**Physics of STM (scanning tunneling microscope)**

**Masatsugu Sei Suzuki**
**Department of Physics, SUNY at Binghamton**
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## 1. Introduction

The scanning tunneling microscope (STM), developed by Gerd Binning and Heinrich Rohrer, delivers pictures of a solid surface with atomic resolution. A direct real-space image of s surface is obtained by moving a tiny metal tip across the sample surface and recording the electron tunnel current between tip and sample as a function of position. In this sense, the STM belongs to the

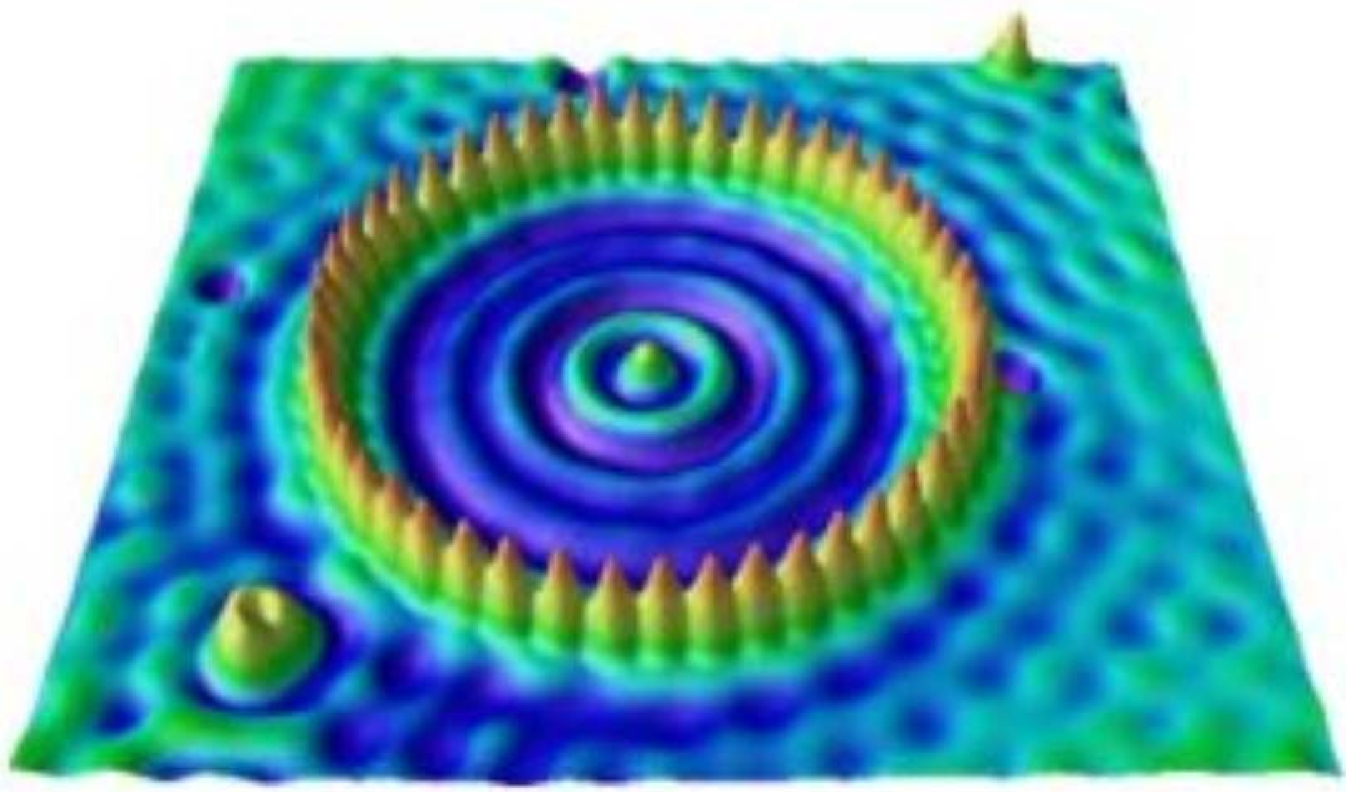


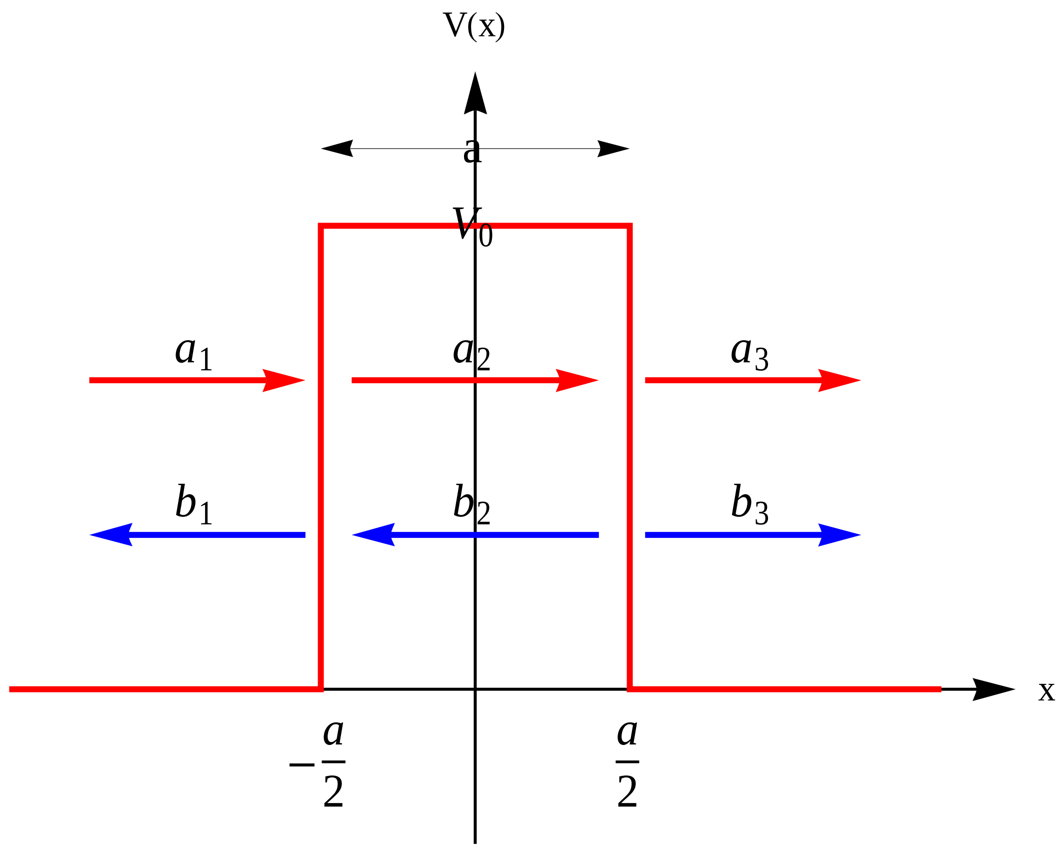
**Fig.** Constant-tunneling current STM image of a quantum corral consisting of 48 Fe atoms assembled in a ring on a Cu(111) surface at 4 K (imaging bias: 0.02 V). The ring with a diameter of 142.6 Å encloses a defect-free area of the surface. Inside of the corral a circular standing wave of electrons in sp-like surface states of the Cu(111) surface is visible.

## 2. Electron tunneling

For the description of the phenomenon called electron tunneling, we assume a rectangular potential barrier with spatial extension a (width) on the x axis and energetic height $V_0$ on the energy scale. The tunneling problem can be described in terms of a stationary flux of electrons left and right of the barrier and the potential in the time independent Schrodinger equation is assumed piecewise as constant.

For simplicity, we assume a symmetric potential. The energy of the electron ($\varepsilon$) is assumed to be lower than the top of the potential barrier $V_0$; $0<\varepsilon<V_0$.

Because of particle (flux) conservation, both $\psi$ and $d\psi / dx$ must be continuous at the barrier borders at $x = -a/2$ and $a/2$.




