# Scanning Tunneling Microscope

Advanced Laboratory, Physics 407

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Abstract

A scanning tunneling microscope is used to demonstrate the principle of quantum mechanical tunneling between the microscope tip and the surface of a conducting sample. Measurements are made on a gold-coated holographic grating and a pyrolytic graphite sample. Since the apparatus is capable of atomic resolution, atomic features of the graphite surface can be directly observed. Mathematical filter algorithms are used to process the sample images and reduce the image noise. The bond angles and bond lengths of the graphite sample are determined.

## 1.1. How the STM Works

There are five scientific and technical processes or ideas that the STM integrates to make atomic resolution images of a surface possible. Each of these processes was used in other areas of science before the invention of the STM.

- The principle of quantum mechanical tunneling.
- Achievement of controlled motion over small distances using piezoelectrics.
- The principle of negative feedback.
- Vibration isolation.
- Electronic data collection.

This Chapter discusses each of these five concepts. The most detail is provided on the process of quantum mechanical tunneling, since this is the fundamental concept that allows the microscope to work. At the end of the discussion of all these concepts, one can see how they integrate to make an STM.

## 1.2. Ouantum Mechanical Tunneling

Quantum mechanical tunneling is not some obscure process that only occurs under extreme conditions in a crowded basement laboratory of a research university. Quantum mechanical tunneling explains some of the most basic phenomena we observe in nature. One example is the radioactive decay of plutonium. If quantum mechanical tunneling did not occur, plutonium would remain plutonium instead of changing into elements lower on the periodic chart. Plutonium converts to other elements when 2 neutrons and 2 protons are ejected from the nucleus because of tunneling. Even the fundamental force that binds atoms into molecules can be thought of as a manifestation of quantum mechanical tunneling. In this lab, we will look at how tunneling manifests itself in another way. We will attempt to understand how a single electron starts out in one metal and then reappears in another metal, even though they are not touching.

To begin, let's examine what electron tunneling means in the real world. Consider two pieces of metal. Metals are good conductors of electricity, i.e. electrons can move very easily and quickly from one end of the metal to the other. Imagine connecting one of the pieces of metal to the negative terminal of a battery and the other piece of metal to the positive terminal, as shown in Figure 2.1. If the metals are not touching, no current will flow through the battery. The electrons are free to move around the metal but cannot leave it. The electrons are analogous to water in a reservoir that is blocked by a dam. They can move about the reservoir but have no access to the river below. If the metals are brought together so that they touch, current will flow freely through the contacting area. The electrons have a free path from the negative terminal to the positive terminal of the battery. This current flow is analogous to opening up the gates of the dam and allowing the water to flow down the river into the ocean.

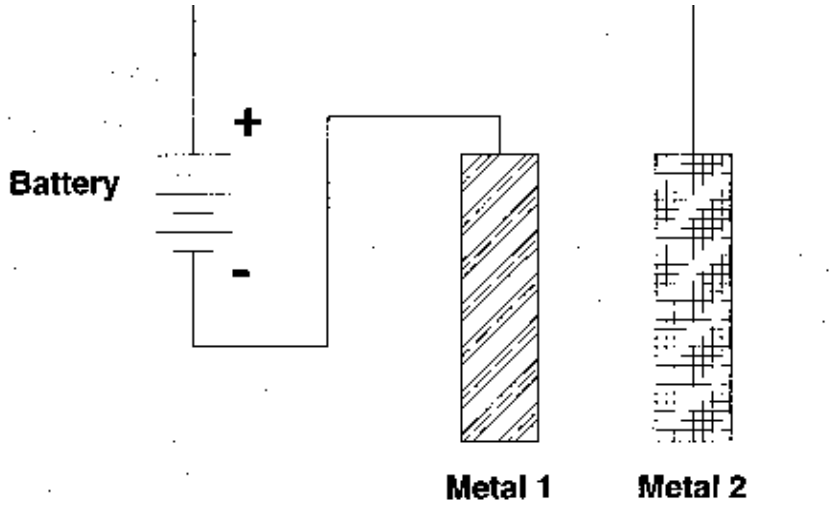


**Figure 1.1. Two pieces of metal, each connected to a battery terminal. While the metals are well separated no current flows through the battery.**

