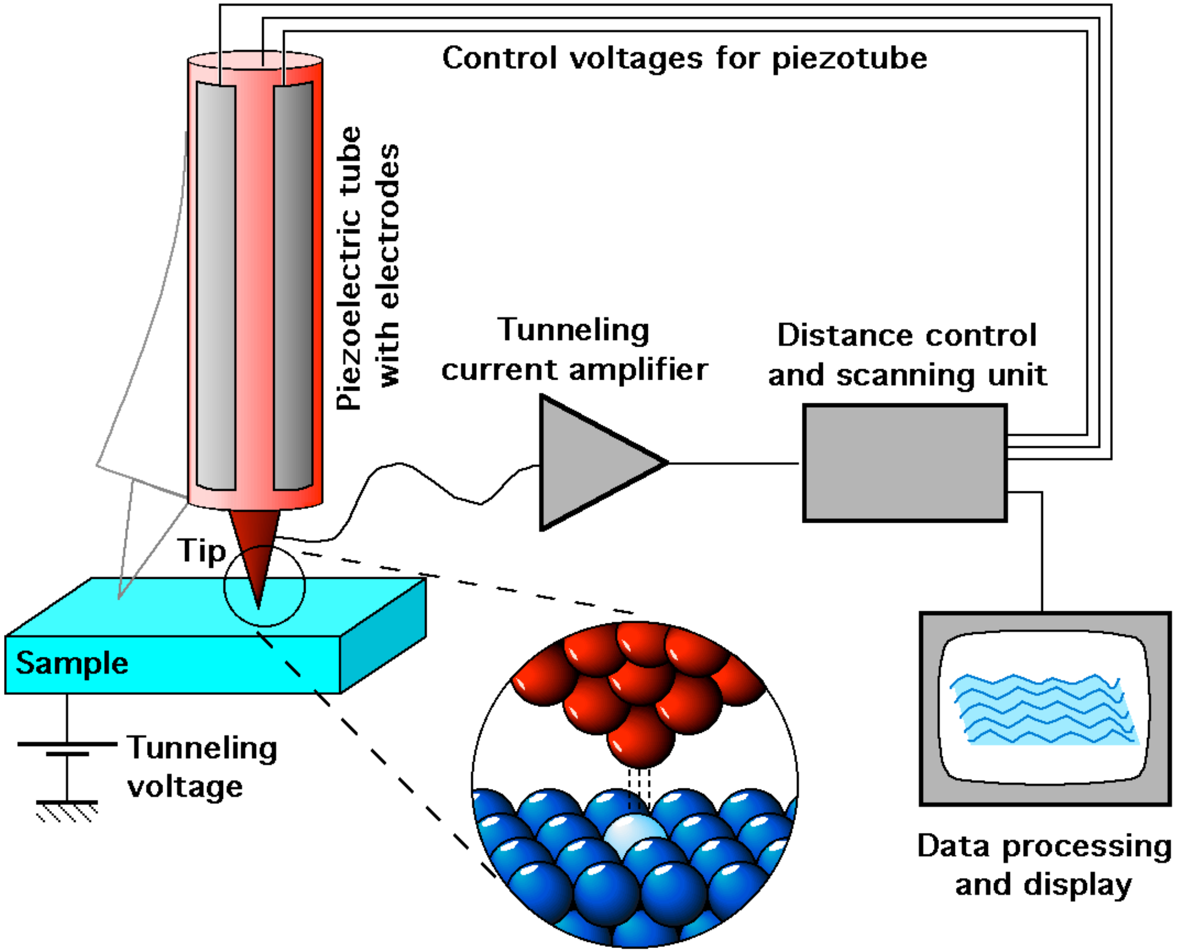
Scanning Tunneling Microscopy

A scanning tunneling microscope (STM) is an instrument for imaging surfaces at the atomic level. Its development in 1981 earned its inventors, Gerd Binnig and Heinrich Rohrer (at IBM Zürich), the Nobel Prize in Physics in 1986. For a STM, good resolution is considered to be 0.1 nm lateral resolution and 0.01 nm (10 pm) depth resolution. With this resolution, individual atoms within materials are routinely imaged and manipulated. The STM can be used not only in ultra-high vacuum but also in air, water, and various other liquid or gas ambients, and at temperatures ranging from near zero kelvin to over 1000°C.

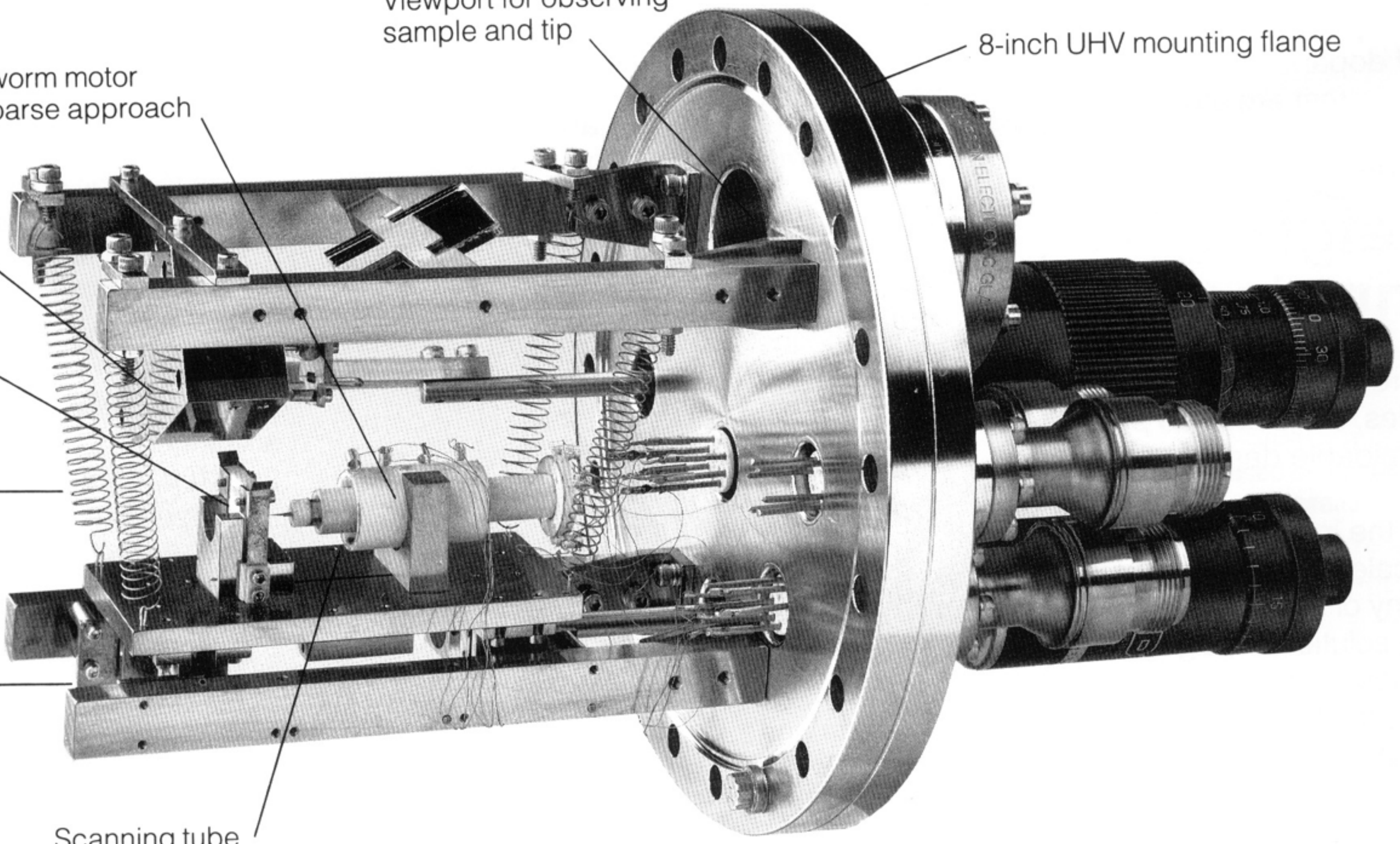
References:

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).

Scanning Tunneling Microscopy



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"

