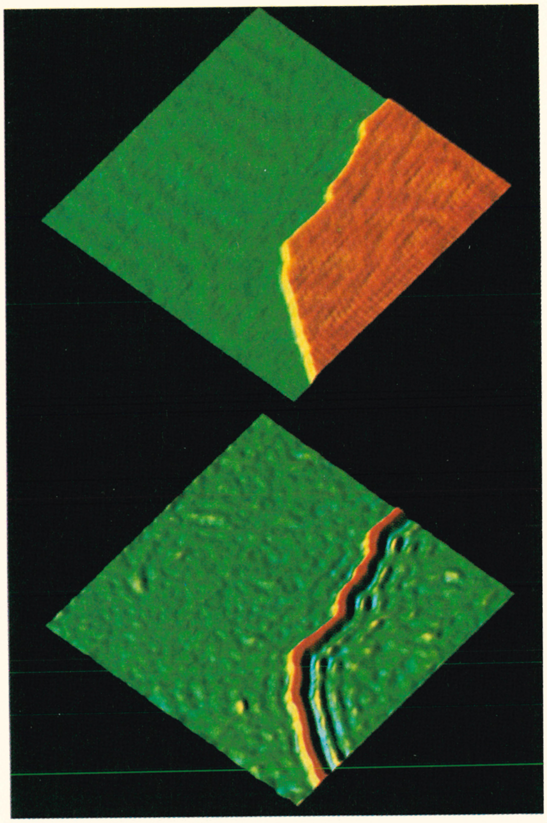
STM ROUNDS UP ELECTRON WAVES AT THE QM CORRAL

Everyone who has completed an elementary quantum mechanics course has seen plots of solutions of the Schrödinger equation for the archetypal "particle in a box." Now IBM researchers have used scanning tunneling microscopy to image the rippled density of states of electrons inside a "corral" built with a few dozen carefully positioned iron atoms on a copper surface.[1] (See the cover of this issue.) The spectacular results closely match theoretical models of the system.

On a high-quality (111) surface of a noble metal such as copper some electrons go into surface states and form a two-dimensional electron gas. These electrons are sandwiched by the work function on the vacuum side and by a bandgap in the energy spectrum of the bulk electrons on the other side, but are essentially free to move in the plane of the surface. The quantum waves of these surface-state electrons reflect off defects such as one-atom-high steps between different terraces of the surface and individual impurity atoms adsorbed on the surface (adatoms). (See the article by Max Lagally on page 24 of this issue.) These reflections result in a variety of interference patterns that have been imaged at both room temperature and 4 K.



Standing waves at a step on a gold (111) surface at room temperature. Upper image shows a topograph of the surface at a one-atom-high step from one terrace (red) down to a lower terrace (green). Lower image maps the local density of electron states 0.15 eV above the Fermi level and shows high density at the step and standing waves on the higher side of the step. (Courtesy of Phaedon Avouris, IBM, Yorktown Heights.)

The work has been carried out independently by two groups of IBM researchers. At IBM's T. J. Watson Research Center, in Yorktown Heights, New York, Phaedon Avouris and Yukio Hasegawa (now at Kyoto University) have produced images of standing waves in the surface-state density on gold and silver surfaces at room temperature.[2,3] Meanwhile, at IBM's Almaden Research Center in California, Michael Crommie, Christopher Lutz and Donald Eigler have imaged copper surfaces cooled to 4 K and have built the first quantum corrals.[1,4]

In addition to providing remarkable pictures of the density distributions of quantum states, the work is answering questions about how electrons interact with atomic-scale structures. The wave-imaging techniques open up many new avenues for research on electron scattering and surface properties, and the corrals might allow direct imaging of state densities associated with quantum chaos. (See the article by Eric Heller and Steven Tomsovic in PHYSICS TODAY, July, page 38.) Harald Hess of AT&T Bell Labs hails the work as "a wonderful demonstration of scanning tunneling microscopy and scanning tunneling spectroscopy."

Foresight and serendipity

A scanning tunneling microscope works by positioning its tip close enough to the target surface that electrons tunnel across the gap between tip and surface at an appreciable rate. The tunneling current depends on many factors, including the distance of the tip from the surface, the bias voltage between the surface and the tip, and the electronic states available in the surface at the energy corresponding to the bias conditions. A common mode of operation is the constant-current topograph, in which the bias voltage between the tip and the surface is kept constant and the height of the tip is adjusted, as it scans across the surface, to keep the tunneling current constant. In another mode of operation, called scanning tunneling spectroscopy, the voltage is varied at each location and the quantity $(dI/dV)/(I/V)$ is measured, yielding the electronic local density of states in the surface at the position of the outermost tip atom. Similar spectroscopy has been carried out with electron states confined to two-dimensional "artificial atoms" by doping and biasing in semiconductors. (See the article by Marc Kastner in PHYSICS TODAY, January 1993, page 24.) "What's completely new is that you can measure the current at different points within the electron gas," says Kastner (MIT). "It really tells you what the wavefunctions look like."