The unusual experimental feature of tunneling is this: when the metals are brought together, but are not quite touching, a small electric current can be measured. The current gets larger the closer the metals are brought together, until it reaches its maximum value when the metals are touching. The concept is analogous to making the dam thinner and thinner by removing cement and noticing that more and more water is leaking through the walls. However, there is a difference between the two analogies. The water physically moves through the pores between the cement, while the *electrons do not move in the space between the metals: they just suddenly appear in the other side.* The metals must be only 10 angstroms apart to produce detectable tunneling current. Figure 2.2. shows current as a function of the separation between metals [a]. Also plotted in this graph is the measured tunneling current if quantum mechanical tunneling did *not* occur [b]. The distances involved are so small that special tools are needed to adjust the distances or the small electric currents will not be detected. We will describe these tools in the section on piezoelectrics (see Section 2.4.).

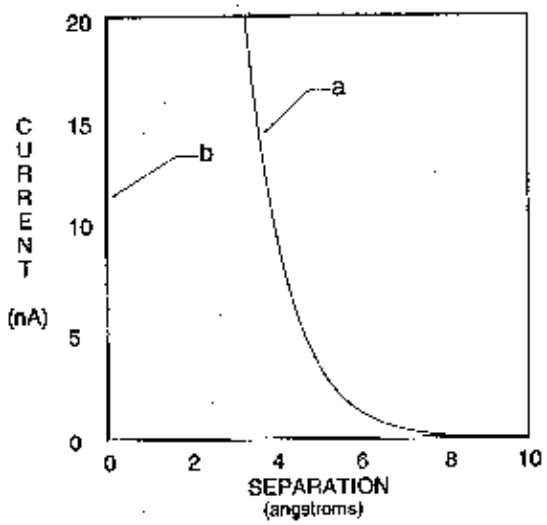


**Figure 2.2. This graph shows a plot of current flowing through the battery as a function of the separation of the metals. [a] shows an exponential increase in current as the metals get closer; [b]: in the absence of quantum mechanical tunneling, no current flows until the metals touch.**

To understand why these small currents occur, the energies involved as the electron moves between the metals must be considered. An electron's energy can be split into two contributions: kinetic energy and potential energy. Kinetic energy (the energy of motion) is large for electrons moving fast and small for electrons moving slowly. Potential energy is the energy available for an electron to convert to kinetic energy if it moves along an electric field. Figure 2.3 plots the potential energy of the electron as it travels from one metal to the other metal. The potential energy shown neglects the complicated aspects of metals, including extra charges from atoms and other electrons on the metals, but does include the general concepts. The potential energy is lower in Metal 2 because this side is connected to the positive terminal of the battery (the terminal to which the electrons are attracted). There is also a large potential energy between the two metals. This is what tends to keep electrons inside their respective metal.

