Name Partners Date

Visual Quantum Mechanics
The Next Generation

Investigating Nano-Space

Goal
You will apply your knowledge of tunneling to understand the operation of the scanning tunneling microscope. You will learn how modern instrumentation can be used to map the location of atoms and to move individual atoms.

Introduction

In the fifth century BC the Greek philosopher Democritus first postulated that atoms were the fundamental building blocks of the visible world. Since then, many advances in science have been driven by human attempts to understand these atoms. All things around us are made from atoms and the differing properties of individual objects depend on the type and arrangement of these atoms. For example, one arrangement of carbon atoms is graphite (as in a pencil lead); another is diamond. Our ancestors carved stones consisting of trillions and trillions of atoms and used them to make tools. Present day fabrication techniques build on the same tradition. Microelectronic technology enables us to manipulate much smaller numbers of atoms to create devices as small as a millionth of a meter. While these devices are tiny compared to the tools made by prehistoric people, they are still enormous compared to the sizes of individual atoms.

An exciting new development – nanotechnology – has given us the ability to manipulate individual atoms directly, with control and precision, to form structures of atomic size. For example, the IBM logo shown in Figure 1 is made of only 35 atoms. Each bump on the surface is one atom. The letters were created by moving individual xenon atoms into specific positions on a nickel surface. In order to manipulate atoms in this manner, we must be able to separate and move each individual atom.

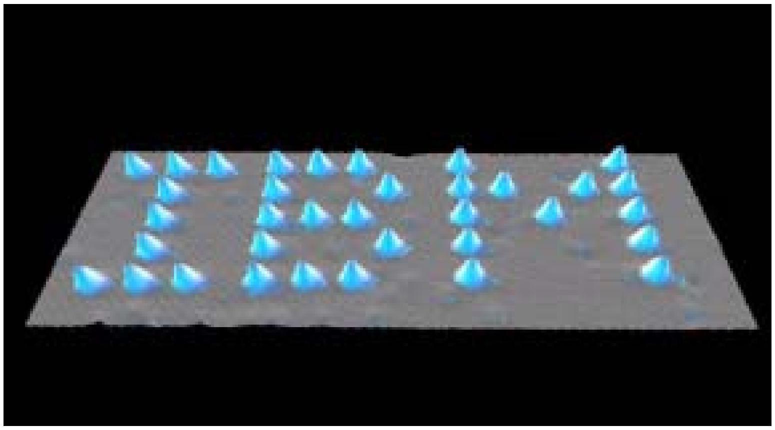

Figure 1: The letters of IBM were created by placing xenon atoms on a nickel surface. (Courtesy of International Business Machines)

To understand the challenge and significance of nanotechnology, we must realize that today's manufacturing methods are very crude at the atomic level. Casting, grinding, milling and other physical manipulations move an enormous number of atoms. Modern manufacturing techniques are cumbersome and imprecise at the atomic level; the equipment cannot efficiently move individual atoms or even small numbers of atoms.

The word "nanotechnology" is being used to describe a broad range of research dealing with structures of approximately *one billionth* of a meter (0.000000001 m), which is about the size of an individual atom. In the future, nanotechnology will let us manipulate the positions of individual atoms directly and construct devices of an atomic size.

In this tutorial we will learn more about how structures like the IBM letters shown in Figure 1 can be fabricated. You will also learn of physical phenomena that must be considered when dealing with structures of such small dimensions.

Using nanotechnology, we can combine atoms — the fundamental building blocks of nature — easily, inexpensively, and in almost any desired arrangement. The ability to manipulate individual atoms will be essential if we are to continue the miniaturization revolution of computer hardware beyond the next decade.
Miniaturization will also allow us to build a broad range of manufactured products more cleanly, more precisely, with more flexibility, and at a lower cost. Many scientists believe that nanotechnology will enable the construction of computer systems with very large numbers of logic elements that are the size of molecules and are interconnected in complex patterns.