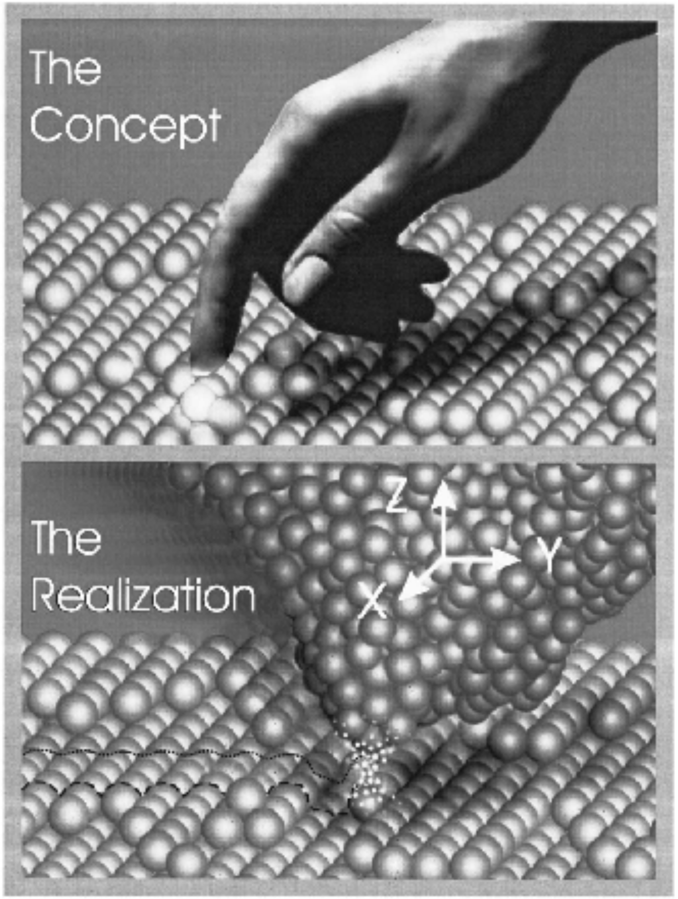
Interchangeable sample holder

Suspension spring for low-frequency vibration isolation

Damping and lockdown mechanism

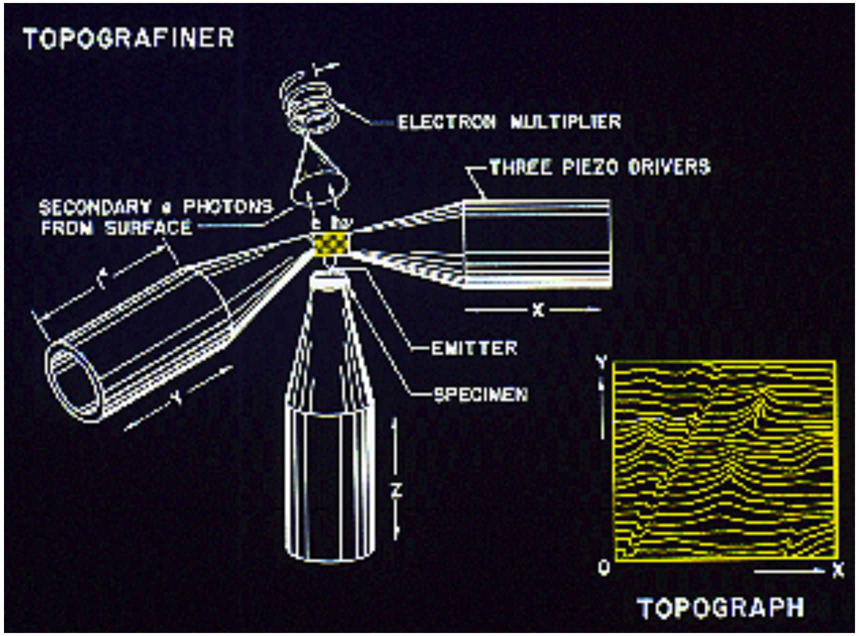
Scanning tube for tip control

Concept: Eye and Finger

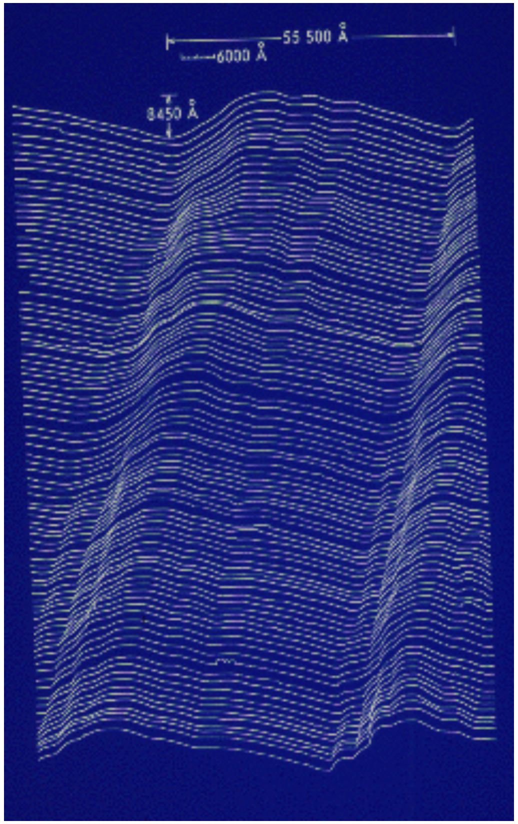


G. Binnig and and H. Rohrer, *Rev. of Mod. Phys.* **71**, S324-S330 (1999).

Topografiner

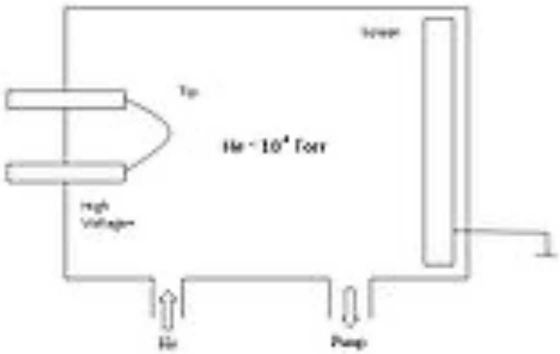


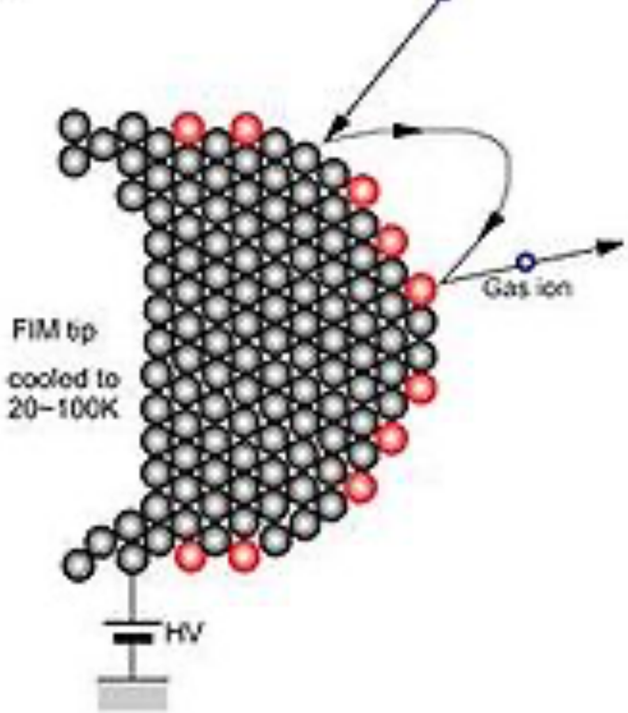
R. Young, J. Ward, and F. Scire, Rev. Sci. Instrum. **43**, 999 (1972).

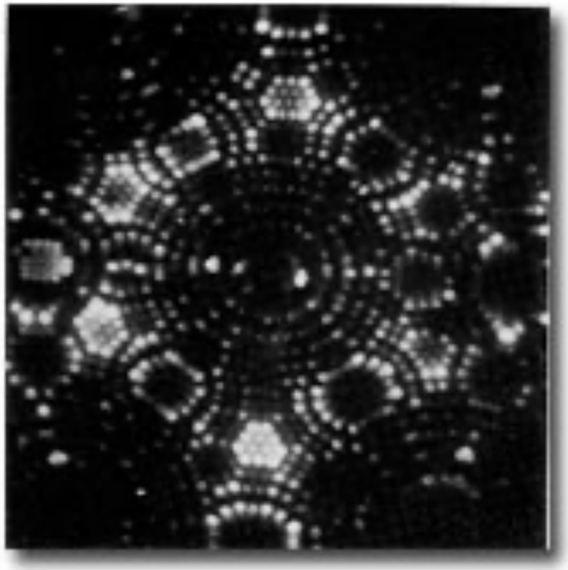


Topographic map of a 180-line-per-mm diffraction-grating replica

Field Ion Microscopy







Erwin W. Müller (1951)

Wave nature of electron

rödinger's equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_n(z)}{\partial z^2}+U(z)\psi_n(z)=E\psi_n(z)$$

J(z)

$$\psi_n(z)=\psi_n(0)e^{\pm ikz}$$

where

$$k=\frac{\sqrt{2m(E-U(z))}}{\hbar}$$

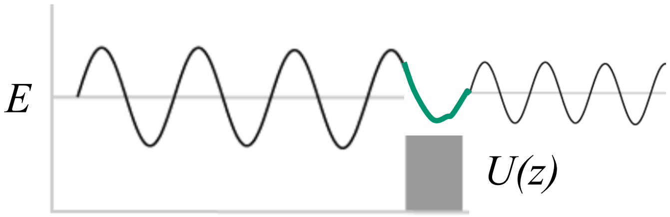
J(z)

$$\psi_n(z)=\psi_n(0)e^{\pm\kappa z}$$

where

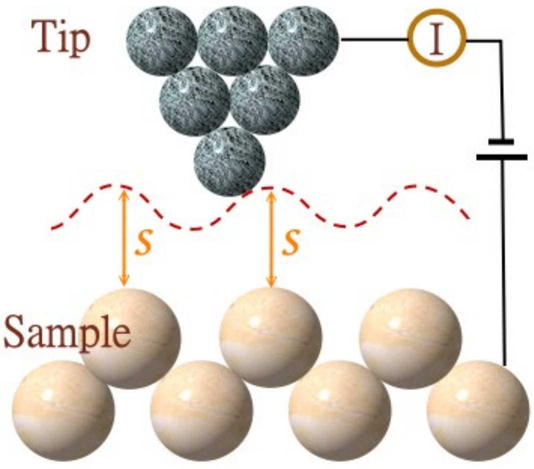
$$\kappa=\frac{\sqrt{2m(U-E)}}{\hbar}$$

Travelling

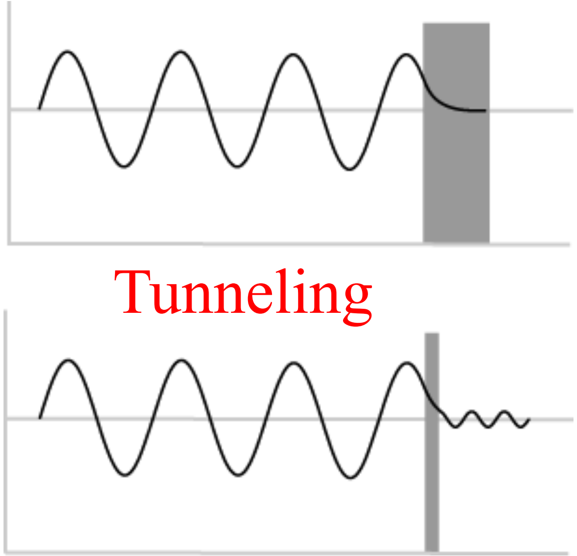


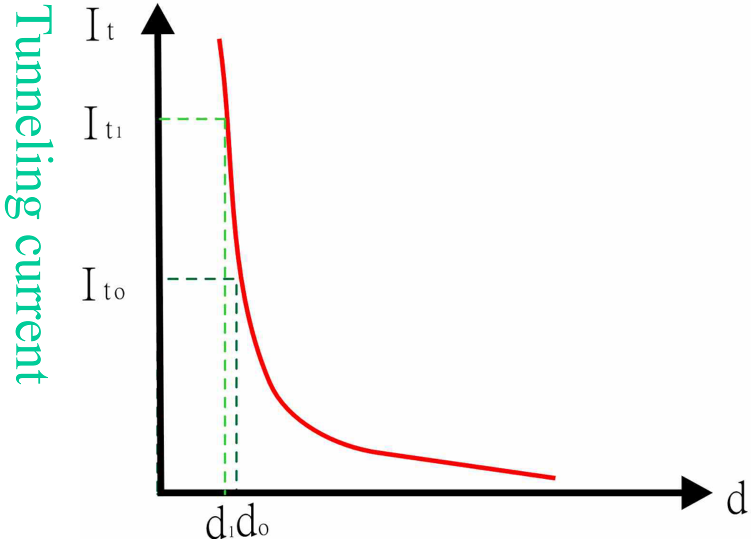
Tunneling

Theory of STM



Constant Current Mode





Tunneling current I_t

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

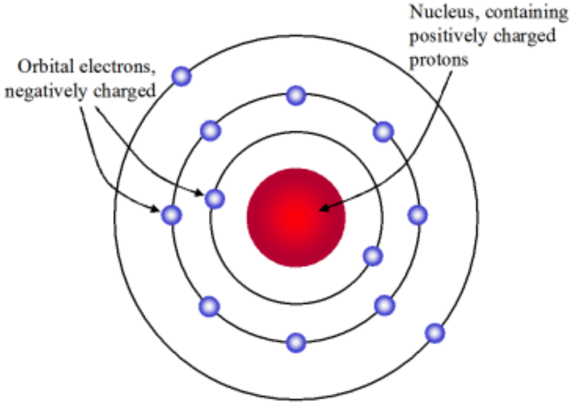
$A = 1.025\ (\mathrm{eV})^{-1/2}\text{Å}^{-1}$