(a) Region I $\quad (x < -\frac{a}{2})$

$$\psi(x) = a_1 e^{ikx} + b_1 e^{-ikx} \qquad \text{for } x < -\frac{a}{2}$$

$$\psi'(x) = ik(a_1 e^{ikx} - b_1 e^{-ikx})$$

(b) Region II $(|x| < \frac{a}{2})$

$$\psi_{II}(x) = a_2 e^{-\rho x} + b_2 e^{\rho x}, \qquad \text{for } |x| < \frac{a}{2}$$

$$\psi_{II}'(x) = \rho(-a_2 e^{-\rho x} + b_2 e^{\rho x}).$$

(c) Region III $x > \frac{a}{2}$,

$$\psi_{III}(x) = a_3 e^{ikx} + b_3 e^{-ikx}, \qquad \text{for } x > \frac{a}{2}$$

$$\psi_{III}'(x) = ik(a_3 e^{ikx} - b_3 e^{-ikx}),$$

where

$$\varepsilon = \frac{\hbar^2 k^2}{2m}, \qquad V_0 - \varepsilon = \frac{\hbar^2 \rho^2}{2m}.$$

(a) Boundary condition at $x = -\frac{a}{2}$;

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = M(-\frac{a}{2}) \begin{pmatrix} a_2 \\ b_2 \end{pmatrix},$$

where

$$M(-\frac{a}{2}) = \frac{1}{2k} \begin{pmatrix} (k + i\rho)\exp[\frac{a(ik+\rho)}{2}] & (k - i\rho)\exp[\frac{a(ik-\rho)}{2}] \\ (k - i\rho)\exp[\frac{a(-ik+\rho)}{2}] & (k + i\rho)\exp[-\frac{a(ik+\rho)}{2}] \end{pmatrix}$$

and

$$\det[M(-\frac{a}{2})] = \frac{i\rho}{k}$$

(b) Boundary condition at $x = \frac{a}{2}$;

$$\begin{pmatrix} a_3 \\ b_3 \end{pmatrix} = M(\frac{a}{2})\begin{pmatrix} a_2 \\ b_2 \end{pmatrix}$$

where

$$M(\frac{a}{2}) = \frac{1}{2k}\begin{pmatrix} (k+i\rho)\exp[-\frac{a(ik+\rho)}{2}] & (k-i\rho)\exp[\frac{a(-ik+\rho)}{2}] \\ (k-i\rho)\exp[\frac{a(ik-\rho)}{2}] & (k+i\rho)\exp[\frac{a(ik+\rho)}{2}] \end{pmatrix}$$

with

$$\det[M(\frac{a}{2})] = \frac{i\rho}{k}$$

Then we get

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = M(-\frac{a}{2})\begin{pmatrix} a_2 \\ b_2 \end{pmatrix}$$

$$= M(-\frac{a}{2})[M(\frac{a}{2})]^{-1}\begin{pmatrix} a_3 \\ b_3 \end{pmatrix}$$

$$= \begin{pmatrix} \frac{e^{iak}[2k\rho\cosh(\rho a) - i(k^2-\rho^2)\sinh(\rho a)]}{2k\rho} & \frac{i(k^2+\rho^2)}{2k\rho}\sinh(\rho a) \\ -\frac{i(k^2+\rho^2)}{2k\rho}\sinh(\rho a) & \frac{e^{-iak}[2k\rho\cosh(\rho a) + i(k^2-\rho^2)\sinh(\rho a)]}{2k\rho} \end{pmatrix}\begin{pmatrix} a_3 \\ b_3 \end{pmatrix}$$

We now consider the special case of transmission of particles which appraoch the barrier from the left side. $b_3$ must be assumed to be zero ($b_3 = 0$). Then we obtain

$$a_1 = a_3 e^{iak}[\cosh(\rho a) + i\frac{(\rho^2-k^2)}{2k\rho}\sinh(\rho a)] \qquad \text{(transmission)}$$

$$b_1 = a_3[-\frac{i(k^2+\rho^2)}{2k\rho}]\sinh(\rho a) \qquad \text{(reflection)}$$

The transmission amplitude from the left to the right describes the tunneling of the electron through the barrier in terms of an attenuation of the incoming wave amplitude upon transmission through the barrier.

$$t = \frac{a_3}{a_1} = \frac{e^{-iak}}{\cosh(\rho a) + i\frac{(\rho^2 - k^2)}{2k\rho}\sinh(\rho a)]}$$

