IBM Images Surfaces by Electron Tunneling

IBM Zurich laboratory group images metal and semiconductor surfaces with nearly atomic resolution by scanning tunneling microscopy

About a year and a half ago, researchers at IBM's Zurich Research Laboratory demonstrated conclusively that electrons could jump from one metal surface over a small distance through a vacuum to another metal by the quantum mechanical tunneling effect. In itself no surprise, vacuum tunneling was purported to be a promising tool for the investigation of the geometry of solid surfaces. The promise is being fulfilled, as the IBM scientists have published several papers demonstrating the capability of vacuum tunneling to image the topography of metal and semiconductor surfaces with nearly atomic resolution. A recent report on the structure of the silicon surface has, for example, contributed to a burst of model making in an attempt to find an arrangement of silicon surface atoms that is compatible with a diverse array of experimental data.

Tunneling between metals or semiconductors separated by extremely thin layers of insulating material has been known experimentally since 1957. A vacuum is the ultimate insulator, so tunneling through the vacuum should not be a challenge, but it turns out to be quite difficult to verify.

Tunneling is possible because the quantum mechanical wave functions that describe electrons near a surface actually extend out of the surface. If two solid materials are close enough together, the wave functions of electrons in the two materials can "overlap" enough so that there is a finite, though small, probability for electrons to crossover. The probability for vacuum tunneling is proportional to $e^{-\phi^{1/2}d}$, where ϕ is the average work function of the materials between which the electrons are tunneling and d is the separation between the two materials. The difficulty in demonstrating vacuum tunneling is that the separation d could only be a few angstroms for there to be a measurable tunneling current. A way had to be figured out to make a mechanically stable fixture reliably to hold samples that far apart in the face of vibrations.

Gerd Binnig, Heinrich Rohrer, Christoph Gerber, and Edmund Weibel of IBM found a solution to this problem and also added a feature that provided the high-resolution imaging capability. In the first version of their setup, the researchers resorted to a two-stage strategy for the isolation of vibrations. The vacuum chamber containing their apparatus sat on a stone table isolated from the laboratory building by inflated rubber tubes. Within the vacuum chamber, the apparatus was levitated above a bowl of superconducting lead by permanent magnets. Rohrer told *Science* that the investigators have recently switched to a less cumbersome approach that is also compatible with the ultrahigh vacuum chambers that are de rigueur for surface studies. Now the apparatus sits on an aluminum ring supported by three springs. The springs, in turn, ride on a second aluminum ring supported in the vacuum chamber by a second set of three springs. The vacuum chamber rests on the laboratory floor with no further isolation.

The IBM researchers can now measure changes in the height of a surface of 0.1 angstrom.

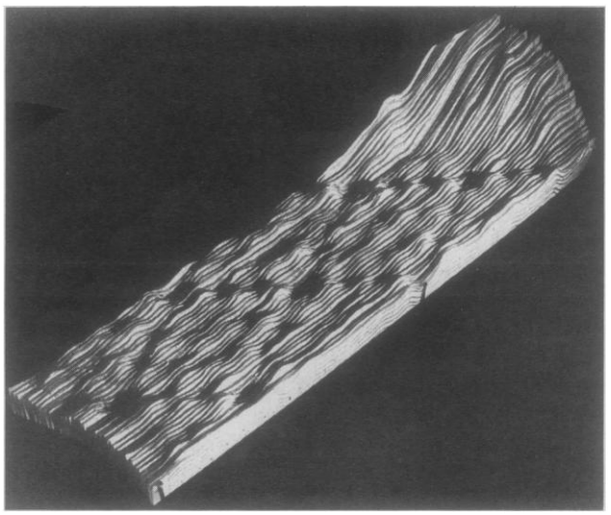
The first IBM demonstration of vacuum tunneling was between a tungsten wire tip and a platinum plate. One proof that true tunneling was taking place was the observation of the characteristic inverse exponential dependence of the tunneling current on the separation between the tungsten wire tip and the platinum surface with a slope corresponding to the work functions of the materials involved.