$\phi \sim 4 - 5$ eV

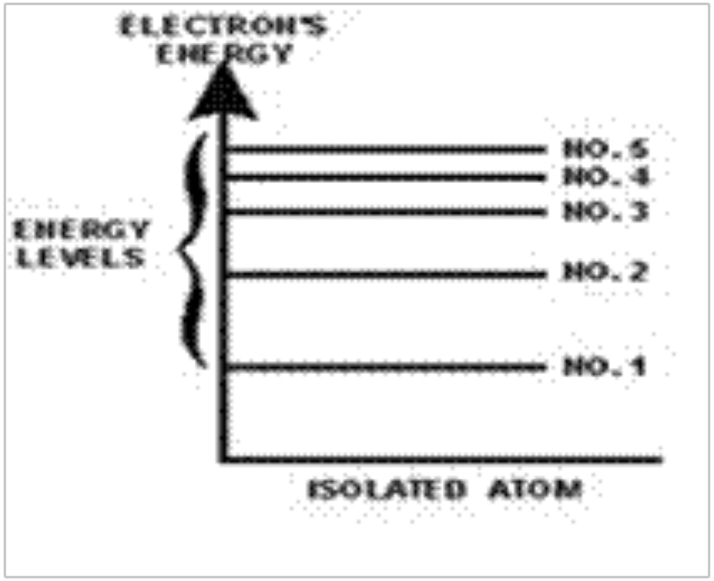
d decreases by 1 Å,

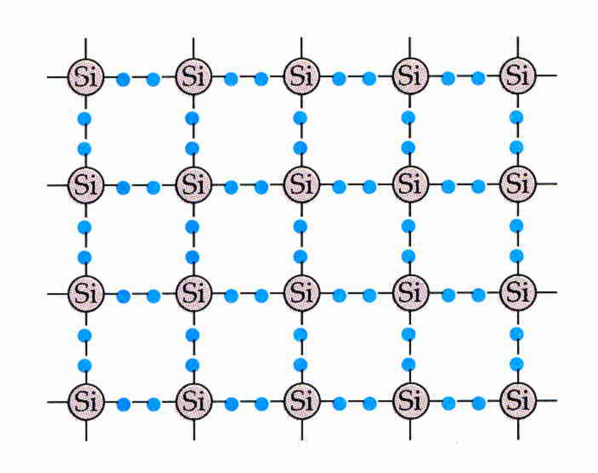
I_t will be increased by ~10 times.

Band Theory of Solids



Isolated atom





Energy Bands in Solids

In solids, the outer electronic energy levels of individual atoms become smeared out to form bands

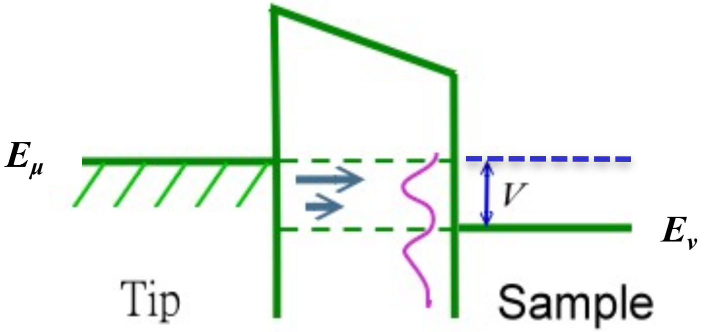
In solids the outer electron energy levels become smeared out to form bands

The highest occupied band is called the VALENCE band. This is full.

For conduction of electrical energy there must be electrons in the CONDUCTION band. Electrons are free to move in this band.

Tunneling current

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



where $f(E)$ is Fermi function,

$E_{\mu,\nu}$ is the energy of state, where μ and ν run over all the states of the tip and surface,

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

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

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

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

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

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

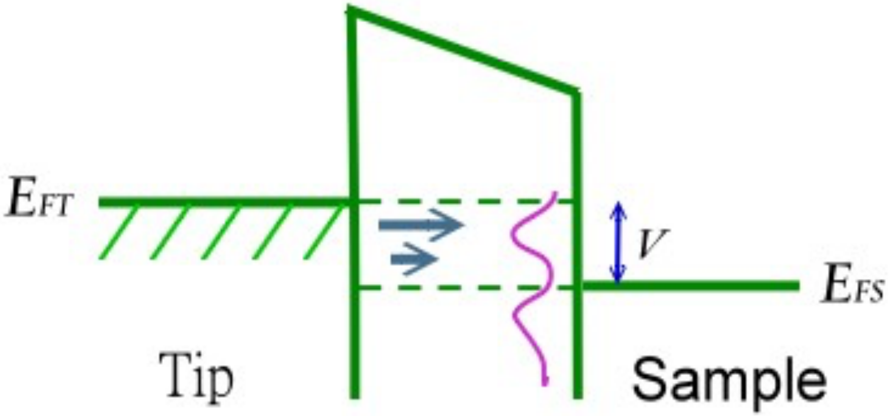
Tunneling current

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

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.

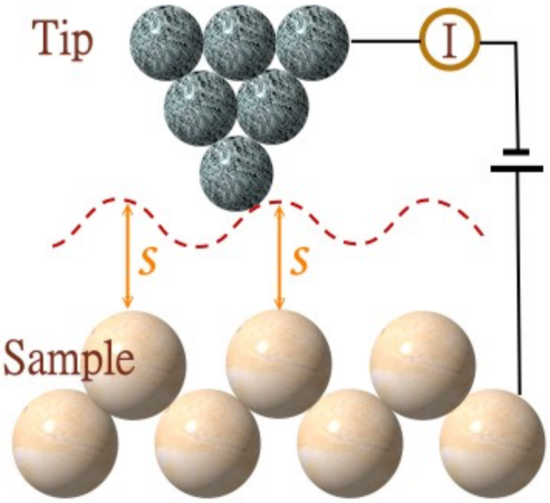
In the low-voltage limit

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

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

$$\rho_S(\tilde{r};E) \equiv \sum_\nu |\psi_\nu(\tilde{r})|^2 \delta(E_\nu - E)$$

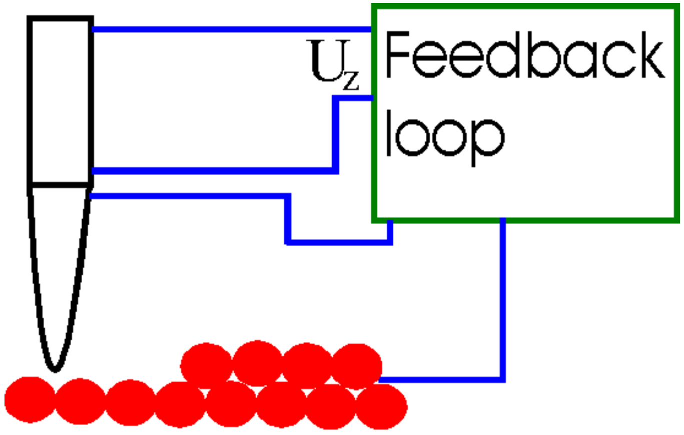
$\rho_t(E_F)$ is the density of states of the tip at the Fermi level and is often regarded as a constant.