The transmission probability is

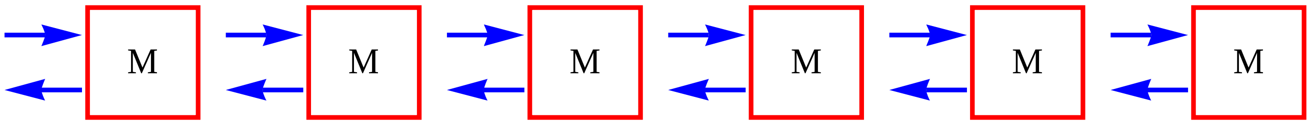
$$T = |t|^2 = \frac{1}{1 + \frac{(\rho^2 + k^2)^2}{4k^2\rho^2}\sinh^2(\rho a)}$$

For high and wide barriers with low transmission probability one has . $\rho a >> 1$, we have

$$\sinh(\rho a) = \frac{1}{2}e^{\rho a}$$

Then

$$T = 16\frac{k^2\rho^2}{(\rho^2 + k^2)^2}e^{-2\rho a} \approx 16\frac{\varepsilon}{V_0}e^{-2\rho} = 16\frac{\varepsilon}{V_0}\exp[-\frac{2}{\hbar}\sqrt{2m(V_0 - \varepsilon)}a]$$




Suppose that there is a 1D barrier potential. When $a$ = d$x$, and $V_0 = V(x)$, then we have the total transition probability as

$$T \propto \exp[-\frac{2}{\hbar}\int\sqrt{2m(V(x) - \varepsilon)}dx]$$

For electron

$$\frac{2}{\hbar}\sqrt{2m(V_0-\varepsilon)}a \approx \frac{2}{\hbar}\sqrt{2mV_0}a = 1.02463\ [V_0(\text{eV})]^{1/2}\ a(\text{Å}).$$

## 3. Mathematica

```
Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};

f11 = a1 Exp[ⅈ k x] +
   b1 Exp[- ⅈ k x];
f12 = D[f11, x];
f21 = a2 Exp[- ρ x] +
   b2 Exp[ρ x];
f22 = D[f21, x];
f31 = a3 Exp[ⅈ k x] +
   b3 Exp[- ⅈ k x];
f32 = D[f31, x];

eq11 = f11 == f21 /. x → -a / 2;
eq12 = f12 == f22 /. x → -a / 2;

eq1 = Solve[{eq11, eq12}, {a1, b1}] // Simplify;

M11 = D[a1 /. eq1[[1]], a2]; M12 = D[a1 /. eq1[[1]], b2];
 M21 = D[b1 /. eq1[[1]], a2];
M22 = D[b1 /. eq1[[1]], b2];
```

```
Ma = (M11 M12
      M21 M22) // Simplify; Ma // MatrixForm
```

$$\begin{pmatrix} \frac{e^{\frac{1}{2} a (i k+\rho)} (k+i \rho)}{2 k} & \frac{e^{\frac{1}{2} i a (k+i \rho)} (k-i \rho)}{2 k} \\ \frac{e^{\frac{1}{2} a (-i k+\rho)} (k-i \rho)}{2 k} & \frac{e^{-\frac{1}{2} a (i k+\rho)} (k+i \rho)}{2 k} \end{pmatrix}$$

```
eq21 = f21 == f31 /. x → a / 2; eq22 = f22 == f32 /. x → a / 2;

eq2 = Solve[{eq21, eq22}, {a3, b3}] // Simplify;

N11 = D[a3 /. eq2[[1]], a2];
N12 = D[a3 /. eq2[[1]], b2];
N21 = D[b3 /. eq2[[1]], a2];
N22 = D[b3 /. eq2[[1]], b2];

Mb = (N11 N12
      N21 N22) // Simplify; Mb // MatrixForm
```

$$\begin{pmatrix} \frac{e^{-\frac{1}{2} a (i k+\rho)} (k+i \rho)}{2 k} & \frac{e^{\frac{1}{2} a (-i k+\rho)} (k-i \rho)}{2 k} \\ \frac{e^{\frac{1}{2} i a (k+i \rho)} (k-i \rho)}{2 k} & \frac{e^{\frac{1}{2} a (i k+\rho)} (k+i \rho)}{2 k} \end{pmatrix}$$

```
(Ma /. a → a1) - (Mb /. a → -a1) // Simplify
```

```
{{0, 0}, {0, 0}}
```

```
eq3 = Ma .Inverse[Mb] // FullSimplify;
```

```
K1 = eq3[[1, 1]];
```

