Revolutionizing Science:
The Scanning Tunneling Microscope

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***Abstract*—We present the basic theory behind the scanning tunneling microscope (STM). The goal of this paper is to explain the fundamentals of the STM in a way that is accessible to audiences in various fields of study. Unlike most conventional forms of microscopy, the results obtained from a scanning tunneling microscope often do not admit an intuitive physical interpretation; an understanding of quantum mechanical principles involved in its operation is required to make effective use of this instrument. In particular, we focus on electron tunneling and the analysis of the tunneling current signal to produce an image. The document concludes with a short overview of how the scanning tunneling microscope is used in various fields, which demonstrates the need for an understanding of this device.**

***Index Terms*—Electron Tunneling, Microscopy, Scanning Tunneling Microscope.**

Contents

I. INTRODUCTION

So why exactly are STMs so special and revolutionary? Unlike normal microscopes, STMs do not just display a closer view of an object through a lens. They obtain detailed profiles of the surfaces that they scan. From these profiles, a contour map of the surface can be generated [1]. This contour map is not only atomic-scaled, but three-dimensional, meaning that the STM gives images that accurately show how atoms and molecules fit together and form certain structures. Questions regarding sizes of atoms and molecules, defects in materials, and the textures of surfaces can all be answered from a few pictures attained with an STM [2]. Information like this would be impossible to derive from two-dimensional pictures of atoms. Since STMs allow us to see how the atoms of the surface conform, it gives us an understanding of the unique properties that result from the structure of the material. This in turn allows us to use and manipulate these materials at an atomic level in ways we would not have been able to otherwise [3].

Although the STM was revolutionary because of the resolution it could display, its predecessor, the topografiner, was the first instrument to utilize a tip that was kept a small distance away from the surface of a material to capture images. Invented by Russell D. Young of the National Bureau of Standards, the topografiner attempted to map out a surface by recording the x, y, and z coordinates of its tip as it scanned over a material. Instead of relying on electron tunneling like the STM does, the topografiner used field emission to capture profiles. Similar to the STM, the field emission was controlled by using an electronic feedback system to maintain a specified tip height. Before the STM came to fruition, the topografiner gave the greatest resolution of a surface [4]. However, the topografiner was flawed due to too much shaking and vibration of the tip, causing inaccuracy in position recordings [2].

About a decade later, two physicists named Heinrich Rohrer and Gerd Binnig designed the first STM in an IBM Research Laboratory located in Switzerland. Due to precise mechanical design by the two physicists, the STM's tip was much more stable than the topografiner, thus making its mapping of a material's surface far more accurate [2]. The STM was the first microscope that allowed its user to see samples at an atomic level. It was also the first microscope that obtained three-dimensional images of samples. In 1986, Rohrer and Binnig were awarded the Nobel Prize in Physics for their design of the STM [3]. Since then, the STM has become an indispensable tool for scientists around the world.

II. ELECTRON TUNNELING

The first step in understanding the STM is a general knowledge of the physical phenomenon it depends on, known as electron tunneling. The tunneling of electrons is a phenomenon that can be explained by quantum mechanics. In particular, a system of Schrödinger wave equations is used in the analysis this electron behavior. The basic idea of tunneling involves the interaction of two conducting materials, which are brought into close proximity with one another. When these two materials are brought within nanometers of each other and a voltage is applied, electron tunneling occurs. Electron tunneling is illogical in that electrons can overcome the energy barrier separating the two conductors. If the distance between the two conducting materials is small, some electrons from one material can transport to the other, even if they have a lower energy than the potential between the two conductors [5].

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A. Concept of tunneling

The idea of electron tunneling can be easily grasped when considering a macroscopic example. The figure below illustrates the idea on a tangible scale.

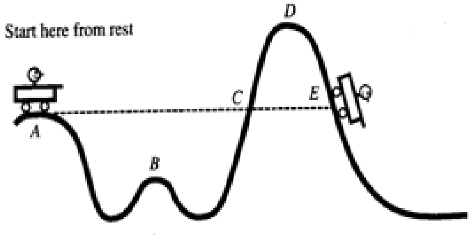

Fig. 1. The concept of electron tunneling on the macroscopic level. [6]

If one imagines an electron as a cart on a roller coaster and the track as a potential energy curve, then the concept of quantum tunneling is intuitive. From the figure, it is clear that the person in the cart at point A has an insufficient amount of energy to travel over the height represented by point D. The figure, however, shows the person traveling beyond this potential barrier. Even though this may be impossible for a roller coaster, electrons naturally behave this way on the nanoscale. This behavior is one of the fundamental principles behind the STM microscope [6].