Avouris and Hasegawa carried out such spectroscopy on a gold surface in February 1992. Previously they had been studying the surface conductivity of a very smooth silicon surface with some nanometer-sized, one-atom-thick islands of silicon spotted about the surface. In that work they saw evidence that electrons were scattered from the island boundaries, and they decided to investigate a metal, believing that the larger density of free electrons might enable them to image the scattering. Their belief proved correct, but they chose to study other phenomena before returning to further imaging[2] of the electron waves in late 1992.

Eigler's group at Almaden, on the other hand, stumbled onto the ripples in January of this year while studying other processes. The Almaden researchers were trying to learn what happens when adatoms on a surface have a magnetic moment, and they switched from platinum surfaces to copper in the hopes of seeing the effects of Kondo scattering.

"When we put the copper sample into our microscope I was the first person to look at it," Eigler told us, "and the very first image I saw, I said, 'Wait a second—something funny is going on here.'" Unlike the (111) surfaces of copper, silver and gold, the Pt(111) surface doesn't support a confined surface state, which is essential for the results described here.

Ripples on the electron sea

Both the Almaden topographs and the Yorktown Heights spectroscopy experiments image the local density of states of the electrons in the surface states. Where the local density of states is larger, so too is the tunneling current.

In the work by Avouris and Hasegawa, which they have continued along with In-Whan Lyo and Robert E. Walkup of Yorktown Heights, ripples were seen parallel to steps on the surface.[2,3] (See the figure on page 17.) In their experiments the ripples extend only a few wavelengths from the steps, because the coherence length is relatively short at room temperature. The ripples are interpreted as interference effects caused by the partial transmission and reflection of the electron wavefunctions at the steps. By varying the tip voltage and seeing how the observed wavelengths changed, the researchers measured the effective mass and the full dispersion relation of the surface-state electrons.

The Yorktown Heights group models its results by allowing for the effects of operating at room temperature. In particular, at any selected bias thermal effects cause one to probe a range of electron wavenumbers. Because of the corresponding range of wavelengths probed, the observed ripples lose coherence after only a few oscillations.[3] "The ideal instrument for these studies would be a variable-temperature STM," says Avouris. "Doing the experiments at variable temperatures will bring a wealth of new information."

His group found that for electrons with low wavenumbers, a step acts like a hard barrier, so that the corresponding surface states on adjacent terraces are relatively isolated. At higher wavenumbers the steps become permeable. The ripples are stronger on the upper terrace at a step, suggesting that an electron coming from that side sees a harder barrier than an electron coming from the lower terrace.

Radial oscillations are observed around point defects on the surface, such as isolated adatoms. Again, these are interpreted as due to the reflection and subsequent interference of an electron wavefunction hitting the defect. The results obtained by the Yorktown Heights group are consistent with the adatoms' acting as quite hard spheres at low wavenumbers but they seem to permit some transmission at higher wavenumbers.

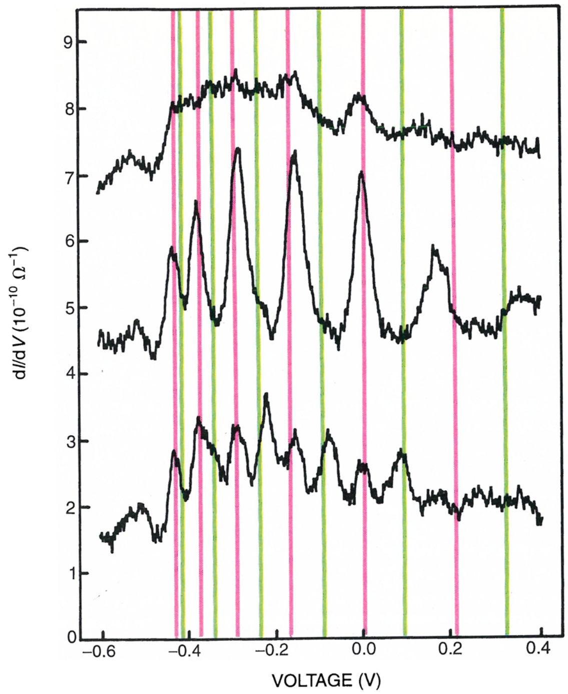
From the detailed properties of the local density of states around a point defect, it may be possible to identify the type of defect, for example, the type of atom and the charge it carries. As Eigler explains, "We can make an energy-dependent study of the amplitude and phase of the scattering of a surface state at an adsorbate. From that we can learn a lot about the scattering potential that the surface-state electron sees."