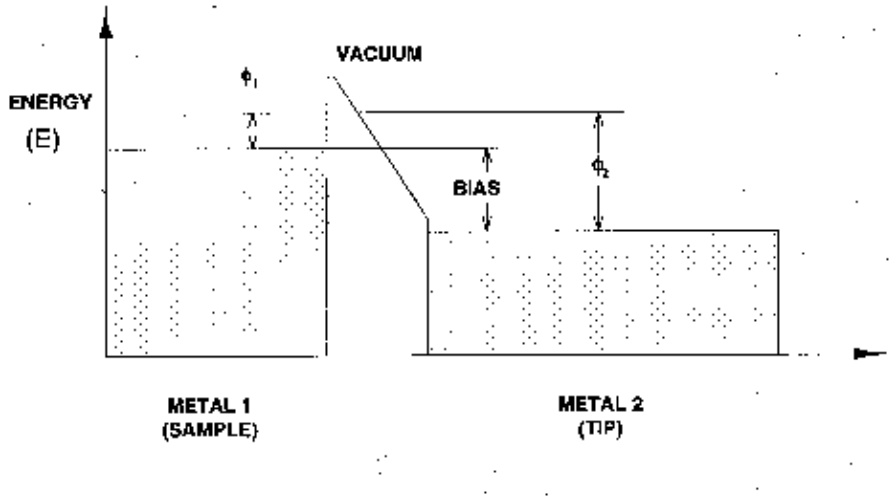


**Figure 2.3. The potential energy that the electrons encounter as they travel from one metal to the other. $\phi_1$ and $\phi_2$ indicate the minimum amount of energy required to remove an electron from the metals (the work function). Note that Metal 2 is attached to the positive terminal, so its electrons have lower potential energy.**

This picture shows that electrons are free to move around in their respective metals but cannot leave them. No electron in a metal has sufficient kinetic energy to go over the barrier. One of the basic tenets of quantum mechanics is that electrons have both a particle and a wave nature. So we should picture the electron not as a hard ball impinging on the barrier, but as a cloud. The size of the cloud is related to the wavelength of the electron (a few angstroms). When the cloud collides with the barrier, part of the cloud may penetrate it. For thick barriers, the cloud will be reflected like a hard particle (see Figure 2.4). For thin barriers, however, part of the cloud may penetrate the barriers and appear on the other side. This process is called tunneling because the electron does not have enough kinetic energy to travel over the barrier, but is able to exist on the other side (see Figure 2.5). It is as if the electron found a way to dig a tunnel *through* the barrier.

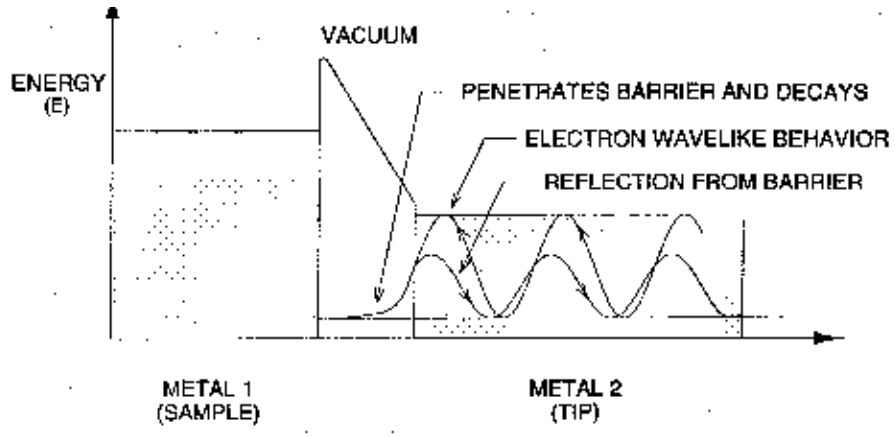


**Figure 2.4. Electrons have a wave and particle nature. Upon impinging on the barrier they will be reflected from and penetrate the barrier. If the barrier is too "thick," the electron cloud will decay and no electron will tunnel to the other side of the barrier.**

