sure. Most stellar reactions occur at low energies and proceed at a pace that is too slow to be measured in the laboratory. Researchers get around the difficulty by measuring the reactions at higher energies, at which the reactions proceed more quickly, and then extrapolating the rates down to stellar energies. That procedure does not work for the oxygen-producing reaction, however. When the carbon and helium nuclei interact, they do not always produce a tightly bound oxygen nucleus immediately; instead, they sometimes first form an oxygen nucleus with loosely bound constituents; this energetically excited state then decays by emitting gamma rays. The intermediate step affects the overall reaction rate and makes the extrapolation unreliable.

Nevertheless, by using a rather complicated argument, physicists can deduce the influence of the loosely bound oxygen state. To treat the state they need to know how it couples to both the $^{12}C + {}^{4}He$ initial state and the $^{16}O + \gamma$ final state. They can measure the latter coupling easily, first by producing the loosely bound oxygen state and then by observing its gamma decay rate. However, the $^{12}C + {}^{4}He$ coupling has long been out of reach. The new experiments use a completely different reaction, the beta decay of nitrogen-16 to oxygen-16, to deduce the missing coupling. Part of the time the beta decay proceeds to the loosely bound oxygen state, yielding $^{12}C + {}^{4}He$ instead of ^{16}O. The energy spectrum of the ^{4}He is thus sensitive to the coupling of the loosely bound oxygen state. The new experiments measured this beta decay reaction. Because the energy of the ^{4}He is so low, the experiments were rather difficult to carry out. Both groups saw the influence of the loosely bound state and interpreted their results in terms of the basic nucleosynthetic reaction. The previously accepted rate for the reaction was 100, measured in units that include effects of the electrostatic repulsion between the nuclei. The new measurements give values in the range of 50–100 units.

Once a star runs out of ^{4}He and can no longer produce ^{16}O, the stage is set for later nucleosynthetic reactions that make heavier elements. If, prior to this time, the $^{12}C + {}^{4}He$ reaction was proceeding slowly, then the heavier elements are formed in a reaction chain that starts from carbon. On the other hand, if the ^{16}O-forming reaction was proceeding quickly, the heavier elements are formed from ^{16}O and at a higher temperature. Depending on these initial conditions, the mix of elements that will be expelled into the cosmos upon the star's explosive death can be quite different. In fact, their production depends so sensitively on the environment that the rate of the reaction $^{12}C + {}^{4}He \rightarrow {}^{16}O + \gamma$ has been inferred from the abundances of different elements observed in the solar system. That analysis yielded a rate of 170 units, which is higher than the new measurements imply. Several uncertainties, however, may reconcile the apparent disagreement. In astrophysics the temperatures depend on somewhat uncertain assumptions about the heat transfer within the star. In nuclear physics additional states with differing quantum numbers might also contribute to the reaction. The additional states would increase the rate, possibly bringing it closer to the number inferred from the elemental abundances.

—George Bertsch and Sharon McGrayne

Condensed-matter physics

Scientists working in the area of atomic manipulation on surfaces scored a major success in 1993. Using the scanning tunneling microscope, they constructed atomic-size enclosures in which they were able to observe quantum confinement directly. Theoretical studies, combined with first-principles calculations, continued to play an important role in condensed-matter physics; the contribution of theory was highlighted by experimental confirmation of the prediction of a new, very hard solid. The changing world order produced a benefit in the form of increased availability of pure, stable isotopes from separation facilities in the former Soviet Union. As a result, isotopically controlled crystals were being grown that enabled a variety of elegant and exciting experiments. Researchers also reported incremental advances in so-called high-temperature superconductivity.

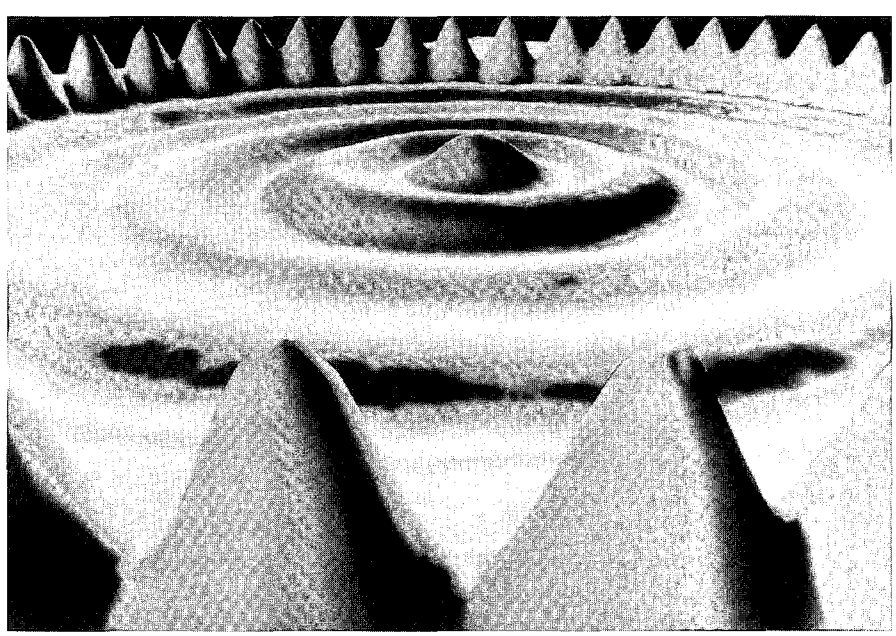
Quantum corrals. The scanning tunneling microscope (STM), invented by Gerd Binnig and Heinrich Rohrer at the IBM Zürich (Switz.) Research Laboratory in the early 1980s, already has had a tremendous impact on surface science. The instrument allows researchers to image the surface of conducting materials with atomic-scale resolution; in addition, the STM can be used for spectroscopy, probing the electronic structure of the surface on an atomic scale. These unprecedented achievements have been accomplished with an instrument that is, in essence, quite simple. It consists of a metal probe ending in a very sharp (atomic-size) tip; the tip is scanned over the surface of the sample by means of piezoelectric controls. A voltage is applied between tip and surface, and even though the tip is not in contact with the surface, a current flows because of the quantum-mechanical tunneling effect. The tip-surface separation is less than a nanometer (nm; a billionth of a meter); typical atoms are a few tenths of a nanometer in size. A feedback loop keeps the current constant while scanning, which usually translates into keeping the tip at a constant distance above the surface. Measuring the displacement perpendicular to the surface produces a map of the trajectory of the tip, reflecting both the topography and the electronic structure of the surface.