Building *nanoscale* electronic devices is indeed difficult now. At present it can be done only in research labs. In this tutorial you will learn about some of the research methods that are used to complete the task. As physicist Richard Feynman said in a classic talk in 1959, "The principles of physics, as far as I can see, do not speak against the possibility of maneuvering things atom by atom." (See http://www.zyvex.com/nanotech/feynman.html for the full text.) We now know that it can be done.

To learn more about nanostructures, browse the World Wide Web. You may search for terms such as "nanotechnology" or "molecular manufacturing." To help you get started, a few links are available at http://www.phys.ksu.edu/perg/vqm/links/micro.html.

A. Scanning Tunneling Microscope

One method of moving atoms involves an instrument called the scanning tunneling microscope (STM). As the name implies the first use of the instrument was to look at very small objects by scanning them and using quantum tunneling.

The scanning tunneling microscope (STM) consists of an extremely fine metal tip called a "probe" which is placed a few tenths of a nanometer above the surface of the sample (Figure 2). By moving the tip over the surface, the scanning tunneling microscope "maps" the surface of the sample and generates an image. In this activity you will learn how the scanning tunneling microscope completes these measurements.

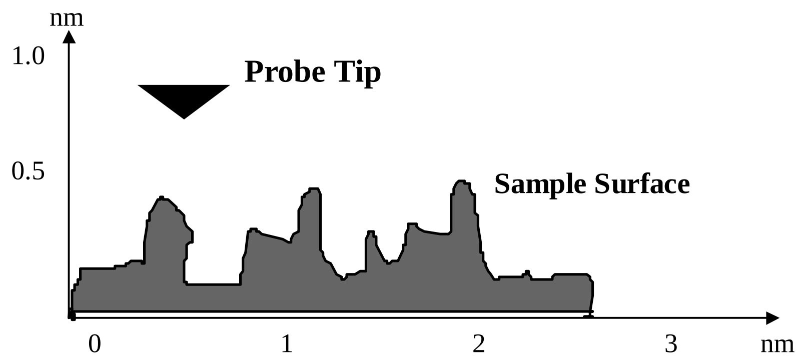

Figure 2: A diagram of the nanometer scale features on a surface. The probe tip of a scanning tunneling microscope is suspended a few tenths of a nanometer above the surface.

A typical image taken by a scanning tunneling microscope is shown in Figure 3 . The dark and light areas represent regions of high and low elevation respectively.

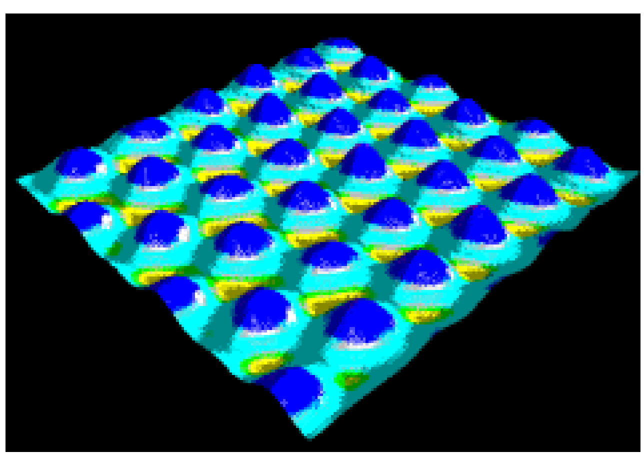

Figure 3: An STM image of carbon atoms on a graphite surface.

Now we will look more closely at how the scanning tunneling microscope works. The tip of the scanning tunneling microscope is typically a few tenths of a nanometer away from the surface and measures locations without ever touching it. This lack of physical contact is important. By moving over the surface without touching it, the probe can determine the location of atoms without disturbing them.

The primary goal of this tutorial is to understand how the scanning tunneling microscope can create pictures of surfaces without using light and without physical contact with the surface. The scheme involves electrons moving from individual atoms on the surface to a probe tip. By knowing where the electrons are we can gain information about the locations, sizes and types of atoms.