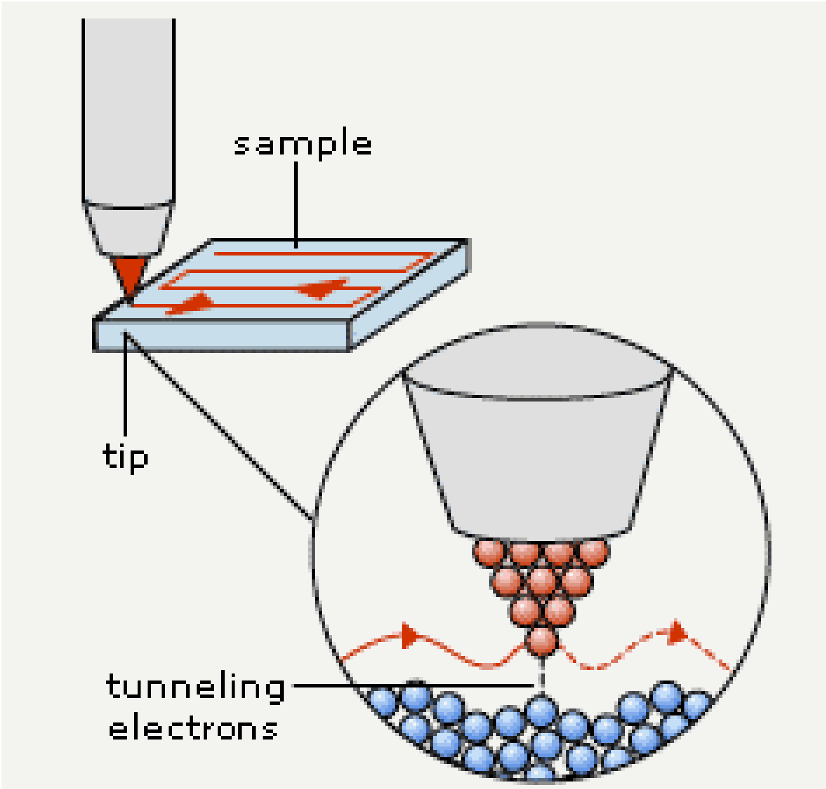
$$T1 = \frac{1}{K1\, K1^*} \text{ // FullSimplify}$$