B. Schrödinger's equation

As mentioned before, the behavior of electron tunneling can be investigated by the use of Schrödinger equations. The motion of the electron is limited to one direction, which simplifies the analysis. Limiting motion to the x direction, Fig. 2 depicts the potential between two conducting materials as a function of x.

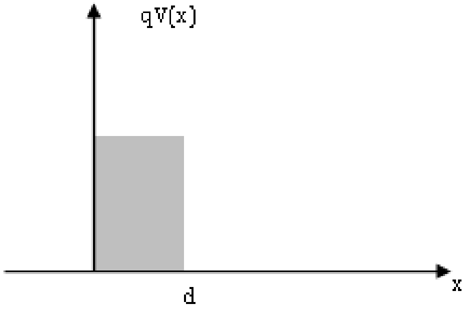

Fig. 2. One-dimensional potential between two conducting materials. [5]

The electron behavior can be described by the following wave equation where the potential is equal to zero. This occurs for $x < 0$ and for $x > d$.

$$\frac{d^2\psi}{dx^2} = \frac{-2m_nE}{\hbar^2}\psi \tag{1}$$

In this equation m_n is the effective mass of an electron, $\hbar$ is Planck's constant divided by 2π, E is the kinetic energy of the electron and ψ is the wave function of the particle. The solution to this second order differential equation is well known and has the following solutions depending on the value of x.

$$\psi(x) = \begin{cases} Ae^{j\sqrt{2m_nE/\hbar^2 x}} + Be^{-j\sqrt{2m_nE/\hbar^2 x}} & , x \leq 0, \\ Ce^{j\sqrt{2m_nE/\hbar^2 x}} & , x \geq d. \end{cases} \tag{2}$$

Inside the area where the potential is greater than zero, Schrödinger's equation describing the motion of the particle is slightly modified. Since the potential in the region $0 < x < d$ is non-zero an extra term is added. The equation below is the corresponding Schrödinger equation for this region of electron behavior.

$$\frac{d^2\psi}{dx^2} = \frac{2m_n(qV_0 - E)}{\hbar^2}\psi \ , \ 0 < x < d \tag{3}$$

Here, the added term qV_0 is the energy associated with the potential barrier between the two materials. As before, the electron motion is described with a second order differential equation with a well know solution. The solution to the above equation is given below.

$$\begin{aligned} \psi(x) &= Fe^{\sqrt{2m_n(qV_0-E)/\hbar^2 x}} \\ &\quad + Ge^{-\sqrt{2m_n(qV_0-E)/\hbar^2 x}} \\ &\qquad , 0 < x < d \end{aligned} \tag{4}$$

This solution has no imaginary component since qV_0 is greater than the kinetic energy of the electron [5].

Solving these simultaneous equations that describe the behavior of the electron is not possible. In the above equations, there are five unknowns: A, B, C, F and G. To successfully solve for all the constants, five equations are needed. Ratios of these constants, however, can be used to predict electron behavior. Of particular interest is the ratio of constants C and A. The ratio of these two constants yields an equation known as the transmission coefficient. In other words, this equation gives the probability of finding an electron that has traveled across the potential barrier. The transmission coefficient is given by the following equation [6].

$$\left(\frac{C}{A}\right)^2 = \left[1 + \frac{qV_0 \sinh\sqrt{2m_n(qV_0 - E)/\hbar^2 d}}{4E(qV_0 - E)}\right]^{-1} \tag{5}$$

III. INTERPRETATION OF TUNNELING CURRENT

An STM can be operated in several modes, but the one most commonly used is the constant-current mode. In this mode, the electron tunneling current between the probe tip and the sample is kept constant by an electronic feedback system controlling the height of the probe, as depicted in Fig. 3. Since the tunneling current is, to a first approximation [7], proportional to the width of the potential well (d in equation 5), this feedback loop prevents the probe tip from crashing into the surface.