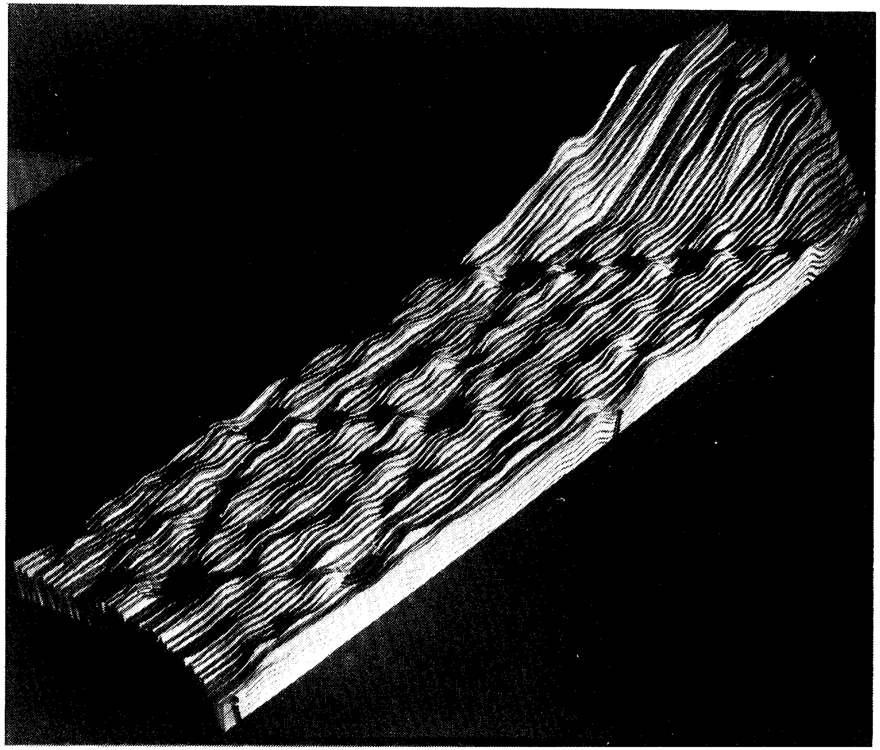
Constant Current Mode

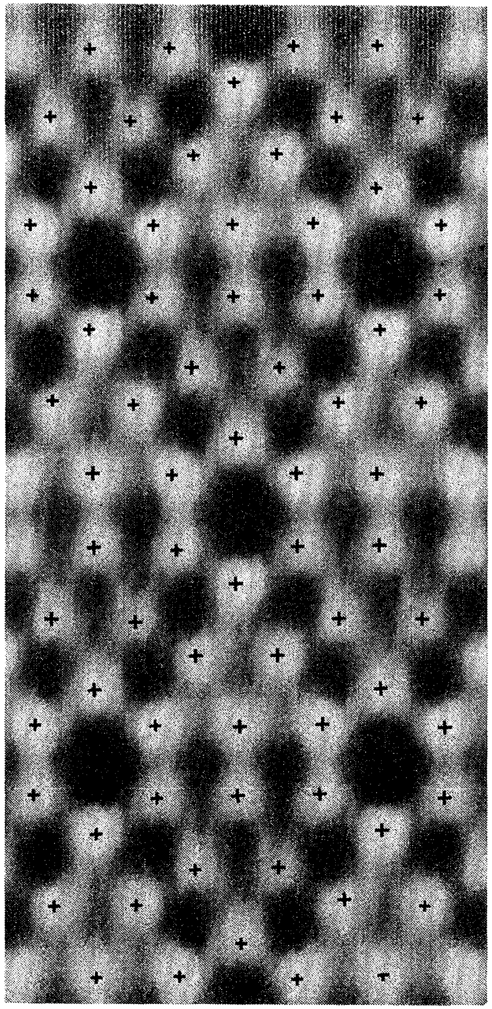
Modes of Operation

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.



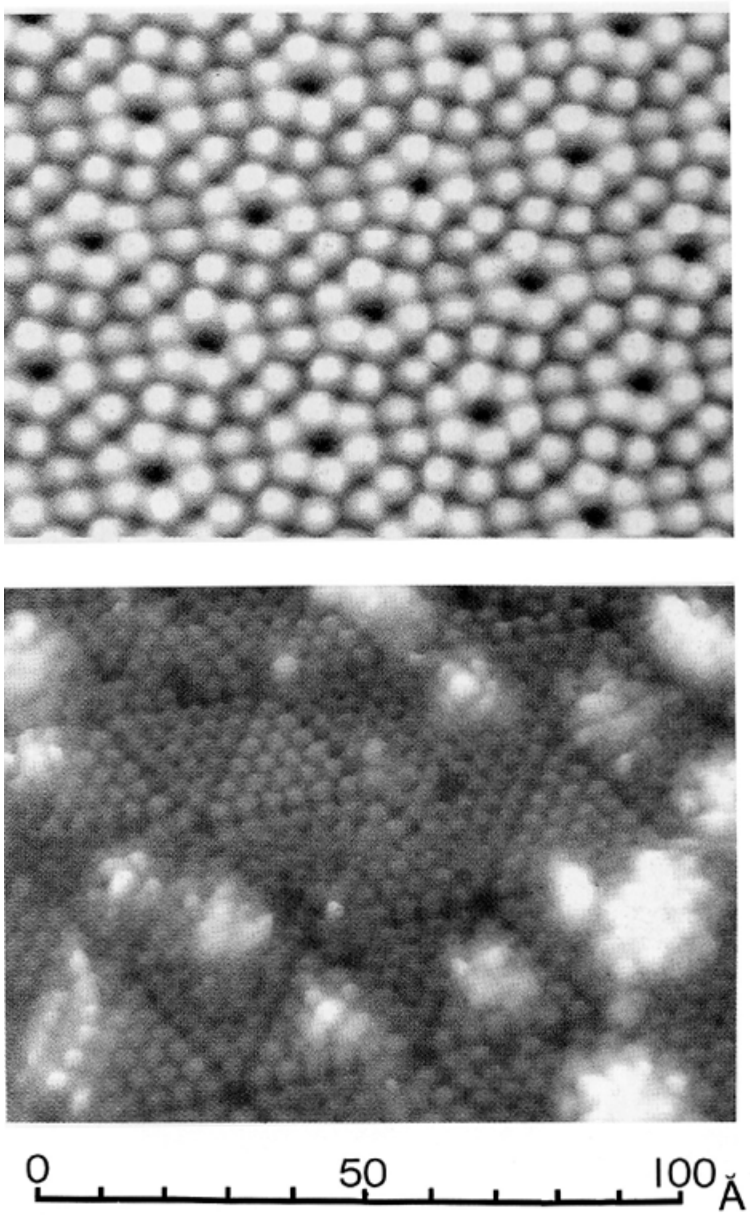
7 × 7 Reconstruction on Si(111) Resolved in Real Space



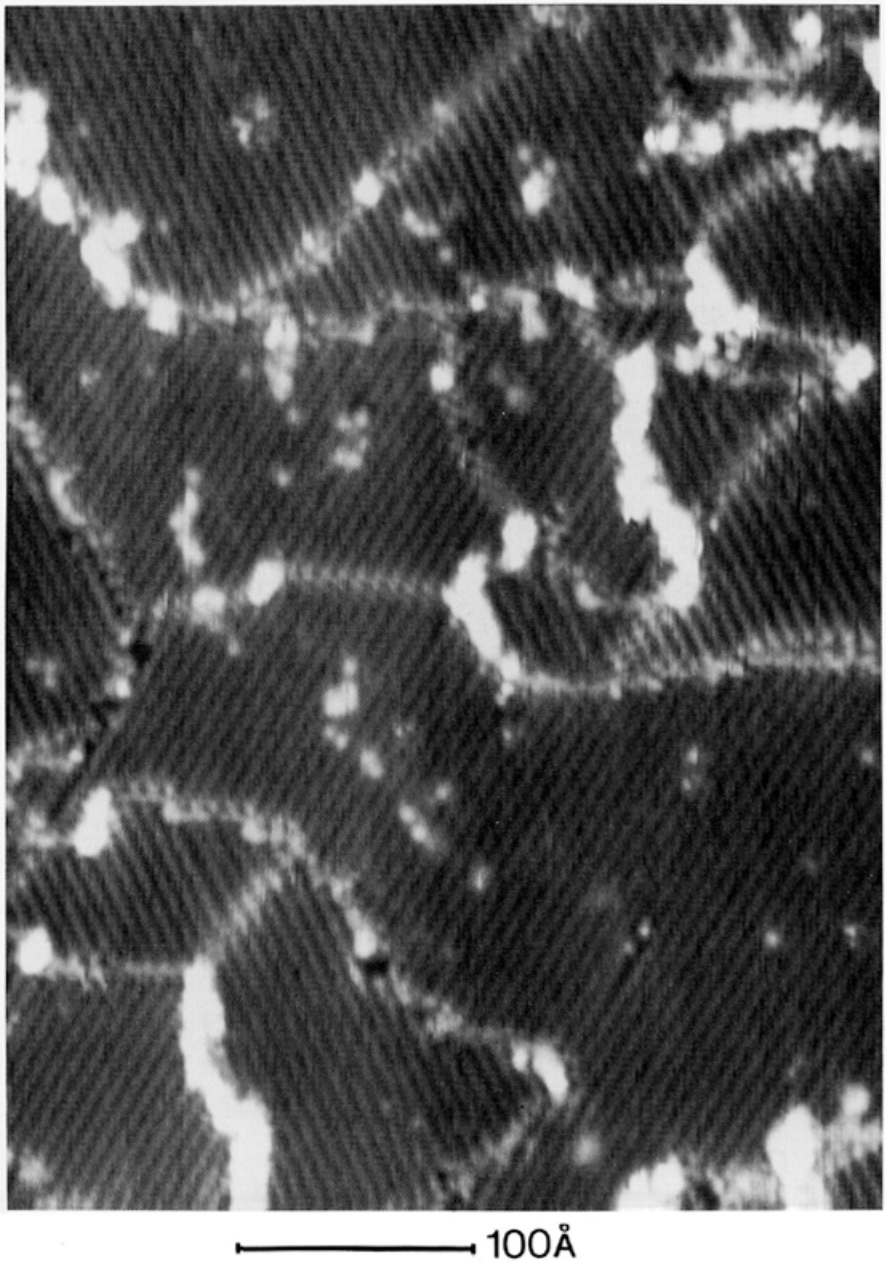


G. Binnig, H. Rohrer, Ch. Gerber, and E. Weibel
Phys. Rev. Lett. 50, 120 (1983)

Si(111)-(7x7)