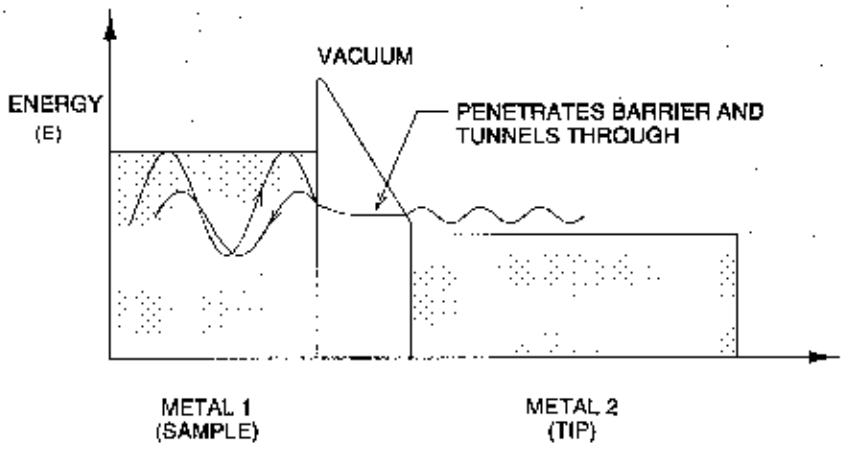


**Figure 2.5. If the barrier is "thin," the electrons might tunnel and transmit through the barrier, thus creating an electrical current that can be measured.**

In the scanning tunneling microscope, one of the metals is the sample being imaged (sample) and the other metal is the probe (tip). The sample is usually flatter than the probe, as shown in Figure 2.6. If the probe is sharpened into a tip it will most likely have one atom at the end. All of the tunneling electrons will pass through this atom. As we will discuss later, this feature leads to the atomic resolution capabilities of the microscope.

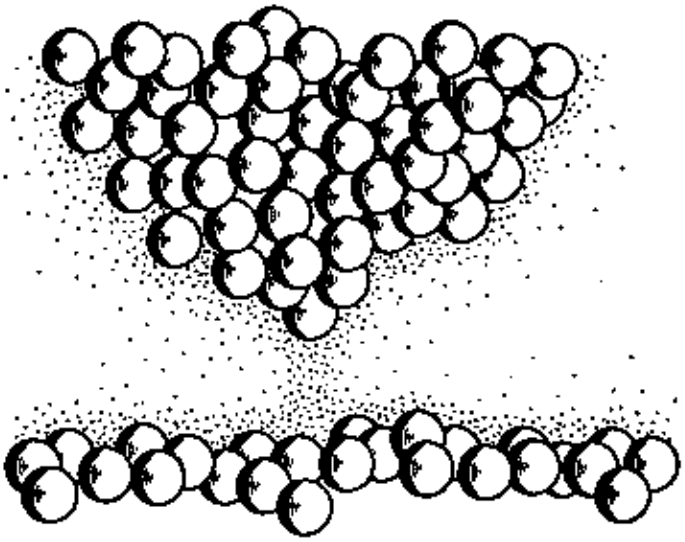

**Figure 2.6. The tip consists of clusters of atoms in which one atom usually sticks out more than the others. This atom is primarily responsible for tunneling between the tip and sample.**

## 1.3. Ouantifying the Tunneling Process

Using Schrödinger's equation of quantum mechanics, we can actually predict how tunneling current increases as separation between two metals decreases. However, the final results of your tunneling experiments can be understood without knowing quantum mechanics. This more complete description is not necessary for understanding how the STM works; it therefore may be thought of as supplemental.

The Drude model of a metal states that the potential energy of a metal is given by the solid line in Figure 2.3. The energy of all the electrons in the metal is lower than the height of the wall. The difference in energy between the most energetic electron and the vacuum energy is called the workfunction and is denoted by the symbol $\Phi$.

The wave nature of an electron, illustrated in Figures 2.4 and 2.5, is critical to explaining tunneling. The movement and shape of the electron wave is governed by Schroedinger's equation, which might be thought of as the quantum mechanical analog of Newton's equation of motion, **F = ma.**