Relative motion of the plate and the wire tip is also achieved in two stages. For "rough" motion of steps of 100 angstroms or larger, the plate lies on a piezoelectric ceramic slab, which contracts or expands in the plane of the slab according to voltages applied to it. The slab is supported by three metal legs, which can be "clamped" to a metal plate by means of applied voltages. The "louse," as it has come to be known, moves like an inchworm when the appropriate sequence of voltages is applied to the piezoelectric slab and to the supporting metal legs.

For finer motion, the wire tip is affixed to an assembly of piezoelectric ceramic elements (piezodrives) that allow the tip to be moved in all three directions, the two in the plane of the platinum plate and the one perpendicular to it. In operation, an electronic control unit uses the measured tunneling current to keep the wire tip at a constant distance from the plate while the tip scans over the plate surface in a raster pattern, as on a television screen, over distances up to a thousand angstroms or so. With this system, the IBM researchers can now measure changes in the height of a surface of 0.1 angstrom (one-thirtieth the diameter of an atom) with a lateral resolution of better than 6 angstroms.

An interesting sidelight is the wire tip. One's first thought would be that it must be exceedingly fine in order to resolve features on the angstrom scale. In fact it is not particularly fine at all. The tip is formed from a 1-millimeter-diameter rod on an ordinary shop grinding wheel, yielding a tip radius of 1 micrometer or less. The key seems to be that there are local filaments or minitips of considerably smaller diameter and that the extreme sensitivity of the tunneling current to distance from the surface "selects" the longest of these. This yields lateral resolutions of about 10 to 15 angstroms, which can be further enhanced by in situ sharpening by means of an applied high electric field. Unfortunately, the reliability of the sharpened tips is uncertain, as the high resolution comes and goes. Stabilizing the high-resolution mode of operation remains one of the problems to be solved. "It is still a matter of luck," says Rohrer.

Nonetheless, the periods of stable high-resolution operation last up to about 2 hours. And even with 15-angstrom resolution, scanning tunneling microscopy provides a new kind of surface image that is not obtainable in other ways. Electron and x-ray diffraction, for example, require ordered surfaces with atoms arrayed on a regular crystal lattice. X-ray absorption techniques like EXAFS can handle disordered surfaces, but the information obtained is an average over the large area illuminated by the x-ray beam. Scanning tunneling microscopy looks at only one or a few atoms at a time and thus requires neither an ordered surface nor averaging over large areas. Consider gold, a material with a cubic structure. The faces of the cube are called (100) planes. The IBM group has been able to show that the (100) surface of gold actually consists of nar-



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Silicon (111) surface

Wood relief model constructed from tunneling microscopy scans shows two complete (7 × 7) unit cells. The "hill" on the right is about 15 angstroms high.

row strips or facets with a (111) orientation. The (111) planes cut diagonally through the cubic unit cell, so the (100) surface of gold is furrowed. On the negative side, it is not yet a quantitative technique, so that accurate measurements of bond lengths are not possible. It also does not yet permit identification of the atomic species being imaged.

The IBM group has used scanning tunneling microscopy to make a detailed investigation of the surface of silicon, as well as gold. Interpretations of the structures of the surfaces of both these materials have been controversial. In general, the energy associated with the missing bonds of surface atoms provides a driving force for a so-called reconstruction in which the surface atoms adopt a lower energy configuration than that expected from the bulk crystal structure. Observing the surface is difficult because to be surface sensitive, probes must interact very strongly with the surface atoms, but the strong interactions are hard to calculate accurately, so that interpretation of the data in terms of basic structural parameters such as the positions of atoms is hindered.