We know that electrons seek the lowest energies available to them. Thus, the number of electrons in a region is an indication of the energy level. If a region has more electrons than in an adjoining region, we can conclude that the region populated with *more electrons* must have a *lower potential energy*. This information can be used to construct a potential energy diagram for the two regions. In Figure 4 the region on the left has more electrons than the region on the right. The related potential energy diagrams are shown in the lower part of the figure.

Figure 4 : The potential energy diagram for an electron in two regions, which is determined based on information about the relative number of electrons in each region. Region 1, with more electrons, has lower potential energy.

For the scanning tunneling microscope the surfaces of the sample and probe tip are electrical conductors. They both contain relatively more electrons than does the gap between them.

A-1. Based on this fact determine the potential energy diagram for an electron moving along the line A-B in the three regions specified in Figure 5. Sketch the potential energy diagram in the lower part of Figure 5.

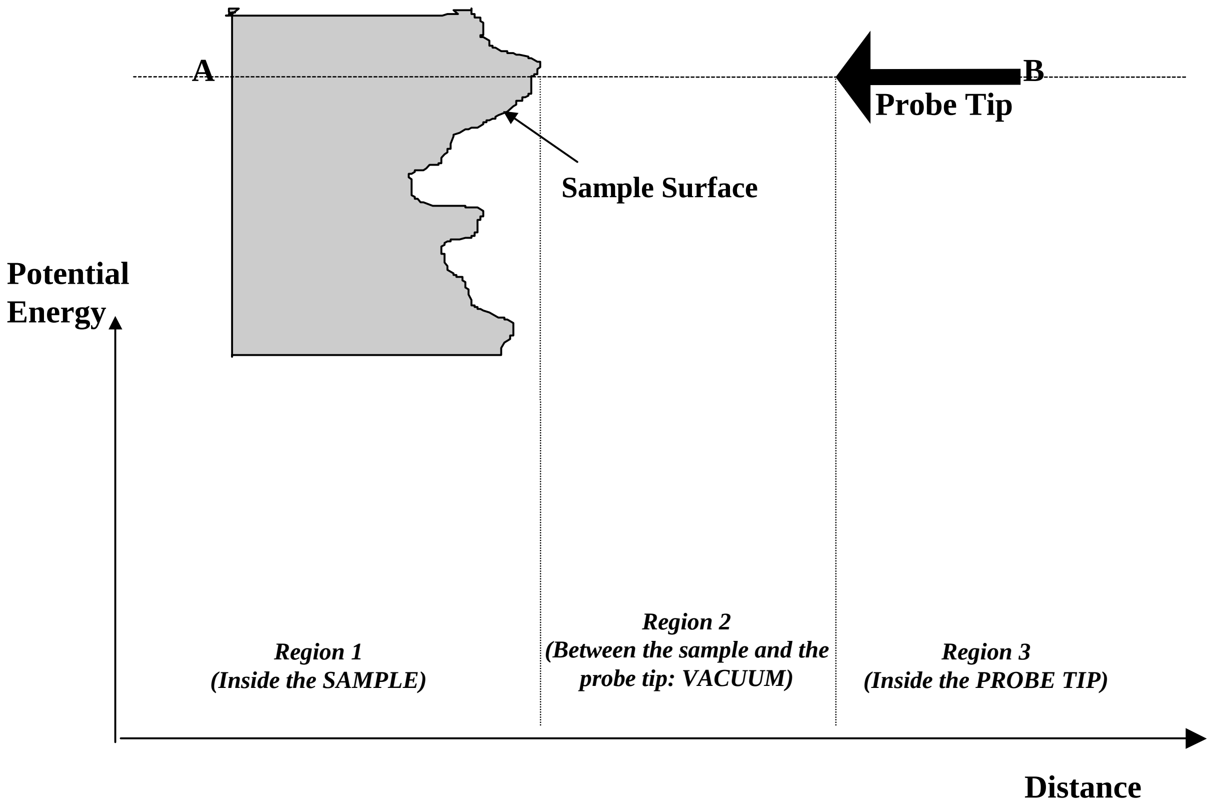

Figure 5: Potential energy diagram for an electron in a scanning tunneling microscope.