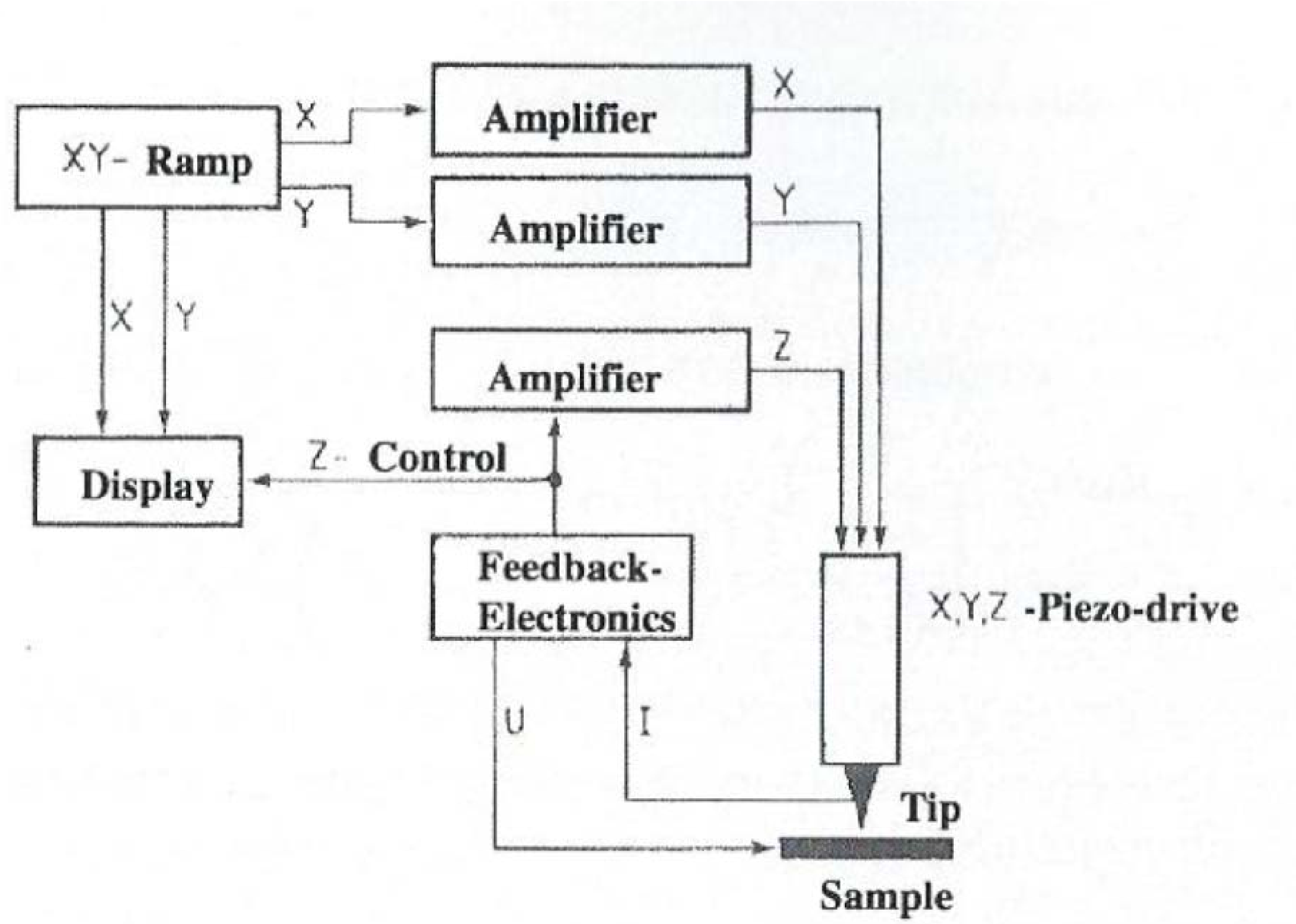
$$\frac{1}{\text{Cosh}[a\,\rho]^2 + \frac{\left(k^2-\rho^2\right)^2 \text{Sinh}[a\,\rho]^2}{4\,k^2\,\rho^2}}$$

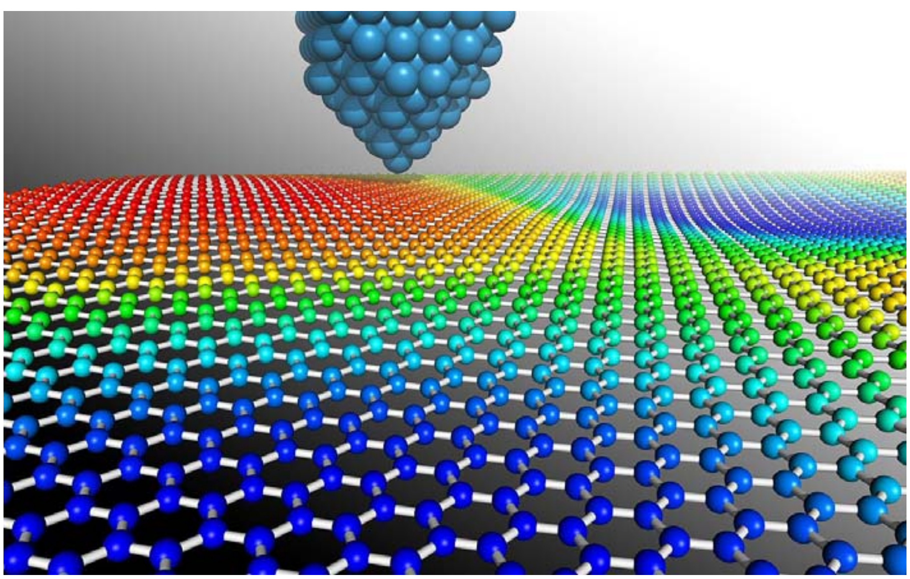
## 4. Scanning tunneling microscope

The scanning tunneling microscope (STM) is an electron microscope that uses a single atom tip to attain atomic resolution. It was developed at IBM at Zurich in 1981 by Gerd Binning and Heinrich Rohrer who shared the Nobel Prize for physics in 1986.