In the STM, tunneling takes place between the tip and the sample. A complete description of the tunneling process requires a solution of the three-dimensional form of Schroedinger's equation, which has the general form:

$$[\mathrm{H}]\Psi = [\mathrm{E}]\Psi \qquad (1.1)$$

where [H] and [E] are the Hamiltonian and total energy operators. The operators are expressed as:

$$\frac{-\hbar^2}{2\mathrm{m}}\nabla^2\Psi(\mathbf{r},\mathrm{t}) + \mathrm{U}\Psi(\mathbf{r},\mathrm{t}) = \mathrm{i}\hbar\frac{\partial\Psi(\mathbf{r},\mathrm{t})}{\partial t} \qquad (1.2)$$

For our purpose it is sufficient to use a one-dimensional analysis, which for the Schroedinger
equation above is given by:

$$\frac{-\hbar^2}{2\mathrm{m}}\nabla^2\Psi(x,t) + \mathrm{U}(x)\Psi(x,t) = \mathrm{i}\hbar\frac{\partial\Psi(x,t)}{\partial t} \qquad (1.3)$$

where the equation:

$$\Psi(x,t) = Ae^{i(-kx-wt)} + Be^{i(k\,x-wt)} \qquad (1.4)$$

is the plane wave representation for an electron wavefunction of wavenumber $k = 2\pi/\lambda$ and angular frequency $\omega$.

In addition, we assume a steady-state (time-independent) situation in which electrons of energy E(x, t) = E encountering a uniform potential barrier of height U(x, t) = U(x) are

continuously flowing from one metal to the other. It is then necessary to solve only the one-dimensional steady-state Schroedinger equation, given by:

$$\frac{\hbar^2}{2\mathrm{m}}\frac{\partial^2\Psi(x)}{\partial x^2}+U(x)\Psi(x)=E\Psi(x) \qquad (1.5)$$

where $E$ is the kinetic energy of the electron. Note that $U(x)$ is the potential energy of the electron as a function of position, as shown in Figure 2.3. $U(x)$ is smaller than the electron energy in the metals and larger than the electron energy in the barrier. For simplicity we can assume $U(x) = U_0$ a constant in the barrier.

In the metal, the general solution to the above equation is given by:

(Metal 1) $$\Psi(x)=Ae^{-ikx}+Be^{+ikx},\ k=\sqrt{\frac{2m(E-U_0)}{\hbar^2}} \qquad (1.6)$$

(Metal 2) $$\Psi(x)=Ee^{-ikx}+Fe^{+ikx} \qquad (1.7)$$

and in the barrier (the classically forbidden region) the solution is:

(barrier) $$\Psi(x) = Ce^{-mx} + De^{+mx},\ m = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}} \qquad (1.8)$$

Equations 1.6 and 1.7 show that the phase of the electron wavefunction varies uniformly in the metals. The wavelength is $\lambda = 1/k$. Higher energy electrons have a smaller wavelength. When a high energy electron wave encounters the boundary of the metal, it "leaks out" a small amount, as discussed in the previous section. The "intensity" of the electron wave decays as a function of distance from the boundary. Mathematically, the argument of the exponential function becomes real and the electron wavefunction decays. (For imaginary arguments, the wave function would have oscillatory behavior.)

To gain a quantitative insight into the electron tunneling phenomena, it is necessary to derive an expression for the transmission coefficient, i.e. the transmitted flux from the sample to the tip through the barrier of width *L*. The barrier is considered wide but finite, such that the electron wavefunction exponential decay in the barrier is significant. Furthermore, the electron wavefunction and its first derivative must be continuous (join smoothly) at the sample-barrier and tip-barrier boundaries to conserve energy and mass. If we set up a coordinate system in which the surface of the sample (Metal 1) is at x = 0 and the tip (Metal 2) is at x = *L*, and apply the boundary conditions for continuity:

$$\begin{aligned} A + B &\approx C \\ ik(A - B) &\approx -mC \end{aligned} \qquad (1.9)$$

(at the sample surface, x = 0) where *D*, the amplitude of the reflected wavefunction at the tip-barrier boundary, is neglected, since $D << A, B, C$. However, *D* is *not* insignificant at the tip-barrier boundary. At the tip-barrier boundary, x = L, continuity would require:

$$\begin{aligned} Ce^{-mL} + De^{mL} &= Fe^{ikL} \\ -mCe^{-mL} + mDe^{mL} &= ikFe^{ikL} \end{aligned} \qquad (1.10)$$