A-2. Explain your reasoning for the potential energy diagram that you sketched above.

For the probe tip to receive any information from the surface, electrons will need to flow from *Region 1 (Sample*) to *Region 3 (Probe Tip)*.

From our previous studies of quantum tunneling we know that an electron has a small probability of moving past the potential energy barriers even though it has insufficient energy. The probability that quantum tunneling occurs is related to the properties of both the electron and the potential energy of the material involved. As you have seen, the transmission coefficient is

$$T = \frac{4\dfrac{\alpha^2 k_0^2}{\left(k_0^2+\alpha^2\right)^2}}{\sinh^2\left(\alpha L\right)+4\dfrac{\alpha^2 k_0^2}{\left(k_0^2+\alpha^2\right)^2}} \approx 4\frac{\alpha^2 k_0^2}{\left(k_0^2+\alpha^2\right)^2}e^{-2\alpha L} \approx e^{-2\alpha L}$$

where

$$\alpha = \frac{\sqrt{2m(U_o - E)}}{\hbar}$$

Thus, the probability of tunneling depends on

- the width of the potential barrier (L),
- the height of the barrier (U_0), and
- the total energy of the electron (E).

We will now investigate how these variables are used to measure the location of atoms on surfaces.

Figure 6 shows a result similar to Figure 5. Here the potential energy diagram has been drawn for you.

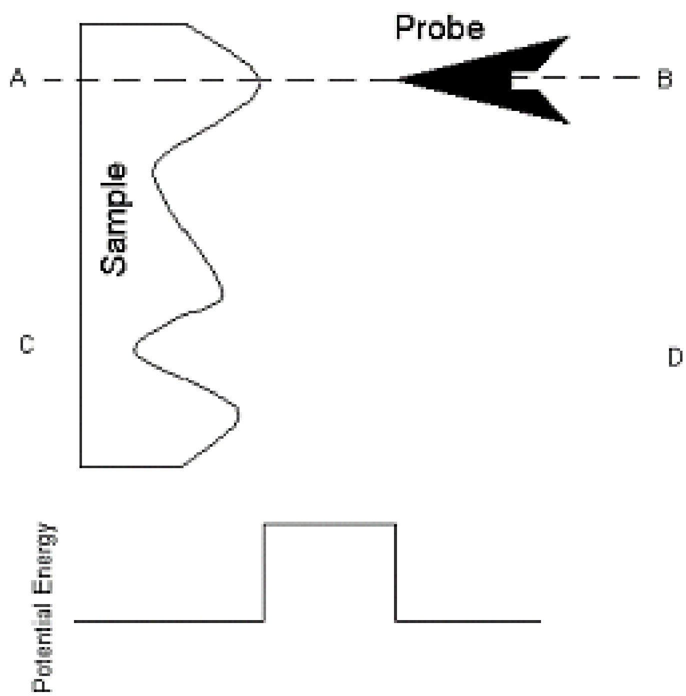

Figure 6: The potential energy diagram for an electron moving on line A-B.

A-3. Suppose the probe is moved to C-D in Figure 6. Sketch the potential energy diagram for this situation.

A-4. Use the approximation for $\alpha L >> 0$ that $T = e^{-\alpha L}$. By what fraction will the transmission probability change when the probe moves down vertically from A-B to C-D?

The potential energy barrier changes as the distance between the probe and surface changes. As a result the transmission coefficient for electrons changes. This conclusion is the basis of the scanning tunneling microscope. The electrical current in the probe is related to the probability that tunneling occurs and, thus, to changes in the surface.

Tunneling occurs without the surfaces ever touching. Because the probe does not touch the atoms, it does not move them. Thus, quantum tunneling provides a way to map atoms on a surface accurately.