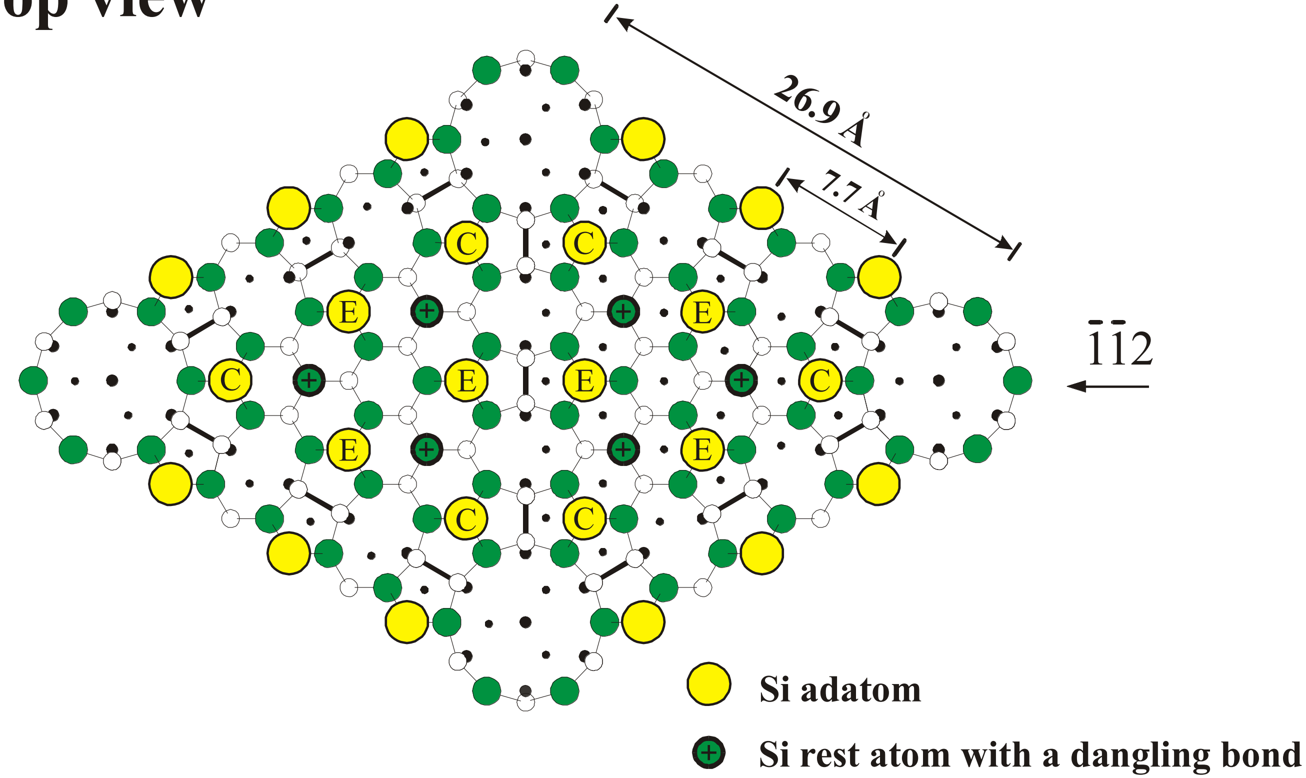


Si(111)-2x1

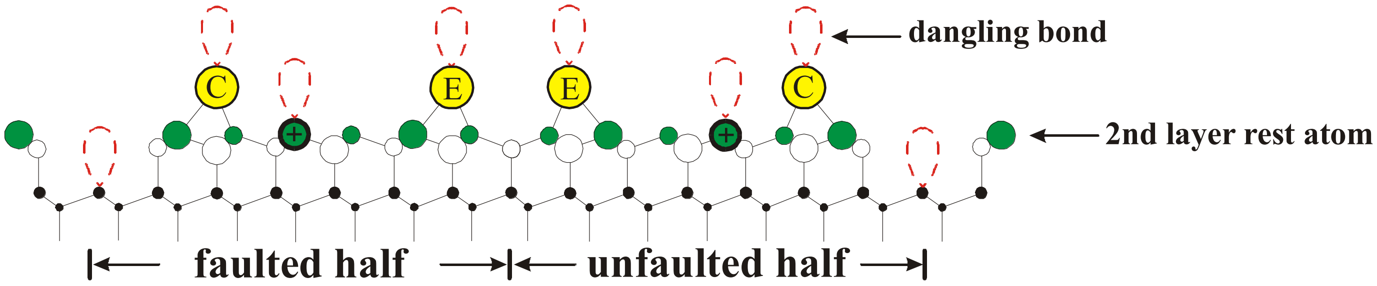


Atomic Model of Si(111)-(7×7)

Top view

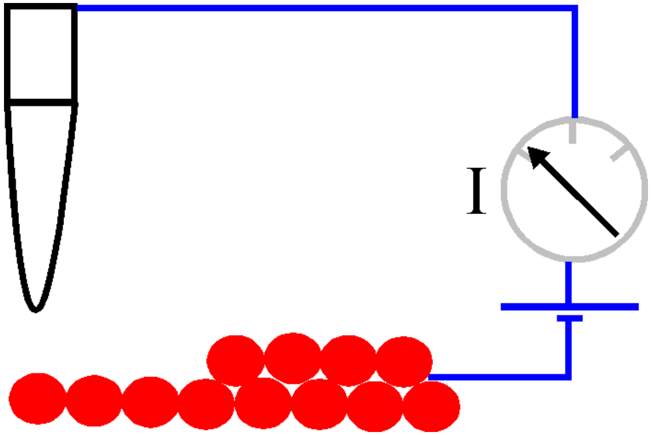


Side view



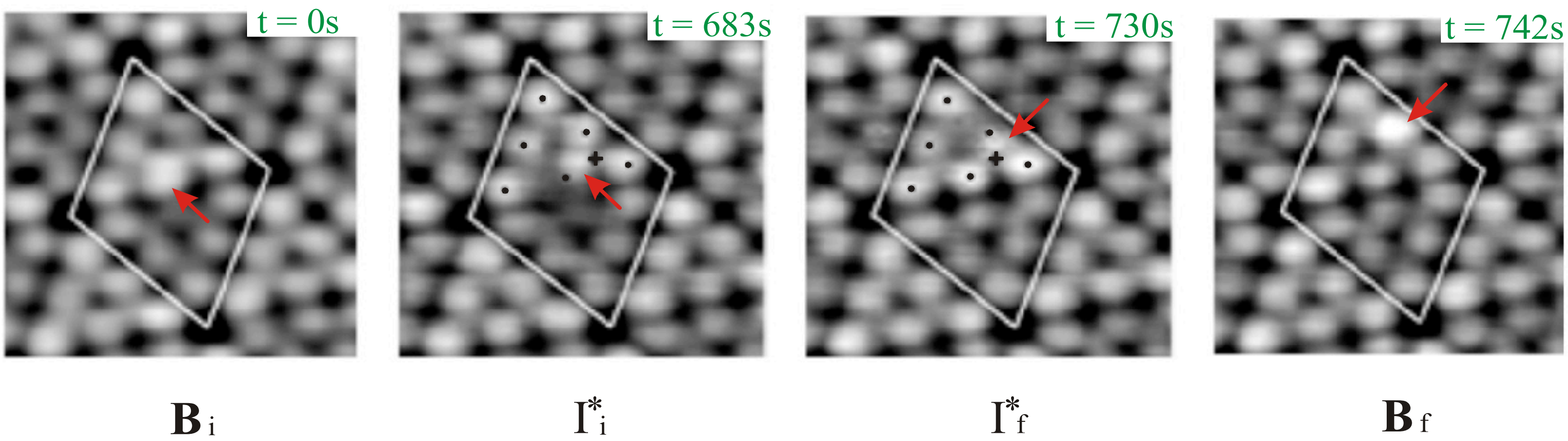
2. Constant Height Mode

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.

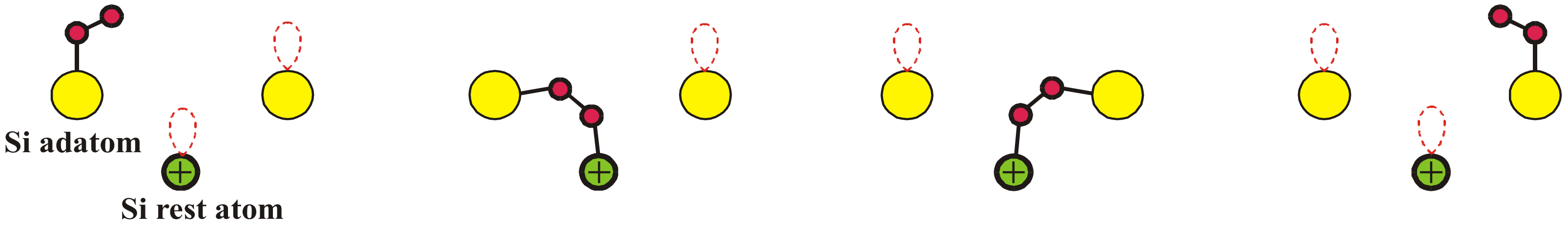


Site Hopping of O_2 Molecule on Si(111)-(7x7)

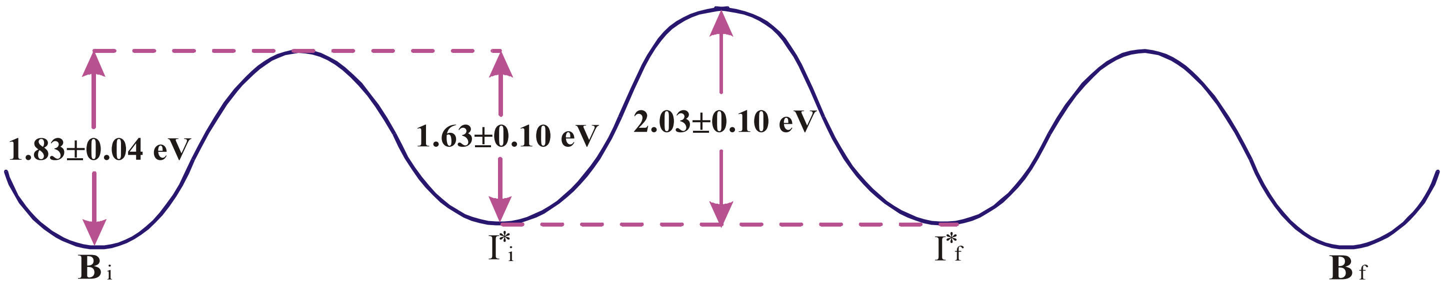
STM images



Atomic model



Potential diagram



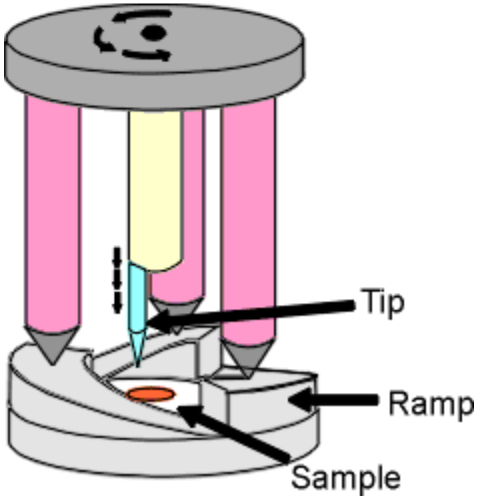
Technical Aspects

Demands:

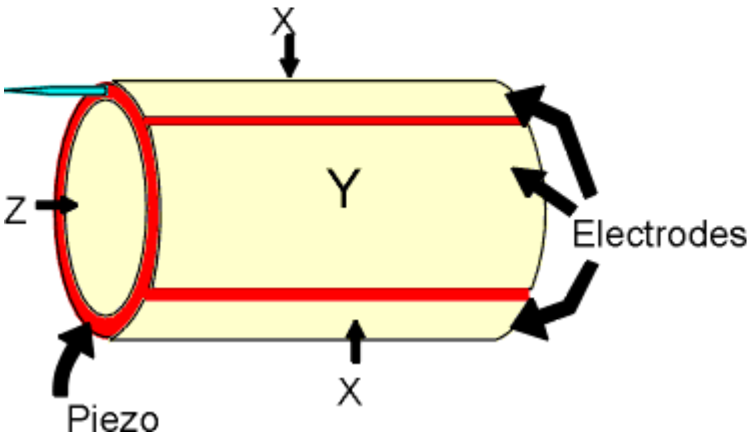
1. Controlling the tip-sample distance from a few mm down to 0.01Å
2. Exact lateral positioning
3. Stabilized tip-sample distance
4. Sharp tip
5. Measuring a current in the range of 0.01nA-50nA

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.