Solving for B/A at x = 0, by solving for C and substituting for it, we get:

$$\frac{B}{A} \approx \frac{-(1+ikd)}{(1-ikd)}$$

(1.11)

where $\delta$ is $1/\mu$, A is the amplitude of the electron wavefunction in the sample surface incident on the barrier, and B represents the amplitude of the reflected wavefunction. The reflection coefficient (R) for the wavefunction is then defined as:

$$R \approx \left|\frac{B}{A}\right|^2$$

(1.12)

where $|\ |^2$ represents the product of a complex number and its conjugate. In this case, it represents the relative intensities of the incident and reflected wavefunctions.

An electron incident at the barrier will either be reflected or transmitted through the barrier. In terms of probability or frequency of occurrence, $R+T = 1$, where $R$ and $T$ are the reflection and transmission coefficients. Thus:

$$R \approx \left|\frac{B}{A}\right|^2 = \frac{-(1+ikd)}{(1-ikd)} \approx 1$$

(1.13)
and, therefore:

$$T = 1 - R \approx 0$$

(1.14)

which indicates that, for an infinitely wide barrier, no electrons would be found in the barrier region. Nevertheless, dividing the first of the sample vacuum-barrier boundary conditions by $A$ results in:

$$1 + \frac{B}{A} \approx \frac{C}{A}$$

(1.15)

The probability of finding an electron in the barrier region at x = 0, due to quantum tunneling, is
given by:

$$\left|\frac{C}{A}\right|^2 \approx \frac{4(kd)^2}{1+(kd)^2}$$

(1.16)

To find the effective tunneling transmission coefficient, $\left|\frac{F}{A}\right|^2$ i.e. the relative probability or frequency of occurrence of an electron tunneling out of the sample surface, across the sample-tip-barrier region, and into the tip, combine the tip-barrier boundary equations (at x *L)* and Equation 1.16 to get:

$$\frac{F}{A} \approx \frac{-4ikd}{(1-ikd)^2} e^{-L(m+ik)}$$

(1.17)

which produces the desired quantitative result:

$$T(E) \approx \left|\frac{F}{A}\right|^2 \approx \left(\frac{4kd}{\left(1+(kd)^2\right)}\right)^2 e^{\frac{2L}{d}} \propto e^{-L\sqrt{2m\Phi/\hbar}}$$

(1.18)
where:

$$k^2 = \frac{2mE}{\hbar^2}$$

$$(kd)^2 = E(U_0 - E) = \frac{E}{\Phi}$$

(1.19)

Substituting typical numbers of $\Phi = 5\text{x}10^{-19}$ joules, $m = 9.11\text{x}10^{-31}$ kilograms, and $\hbar = 1.05\text{x}10^{-34}$ joule-seconds, results in:

$$T(E) = e^{-2L}, \text{ L in Angstroms}.$$

This formula shows that for each angstrom change in separation, the probability that an electron tunnels decreases by an order of magnitude. This demonstrates mathematically that tunneling current is indeed a sensitive measure of the distance between the tip and sample.

In the STM, one of the metals is the sample being looked at and the other metal is the probe. The sample is usually flatter than the probe, as shown in Figure 2.6. Because the probe is formed of atoms, if it is sharpened into a tip, it will most likely have one atom at the end of the tip. The spacing between atoms is about 3 angstroms. Therefore, any tunneling through atoms that are one atom back from the closest atom is a fraction $\left[e^{-(2)(3)} = 0.002\right]$ of tunneling through the atom at the tip, as shown in Figure 2.6. Virtually all of the tunneling electrons will pass through the single atom closest to the surface. This feature produces the atomic resolution capabilities of the microscope.