The more interesting result of this feedback loop is that the probe tip height automatically varies as the tip is scanned

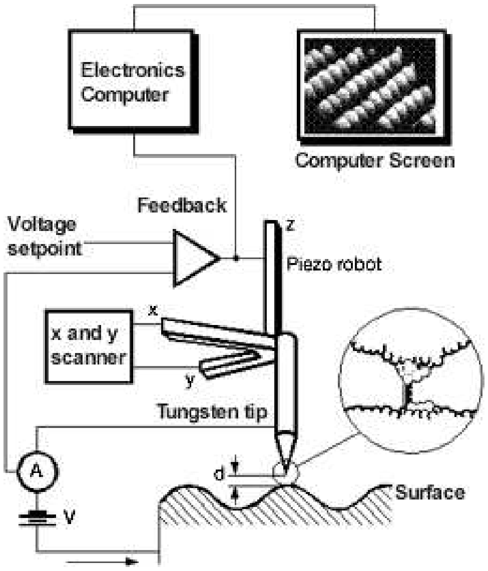

Fig. 3. Schematic of STM operation. [8]

across the surface of the sample, and can easily be recorded. These variations are closely correlated with various local features of the sample – most significantly the contour of constant surface charge density. In other words, a nearly-atomic-scale topograph of the sample, as seen in Fig. 4.

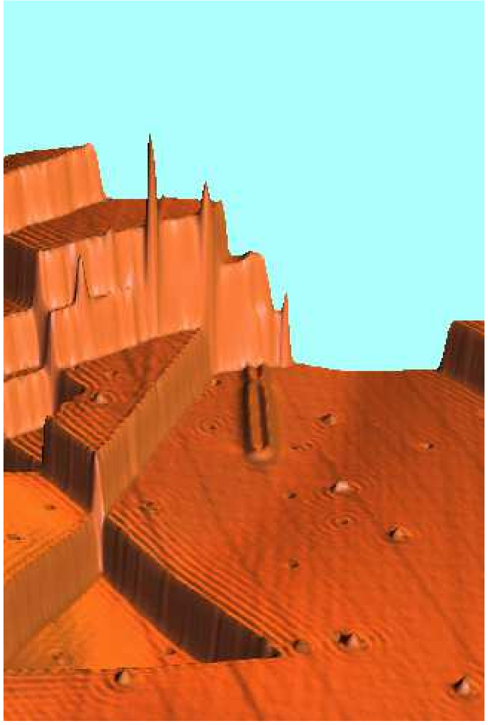

Fig. 4. A three dimensional rendering of a copper surface, based on STM data. [9]

However, this interpretation of the STM signal as a topograph is only a gross approximation. While it is adequate for many purposes, it fails when approaching the atomic scale – note the anomalous "ripples" visible near feature edges in Fig. 4. Indeed, at such small scales it is not even entirely clear what is meant by "topograph". An improved interpretation is needed for work in the atomic-scale and semiconductor domains.

When our mathematical model of the probe-sample system is improved beyond the roughest of approximations, we find that the tunneling current, and thus the height of the probe tip, vary proportionally to a quantity known as the local density of states (LDOS) [7]. This property is closely related to the total charge density, or topography; it is the charge density from states at the Fermi level[1].

Understanding precisely what the STM measures is critical to work at small scales. Proper interpretation of STM signals can even provide greater insight into a sample than any other methods would. Fig. 5 is an STM scan of a gold surface covered with copper phthalocyanine and cobalt phthalocyanine ions. These two compounds are nearly indistinguishable from a crystallographic perspective, yet with an STM each atom can be individually identified [10].

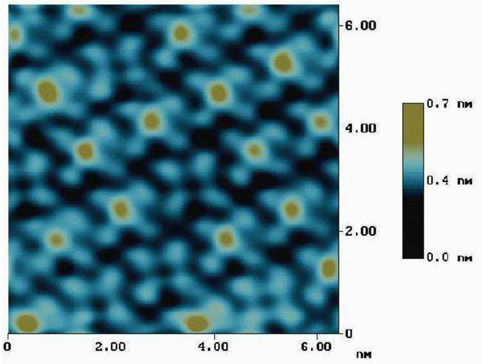

Fig. 5. A layer of CoPc and CuPc on Au(111). The CoPc atoms have bright centers; the CuPc atoms dull. [10]

IV. APPLICATIONS

Since its invention in 1983, scanning tunneling microscopes have been used in many technical and science fields. STM images play an important role in biology, chemistry, materials science, microelectronics, and semiconductor engineering.