To see how this process works, start the *Scanning Tunneling Microscope* program. After starting the program, click in the square and open the file ***Atoms***. This picture is an actual image created from STM data. The program will provide us detailed information about a single scan. So, first you must decide which region of the image you wish to scan. You may choose any straight line across the image. Pick one and use the cursor to draw the line.

Now, select cross-section under the View menu. This window shows a highly magnified cross-sectional view that you would see if you cut the surface along the line that you drew. Use the mouse to move the probe tip straight down, ***closer,*** to the surface and then further away.

A-5. How does the tunneling probability change as you move the probe?

A-6. How is this result consistent with your previous knowledge of tunneling?

A-7. Open the *Potential Energy Diagram View*. Again move the probe so that it comes close to the surface. How is the variation in the potential energy consistent with your knowledge of tunneling?

As you can see, the probability of tunneling is rather small even when the probe is very close to the surface. In a real STM the probe needs to stay a small distance away from the surface. To make the scan efficient we need to “encourage” electrons to undergo tunneling.

A-8. List as many methods as you can, other than getting closer to the surface, to increase the quantum tunneling.

A-9. The voltage control in the lower left places the probe tip at a positive voltage relative to the surface. Gradually increase the voltage from 0 to about 5 volts. After each increase, click *Apply*, sketch the potential energy diagram below and record the tunneling probabliity.

A-10. Describe how this result is consistent with your knowledge of

- potential energy diagrams

- quantum tunneling

Now, open the *Wave Function View*. This window represents the wave function of electrons. Notice that the exponentially decreasing portion of the wave function occurs only in a narrow region so it is a little hard to see.

A-11. Describe how the wave function changes as you

- move the probe away from the surface

- move the probe horizontally

- increase the voltage between the surface and probe.

A-12. Move the probe horizontally above the surface. Stop several times and record the tunneling probability. Describe how the tunneling probability varies with the surface.

A-13. How are these results consistent with your knowledge of quantum tunneling?

In an actual STM one does not measure the transmission probability, but does measure the electrical current that is a result of the motion of electrons which undergo tunneling. This current is displayed below the voltage. As you might expect this current is called the tunneling current. Open the *Current Profile View*.

To obtain a current profile you must do a "scan". The right-most three buttons on the tool bar select different scan modes. Select *Arbitrary Tip Path* (left button of three). Complete a scan by pressing the shift key while moving the probe tip.

A-14. How is the tunneling current related to the variations in the surface?

A-15. How can you get the current profile to closely match the surface?

A-16. Explain how this relation can occur by using your observations of the potential energies, tunneling probability, and wave function.

We have looked at one scan line across a surface. An STM will complete a large number of scan lines. With each one the tunneling current is measured. Putting the currents together from all of the scans creates an image of the surface.

B. Modes of Operation for an STM

You have seen how the scanning tunneling microscope can be used to create an image of a surface by measuring the tunneling current. Normal STMs operate in one of two modes. The constant probe height mode (middle mode button) keeps the probe at the same vertical location. Try this mode with a scan. (Remember to hold down the shift key.)

B-1. How do the current profile and surface variations compare?

In the second mode the probe remains at a constant height above the surface. By moving the probe up and down it can always maintain a constant current and, thus, a constant distance between it and the surface.

In this mode, the STM has an internal mechanism that maintains a constant tunneling current by moving the probe tip vertically as it moves horizontally. Then, the vertical motion of the probe represents changes in the height of the surface. (Figure 7)