Corrals

The Almaden researchers have made use of the hard-sphere nature of adatoms by building enclosures on their copper surface out of small numbers of iron adatoms.[1] They position the adatoms with the scanning tunneling microscope. The image on the cover shows a circular enclosure of 48 Fe adatoms that they built in May of this year. The adatoms are spaced at about 3.7 times the 2.55-Å nearest-neighbor spacing of the Cu atoms. The Fe–Fe repulsion prevents much closer spacing, while a wider spacing would be "leakier." Also, this particular spacing allows formation of an almost perfect circle on the hexagonal grid of allowed sites. (The Cu(111) surface that the Almaden group uses is a hexagonal grid, and the Fe atoms probably sit on the hollows located equidistant from three nearest-neighbor Cu atoms.)

As can be seen in the image on the cover, dramatic patterns appear inside such "quantum corrals." As Eigler explains it, "We build a box for our electrons, put an electron in the box, and we see how the electrons solve the Schrödinger equation in that particular environment." In the topograph scans, the trajectory of the microscope tip just above the surface corresponds to a contour on which the local density of electron states is constant, and the density of states depends on the square of the amplitude of the wavefunctions available to the electrons on the surface.

To further test the particle-in-a-box idea, Eigler and coworkers performed some spectroscopy measurements at selected locations inside the circular corral. These results were complicated by the movement of about one-fifth of the Fe adatoms by one or two lattice spacings during the measurements. This had not been a problem during the topograph scans, which used a lower bias voltage between the tip and the surface. (Kastner comments that finding a way to keep the adatoms in place at high biases and at temperatures higher than 4 K would be a further major advance.) At the circle's center, six or seven peaks are observed in the spectrum. (See the figure on page 19.) These correspond closely to the energies of zero-angular-momentum ($l = 0$) eigenstates for a particle in a circular box and having mass $0.38\ m_e$, the effective mass of a surface electron. At a position 9 Å away



Measured spectra and theoretical eigenenergies for the corral shown on the cover. Top curve was measured 1000 Å away from the center of the 143-Å-diameter corral; middle curve, at the center of the corral; bottom curve, 9 Å from the center. The upper two curves are offset vertically for clarity. The vertical lines indicate the eigenenergies for a particle in a two-dimensional circular box with angular momentum 0 (red) and 1 (green). (Adapted from ref. 1.)

from the center there are four additional peaks—corresponding to the $l = 1$ eigenenergies.

The widths of the peaks in the spectrum correspond to a lifetime of about 3×10^{-14} sec, comparable to the time that would be needed for a free surface-state electron to traverse the diameter of the circle (about 2×10^{-14} sec). The Almaden researchers speculate that leakage out of the corral or scattering into bulk states is responsible for the short lifetimes. The tunneling current corresponds to an electron hopping from the surface to the tip about once every 10^{-10} sec. Each scan line takes about a second, each frame about a minute.

The Yorktown Heights group also has imaged confined states, but in one-atom-high islands rather than corrals. Such islands can be produced by molecular-beam epitaxy and, within the constraints of the underlying lattice geometry, are distributed randomly on the surface in a variety of sizes and shapes. They can be as small as a few nanometers across and remain stable for long times even at room temperature. Avouris and coworkers have successfully imaged standing waves within hexagonal silver islands.[3]

Quantum chaos?

It is possible that corrals can be built that will exhibit quantum chaos. For example, the corrals could be designed with shapes like the "stadium" or the "lemon," which theoretically exhibit chaotic dynamics, as described in the July article by Heller and Tomsovic. Then, it is hoped, instead of the familiar particle-in-a-box waveforms observed so far, one would see eigenstates corresponding to chaotic dynamics.

Indeed, in June the Almaden group sent images and data of circular, triangular and stadium-shaped corrals to Heller (then at the University of Washington, now at the Harvard–Smithsonian Center for Astrophysics). "I dropped everything to try to understand the pictures and other data," Heller says.

Heller explains the images in terms of reflecting traveling waves rather than confined eigenstates. He estimates from the data that when an electron wave meets a line of 10-Å-spaced Fe adatoms, about a quarter of the wave is reflected, a quarter is transmitted, and half is scattered into the bulk states. "What's important are the multiple reflections of the waves," he says. Fully quantum simulations of such reflecting waves accurately model the observed data.[5] Heller considers it remarkable that a single assumption—strong s-wave absorption at an adatom—leads to a theory that explains all the data. Thus far, the Fe corrals on Cu(111) are too "leaky" for observation of quantum chaos, but it is possible that a different combination of surface and adatoms will be less of a sieve.

Investigating quantum chaos is just one of the experimental opportunities opened up by the new imaging techniques—every researcher we spoke to had a long list of possibilities. These include studies of the interactions between electrons and adatoms (for example, the Kondo effect), long-range interactions between adatoms, the coupling between surface and bulk electron states at adatoms and at steps, the effects of electron–phonon interactions and other dephasing mechanisms, and the attenuation of an electron wave moving on a defect-free Cu(111) surface. Also, new structures might be built, atom by atom, with applications in nanoelectronics and surface chemistry. "The work of these groups has demonstrated that you can do things that no one dreamed were possible," says Kastner.

—GRAHAM P. COLLINS

References

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