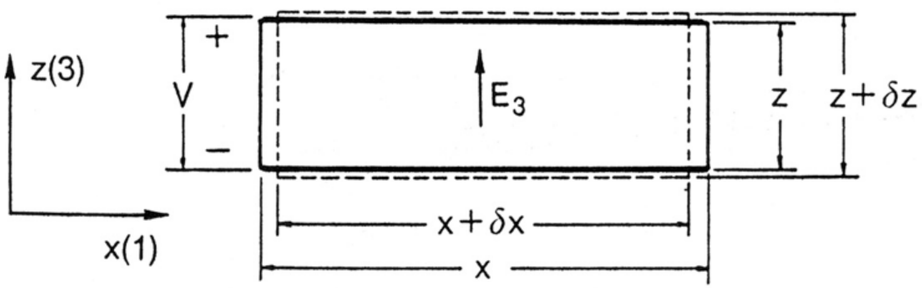


coarse positioner (beetle)

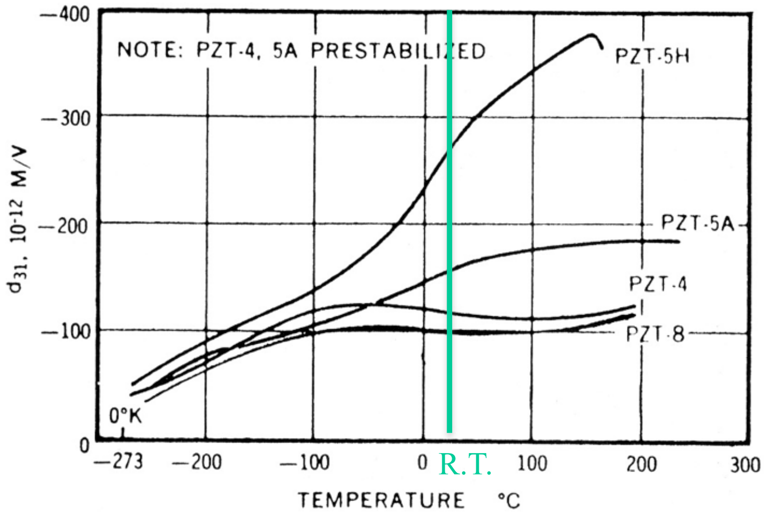


fine positioner/scanner

Piezoelectric Response



Variation of piezoelectric coefficient with temperature.



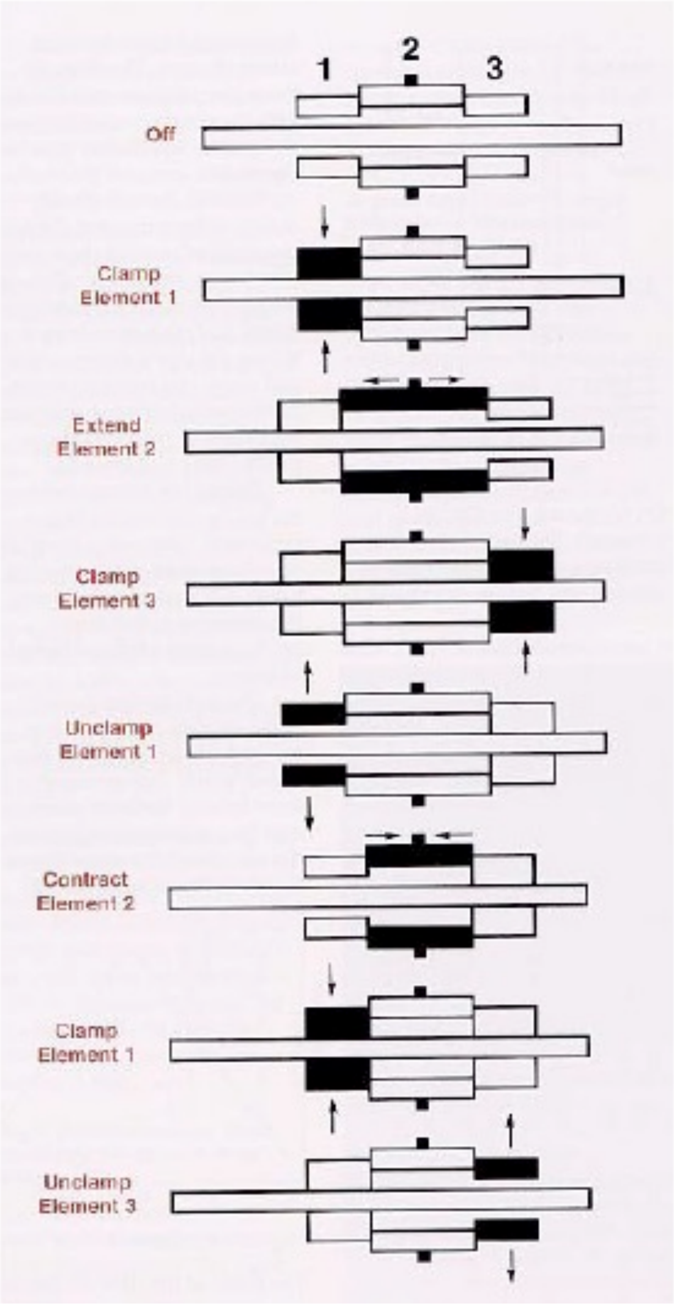
Strain: $S_1 = \delta x/x$, $S_3 = \delta z/z$

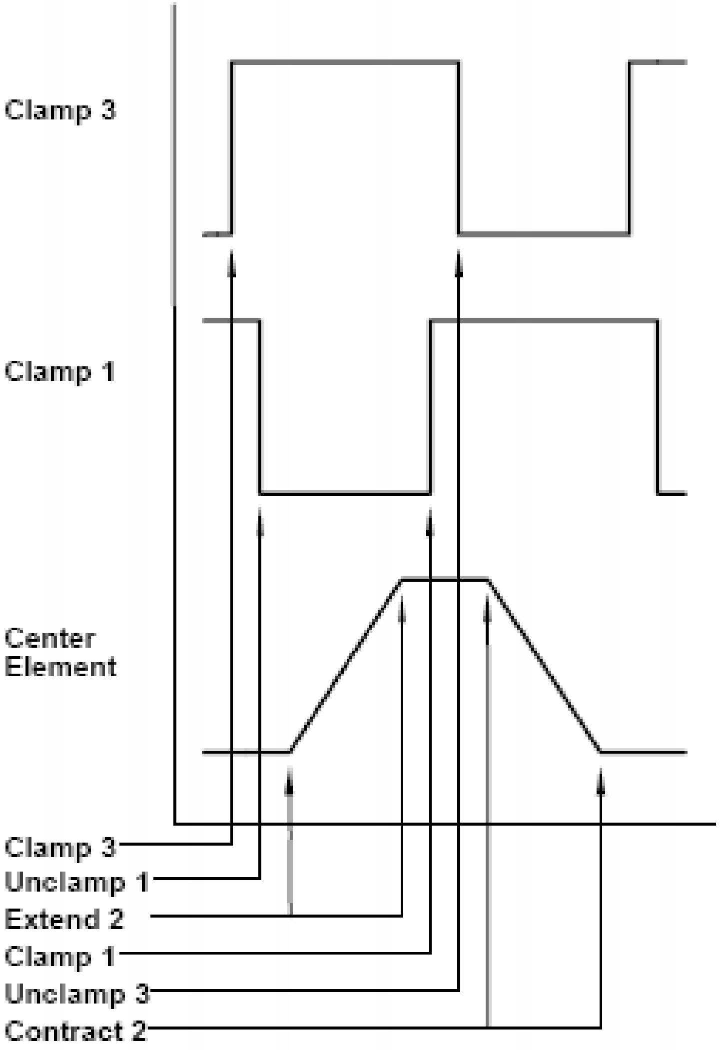
Electric field: $E_3 = V/z$

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

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

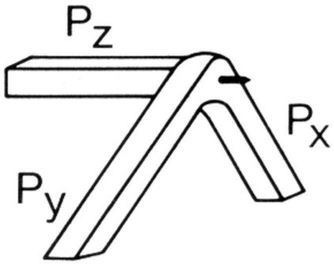
Inchworm Motor





Piezoelectric Scanner

Tripod scanner



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

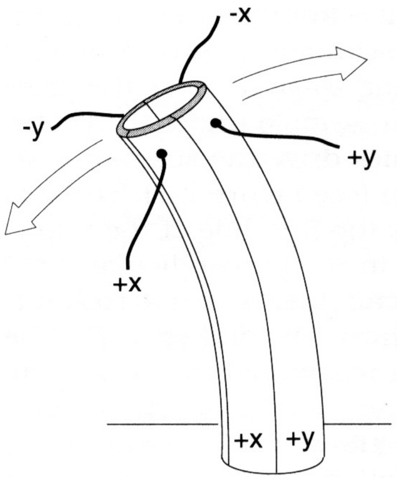
Piezoelectric Constant:

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

Resonance Freq. for bending:

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

Tube scanner



Piezoelectric Constant:

$K = dx/dV = 2\sqrt{2}d_{31}L^2/\pi Dh$

Resonance Freq. for bending:

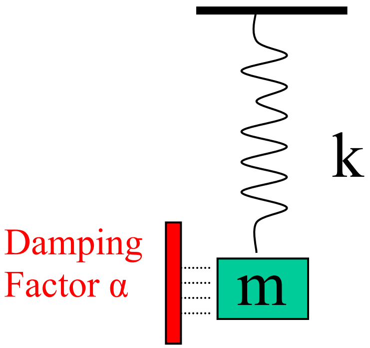
$f = 0.56\ \kappa C/L2\ ,\ \kappa = (D^2 + d^2)^{1/2}/8$

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.