Silicon's (111) surface is a case in point. The atoms in a (111) plane of silicon form a hexagonal array with the alternate points of the hexagon displaced slightly upward and downward. If silicon is cleaved in ultrahigh vacuum so that a (111) plane is exposed, the surface atoms rearrange their bonds slightly so that the threefold rotational symmetry is lost. The resulting surface unit cell is larger, less symmetric, and has the jargon name (2 × 1). If the silicon is annealed at a high temperature and cooled, the structure changes again to a configuration that the clean surface always returns to at room temperature regardless of further treatment. The final structure is called a (7 × 7) and has an even larger and more complicated unit cell than the (2 × 1). The 49 silicon atoms in the (7 × 7) unit cell make impossible the type of detailed calculations needed to enable low energy electron diffraction (LEED) to yield quantitative atomic positions.

Last January, the IBM researchers published a report on their scanning tunneling microscopy study of the silicon (111) surface. The figure shows what they found. Clearly evident are two of the diamond-shaped (7 × 7) surface unit cells, each of which contains 9 minima between atom sites and 12 maxima where atoms sit. The deepest minima are at the corners of the unit cells. The peak heights of the maxima lie 0.7 angstrom above the average for all the atoms in the unit cell; the deep corner minima lie 2.1 angstroms below the average; and the edge and short diagonal minima lie 0.9 angstrom below the average. Two other important features revealed by analysis are the sixfold rotational symmetry of the maxima surrounding each unit cell corner and the threefold rotational symmetry of the pattern of the minima in a unit cell as a whole.

In comparing these findings with the many models of the silicon (111) surface that have been generated in the last two decades, the IBM researchers were able to rule out most of the older ones. As it happens, however, the last 2 years have seen a revival of interest in the technologically important silicon surface, and several new proposals for surface structures have come out and are about to come out. The subject is far from resolved.

One of the questions concerning the evidence from scanning tunneling microscopy is that of surface cleanliness, points out Donald Hamann of Bell Laboratories, who otherwise is an enthusiastic supporter of the technique. To be sure a surface is clean, scientists go through a multistep process that includes several cycles of heating the silicon and bombarding it with argon ions. Then a LEED experiment is done to verify that the characteristic diffraction pattern of the (7 × 7) surface is present. Finally, Auger electron spectroscopy of the surface is done to be sure that contaminating species are absent (to the 1 percent level). The IBM group could clean their silicon but did not have LEED and Auger equipment in their vacuum system when their silicon study was under way. Therefore, it is not certain that their (7 × 7) surface was the same in all details as those other researchers have investigated. This situation is now being remedied, says Rohrer.

As for the future, there are several possibilities. One is scanning inelastic tunneling spectroscopy. Inelastic means that the electrons lose some energy during the tunneling. One way they can lose energy is by exciting surface lattice vibrations. Inelastic tunneling spectroscopy of surface vibrations at the interfaces in metal-insulator-metal sandwiches is now being done at a few laboratories, but the information represents an average for the entire area of an interface. Replacing the insulator layer with a vacuum and using scanning vacuum tunneling would allow spatially resolved measurements of surface vibrations or other phenomena that might be excited by the tunneling electrons.

A second possibility would help clarify the electronic structure (wave functions) of surface atoms. The $e^{-\Phi^{1/2}d}$ dependence of the tunneling current given earlier is actually valid for the case of a large surface extending over thousands of atoms. When tunneling is only between a few atoms at a given instant, the macroscopic average represented by that formula loses its relevance and has to be replaced by a detailed analysis in terms of the actual wave functions involved, if the measured topography is to be related to the atomic positions. The tables can be turned, however, and with such tricks as varying the voltage that drives the tunneling (2.9 volts in the silicon experiment) and the distance between the wire tip and the surface in appropriate ways, it is possible to map out the surface atom electronic wave functions. This would give an electron density map somewhat like those generated in x-ray diffraction studies of complex crystals.

A third possibility, among the many that have been mentioned, is to investigate adsorbed species, such as organic molecules on metal surfaces, the classic heterogeneous catalysis situation.

—ARTHUR L. ROBINSON