The principle of the STM is based on the distance dependence of the quantum mechanical tunneling effect. Maintaining a constant tunneling current by adjusting the height with a piezo-electric crystal, and monitoring the piezo voltage while scanning, allows one to image a surface, under ideal conditions, to atomic resolution. (If the tip is scanned over the sample surface while an electronic feedback loop keeps the tunneling current constant (constant current mode), the tip height follows a contour of constant local density of electronic states and provides information on the topography of the sample surface if the surface is composed of the same atoms). Most of the tunneling current flows through a single protruding atom on the tip and thus sub-angstrom resolution in *z* can be achieved on a clean surface with a sharp tip.


sample
tip
tunneling
electrons



(http://www.britishcarbon.org/images/gallery/7.graphene_8nm.jpg)

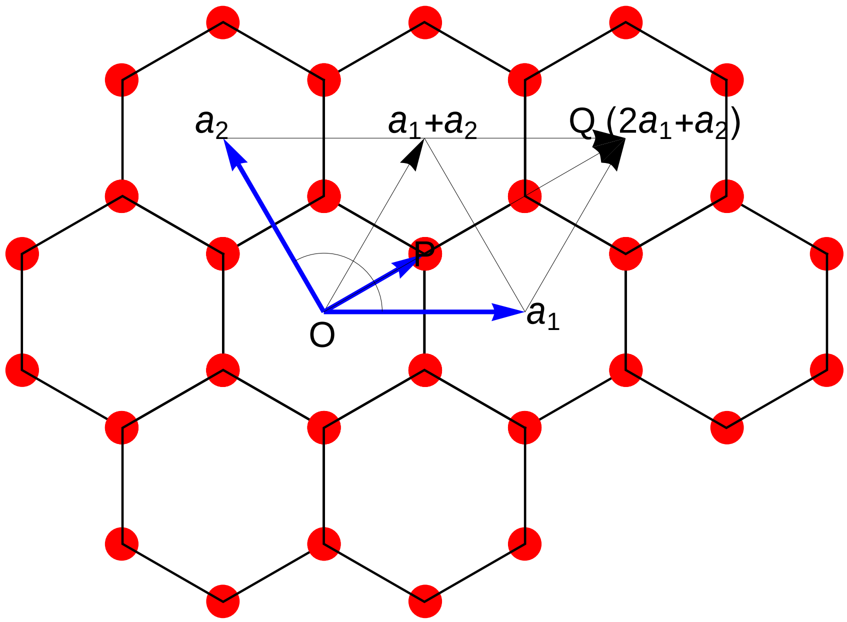



Fig. In-plane structure of graphene. The lattice constant $a_1$ is equal to 2.46 Å.

Tunneling is a genuine quantum mechanical effect in which electrons from one conductor penetrate through a classically impenetrable potential barrier - in the present case the vacuum - into a second conductor. The phenomenon arises from the leaking out of the respective wave functions into the vacuum and their overlap within classically forbidden regions. This overlap is significant only over atomic-scale distances and the tunnel current $I_T$ depends exponentially on the distance d between the two conductors, i.,e., the tip and the sample surface.

$$I_T \propto \frac{U}{d} \exp(-Kd\sqrt{\bar{\phi}})$$

where U is the applied voltage between the two electrodes, tip and sample, $\bar{\phi}$ their wverage work function ($\bar{\phi} >> eU$), and $K$ a constant with a value of about

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

for a vacuum gap. The current $I_T$ is easily measurable for distances d of several tens of Å and, in order to get interesting information about the surface, d must be controlled with a precision of 0.05 - 0.1 Å.

In order to achieve a lateral resolution that allows imaging of individual atoms, the movement of the tiny metal tip across the surface under investigation must be controlled to within 1 - 2 Å. The high sensitivity of the instrument to the slightest corrugations of the surface electron density is due to the exponential dependence of the current on $d$ and $\sqrt{\bar{\phi}}$ .

## REFERENCES

G. Binnig, H. Rohrer, Ch. Gerber, E. Weibel, Appl. Phys. Lett. **40**, 178 (1982): Phys. Rev. Lett. 50, 120 (1983).