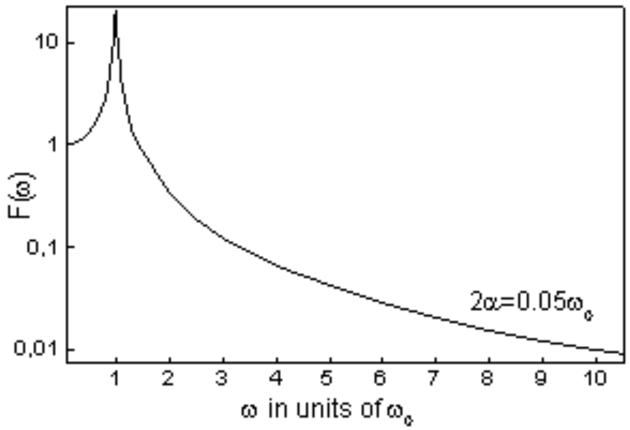
Environmental vibrations are caused by:

- Vibration of the building 15 - 20 Hz
- Running people 2 - 4 Hz
- Vacuum pumps
- Sound



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

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



Damping can be done by

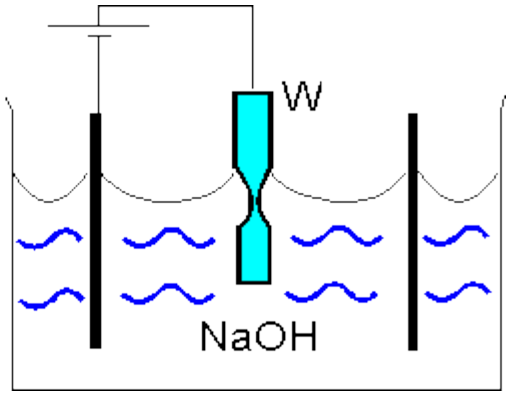
- Suspension with springs (including additional eddy current dampers)
- Stacked plate systems
- Pneumatic systems

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.

Feedback loop in STM

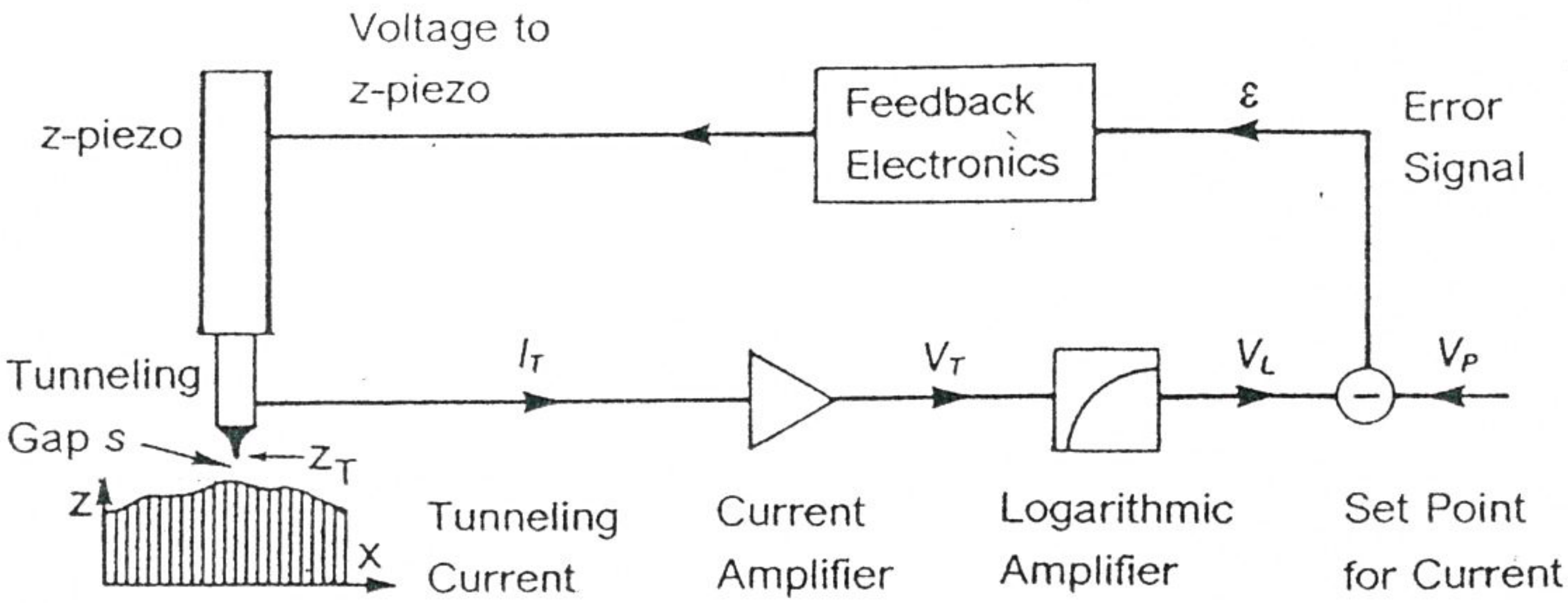
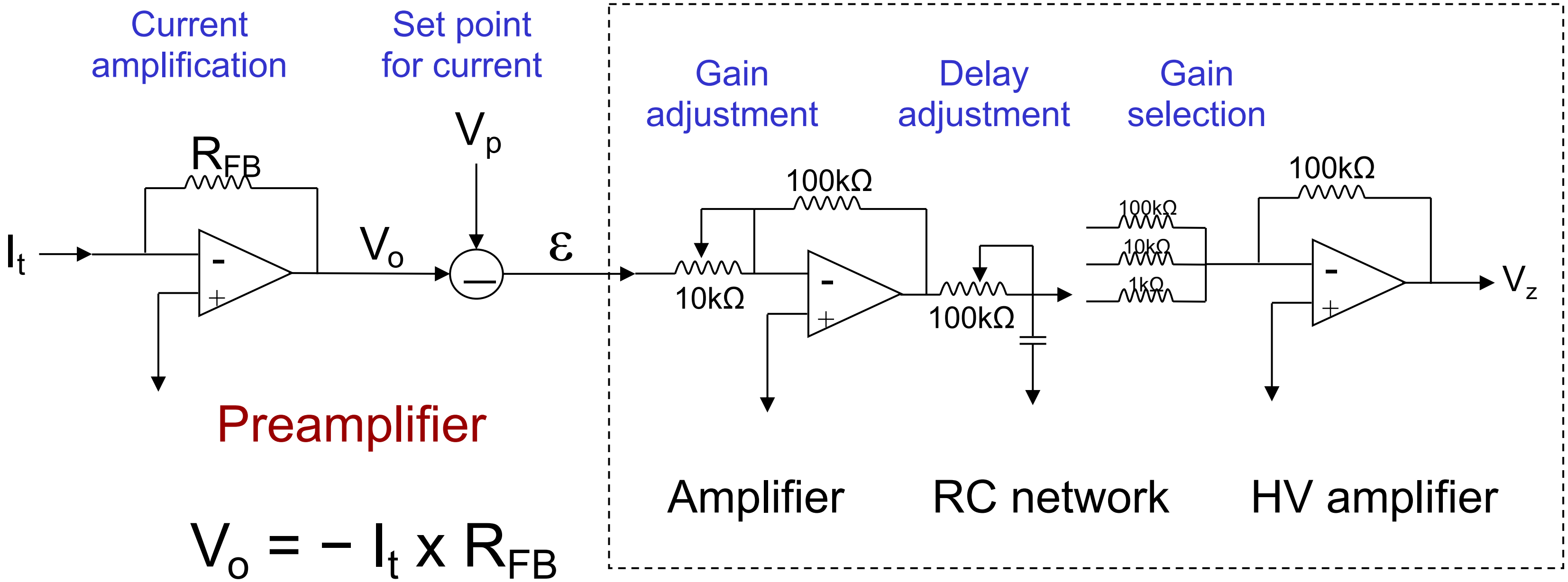


Fig. 11-5. A schematic of the feedback loop in an STM. The tunneling current, after the current amplifier and the logarithmic amplifier, is compared with a current set-point, which represents the reference current. The error signal is processed by the feedback electronics, which typically contains an amplifier and an integration circuit. The output of the feedback electronics is applied to the *z*-piezo, to keep the error between the actual tunneling current and the reference current very small. The voltage applied on the *z*-piezo is recorded as the topographic image.