Biological applications of STMs are a novel idea in that organic material acts as an insulator under low voltage and current conditions. Given this fact it seems that an STM would be unable to scan the surface of organic molecules. However, by evaporating a thin layer of an organic material on a conductive surface, electrons are able to tunnel, and thus an STM is able to image organic molecules [11]. Using STMs, scientists are able to produce images of DNA molecules such as the one shown in Fig. 6.

Chemical applications include the analysis of chemical reactions and chemical bonds at the surface of a metal, and imaging of polymers[2]. Using STMs, scientists can analyze the effectiveness of protective coatings such as Teflon at the atomic level and produce more resistant chemical coatings [13]. Another application is the control of chemical reactions.

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[1] The Fermi level is a certain electron energy level, determined by the sample material.

[2] Long molecular chains usually associated with plastics.

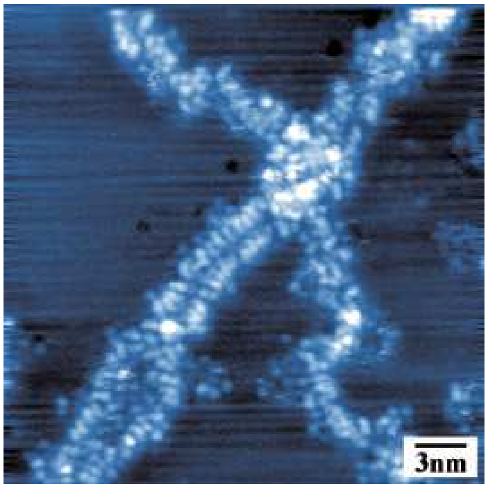

Fig. 6. STM Image of a DNA Molecule. [12]

In large scale chemical reactions, a scientist has no control of individual molecules, however with an STM, a scientist is able to manipulate specific molecules and atoms to control and force specific chemical reactions [14].

Materials science and materials engineering is a relatively new branch of mechanical engineering in which scientists "build materials atom by atom" [15]. Materials scientists are responsible for new composite materials such as Kevlar. STMs allow material scientists to analyze atomic structures to determine a material's important mechanical and thermal properties [15]. Using STMs also allows materials scientists to analyze electrical and thermal insulators. Although STMs normally need conductive materials for electrons to tunnel, STMs can image insulators in the same way as organic molecules – through the process of layering a thin insulating material on a conductive substrate [11].

As technology improves in the fields of microelectronics and semiconductors, the ability to resolve images of objects as small as a few nanometers, such as Intel's 45 nm processor technology, becomes important. Such an image is shown in Fig. 7. At such a small scale, atomic arrangement plays a much greater role in determining a material's characteristics. Using STMs, scientists are able to more closely analyze the atomic make up of semiconductor materials, which are an integral part of modern computers. Comparing these images to known conductors and semiconductors, scientists can determine the effectiveness of a semiconductor in order to engineer transistors with faster switch rates and thus faster processors [11].

V. CONCLUSION

The STM has proven to be invaluable in the science and technical fields. Its importance is amplified by the invention of new unconventional microscopes such as the atomic force microscope and the magnetic force microscope, which both depend on the STM as a building block. Scanning tunneling microscopy is an important development that will continue to have a profound effect on many scientific disciplines.

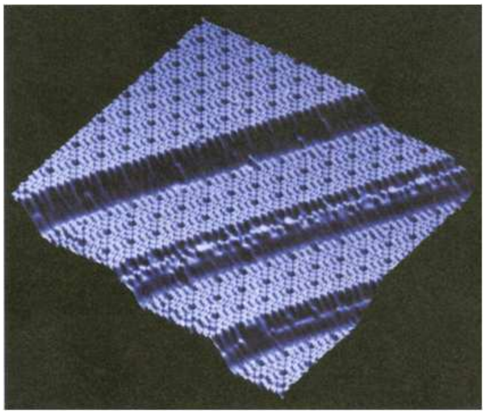

Fig. 7. Binnig and Rohrer's STM image of Si(111) in 7x7 arrangement. [11]

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