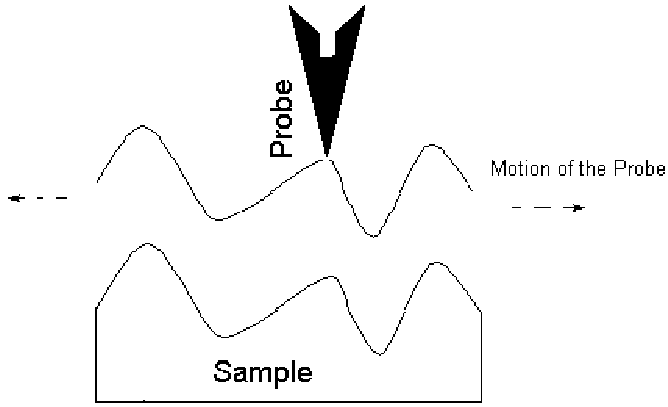

Figure 7: Constant current mode of an STM. At each point the probe moves to a height where the current is identical to other points. Thus, it is always at the same distance from the surface.

C. Moving Atoms

The physical distance between the probe tip and the surface of the sample must be no more than a few nanometers for a current to occur. Because of the small distances involved, the scanning tunneling microscope is a very valuable tool for studying the minutest details of surfaces. When the STM is used to study a surface, the electrons tunnel to create the current. However, electrons are not the only objects that undergo quantum tunneling; atoms can do it too.

While atoms can tunnel, their probability of tunneling in any situation is much smaller than that of an electron. A proton is about 2000 times more massive than an electron. Use the transmission coefficient to compare tunneling for an electron and a proton with the following parameters:

- Total Energy = 3 eV
- Potential Energy = 4 eV
- Potential (Barrier) Width = 5×10^{-10} m

C-1. How do the probabilities for tunneling of an electron compare with that of a proton?

C-2. How would you need to change the potential energy barrier width for a proton to obtain the same tunneling probability as an electron? (You may do this numerically or use the *QuantumTunneling* program.)

Because a proton is the nucleus of hydrogen, the comparisons for the electron and proton give us an idea about how tunneling of electrons compares to that of atoms. We conclude that atoms can tunnel in STMs only when the distances between the surface and probe tip are much smaller than for electrons. However, this situation can be created. Because both the surface and the probe of an STM are electrical conductors, electrons which move from the surface to the probe can move through the probe easily. For atoms, such movement is not so easy. They are big (at least compared to electrons) and they have many negatively charged electrons surrounding the nucleus. Thus, after an atom tunnels, it tends to stick on the tip of the probe.

To get the atom unstuck we need to change the voltage on the probe. Then the atom gains some energy, is repelled from the probe tip and returns to the surface. This process allows STM operators to move atoms, one at a time, along a surface. It is summarized in Figure 8.

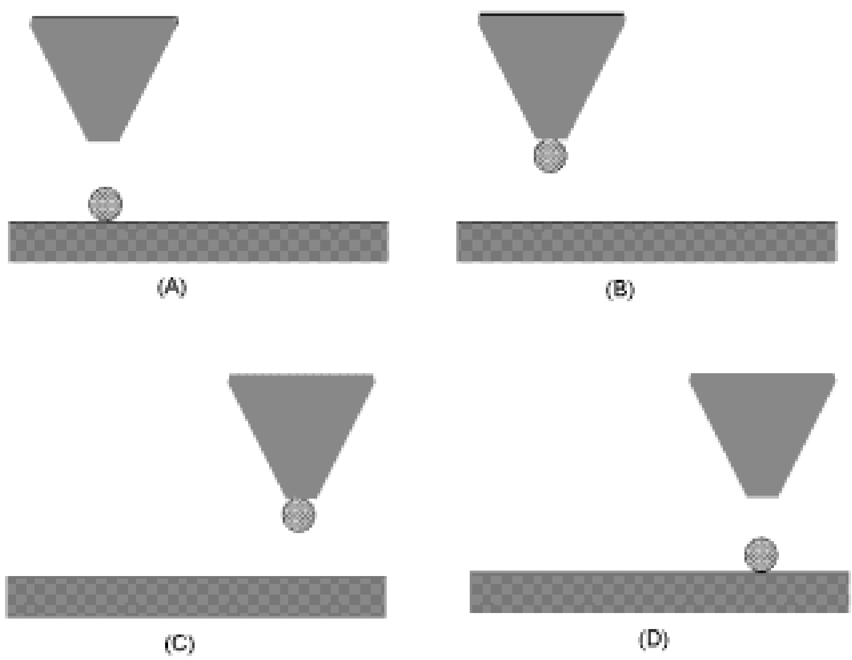

Figure 8: The process of moving one atom. (A) The probe comes very close to an atom on the surface. (B) The atom tunnels and sticks to the end of the probe. (C) The probe moves to a new location. (D) By changing the voltage, the atom is forced back to the surface.