STM electronics and control



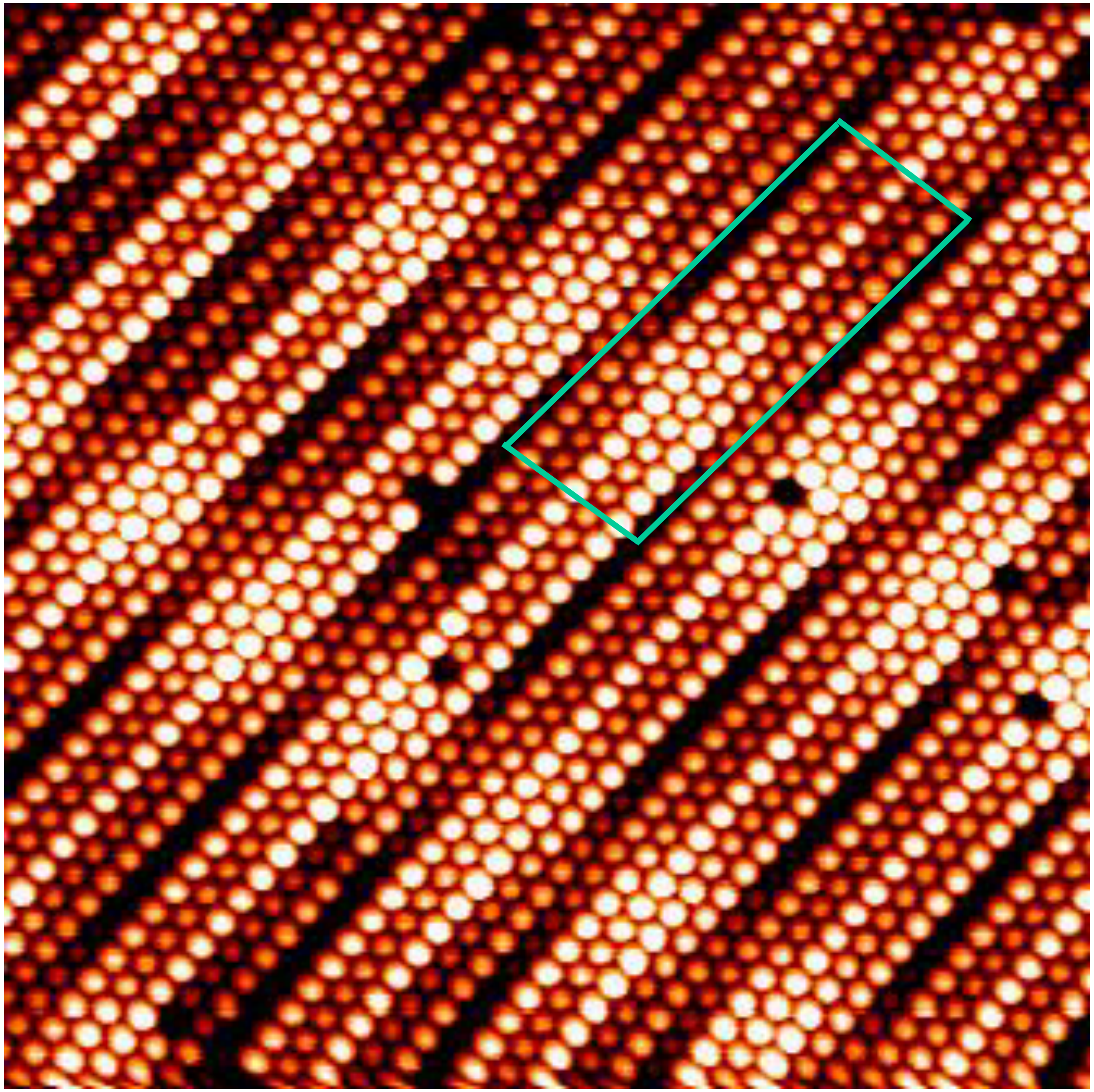
$$V_o = -I_t \times R_{FB}$$

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

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.

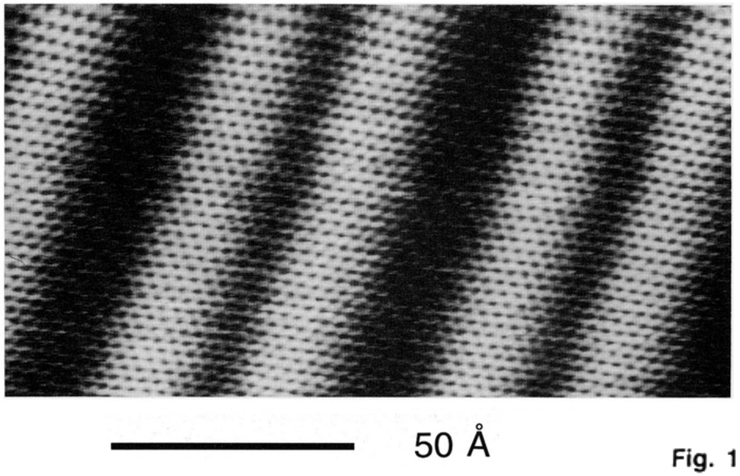
Atomic Structure of the Pt(001) Surface



V_b = 0.1 V

I_t = 1 nA

Surface Science **306**, 10 (1994).



V_b = 0.1 V

I_t = 1 nA

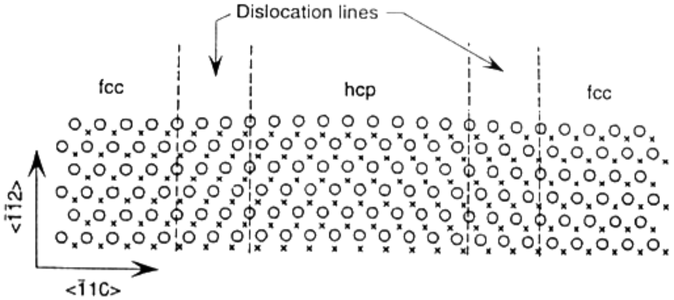
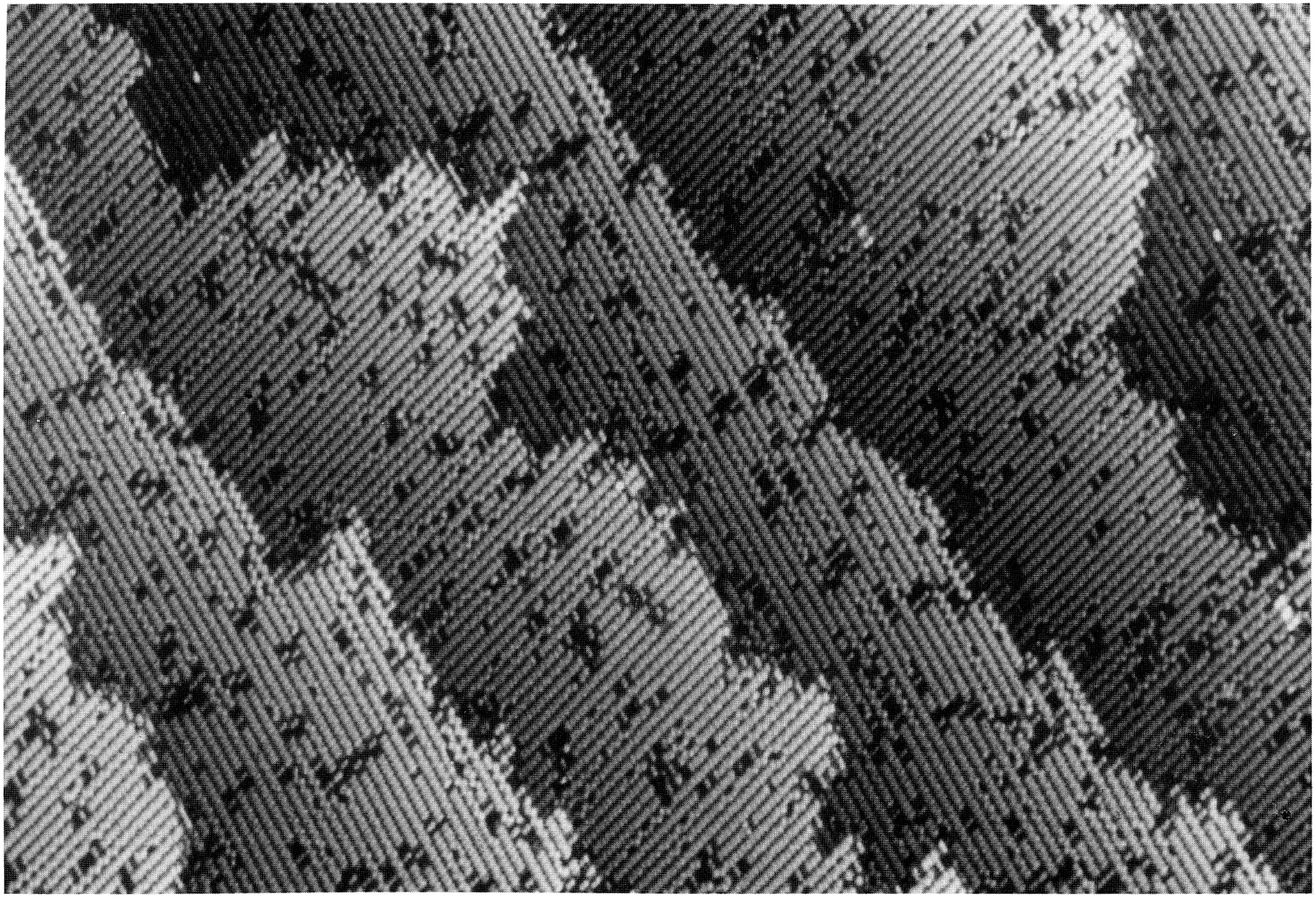


Fig. 1. In-plane structure of the Au(111) surface with a $22 \times \sqrt{3}$ reconstruction. The circles and crosses correspond to atoms in the first and second surface layers, respectively. Surface atoms in both sides of the figure lie on fcc sites, whereas atoms in the center of the figure lie on 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.

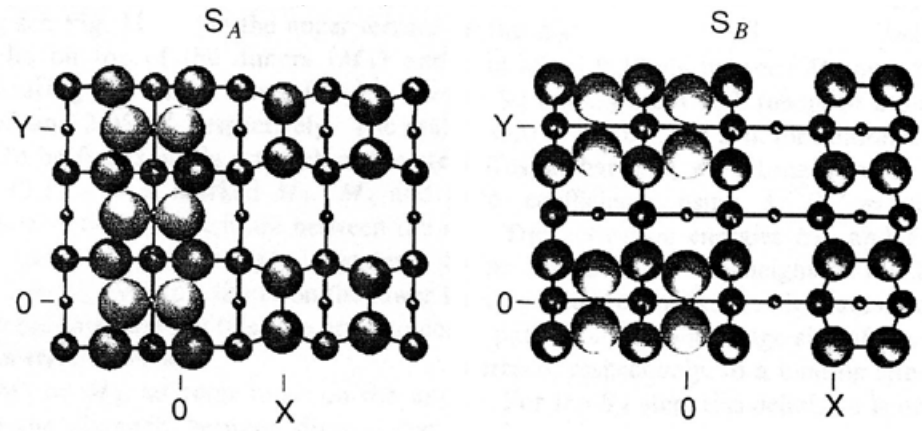
Science 258, 1763 (1992).

Atomic Structure of the Si(001) Surface

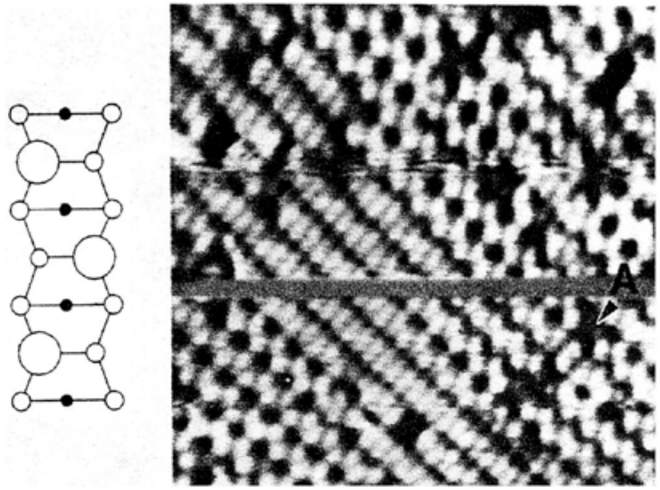


V_b = 2 V I_t = 1 nA

Si(001)-2x1 and 1x2



Si(001)-c(4x2)



Si(111)-(2x1)