By moving atoms scientists have created words such as the Japanese character for atoms, Kanji, shown in Figure 9. They have also created circles of atoms in which electrons were trapped. One of these “electron corrals” is shown in Figure 10. The wave-like surface in the middle of the circle is made up of only electrons. Thus, the STM, which was built after scientists understood quantum mechanics, now has given us a graphic display of the wave properties of matter.

Writing characters and creating corrales is a beginning of nanotechnology. Looking to the future we can imagine people creating tiny machines out of even tinier gears. These machines could perform tasks on a very small scale. For example, some scientists think that nanomachines may some day be able to repair human cells. When we become ill, doctors will inject nanomachines in our blood. These devices will be programmed to “fix up” our cells.

While many people are speculating on benefits of nanodevices, others are concerned about the negative side. Nanomachines could be programmed to reproduce themselves. Suppose they overdid the reproduction and grew in number as viruses do. Then, they could cause great harm.

At present potential positive and negative effects of this technology are speculation. We are still learning how to manipulate atoms. Much work needs to be done before nano-manufacturing is operating on a large scale.

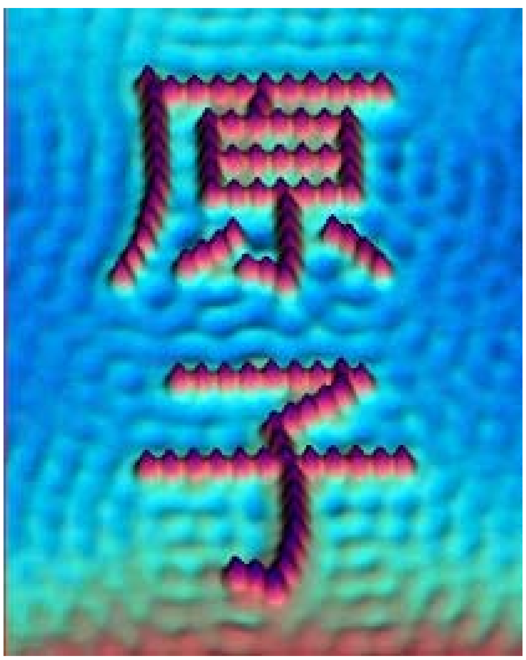

Figure 9: The Kanji character for “atom” — the literal translation is “original child” — created by appropriately placing iron atoms on a copper surface. (Courtesy of International Business Machines)

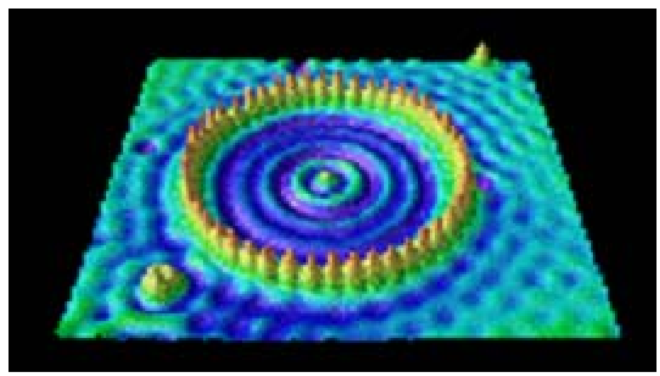

Figure 10: Iron atoms are placed in a circle on a surface. Electrons are trapped inside this “corral.” (Courtesy of International Business Machines)