Recently surface scientists began to use the STM not just to analyze the surface but also to synthesize new structures. By setting the correct current and voltage conditions, one can select an individual atom that is absorbed on the surface, move it around, and place it in a specific location. Donald M. Eigler and co-workers at the IBM Almaden Research Center, San Jose, Calif., pioneered the technique in 1990, manipulating xenon atoms on a nickel surface. (See *1992 Yearbook of Science and the Future* Year in Review: PHYSICS: *General developments.*) In 1993 Eigler, Michael F. Crommie, and Christopher P. Lutz at the Almaden laboratory reported another breakthrough; they demonstrated that iron atoms can be manipulated and placed in specific locations on a copper surface. The whole operation had to be performed at very low temperature, requiring cooling by liquid helium at four degrees above absolute zero, in order to limit thermal motion of the atoms. One of the structures that the researchers constructed was a circle with a diameter of 14.3 nm. The same STM tip that was used to position the atoms was then scanned over the surface to obtain a picture of the location of the atoms. In addition, the STM provided information about the electronic wave functions on the surface.

Quantum mechanics predicts that a particle enclosed in a "box" of small dimensions exhibits quantized behavior. The energy of the particle can assume only discrete values, determined by the dimensions of the box. In addition, the probability of finding the particle in a certain location is not uniform throughout the box but oscillates in space. This behavior is related to particle-wave duality; the particle can be represented by a quantum-mechanical wave, which is reflected at the edges of the box, leading to interference and the formation of a standing-wave pattern. The amplitude of the wave corresponds to the probability of finding the particle in that location. In order for the interference effects to be produced, the size of the box should be comparable to the wavelength of the waves that correspond to elementary particles (electrons in the case of the IBM experiment), which is on the order of nanometers. The box in question actually need not be a three-dimensional object; a two-dimensional shape can be used to confine a particle in a plane. Nor does the box have to be rectangular; a circle works just as well, although the details of the interference pattern depend on the shape and size.

The circle of iron atoms constructed by Eigler and co-workers actually serves as a box in which electrons moving on the copper surface can be trapped. Tunneling spectroscopy indeed revealed the existence of discrete energies, consistent with quantization. The STM, however, made it possible to resolve the quantum states spatially as well as spectroscopically for the first time. The interference pattern produced by the electron wave corresponds to a variation in the local electron density, which is measurable with the STM. Ripples in the electron density indeed were observed, and they corresponded accurately to the quantum-mechanical predictions. The authors of the work referred to their circular enclosure for electrons as a "quantum corral."

The significance of the work goes far beyond the verification and elegant illustration of basic quantum mechanics. For instance, it now is feasible to



A quantum corral made of 48 iron atoms adsorbed on a copper surface encloses ripples in the local density of states of the surface electrons. The iron atoms were positioned with a scanning tunneling microscope (STM); the same STM was then used to make the image. The corral is about 14.3 nm in diameter, and the ripples closely match the quantum-mechanical predictions for a particle in a circular box.

M F Crommie, C P Lutz, and D M. Eigler, IBM Research Division, Almaden Research Center

study the properties of confined electrons in boxes with complicated shapes, such as polygons or stadia. Stadium-shaped boxes have attracted particular attention since they are known to lead to chaotic behavior. One also envisions studying the interaction of surface-state electrons with adsorbed atoms or molecules or with surface defects. Eigler and co-workers, for example, observed oscillations in the electron density in the neighborhood of point defects (associated with impurity atoms) and around step edges (which occur at the boundaries of terraces on the surface). In many respects the quantum corrals indicate that the vision of physicist Richard Feynman, outlined in 1959, has been realized—an era in which "the problems of chemistry and biology can be greatly helped if our ability to see what we are doing, and to do things on an atomic level, is ultimately developed."

New materials by design. First-principles calculations have made significant contributions to condensed-matter physics and materials science. *First principles* refers to the feature that no input from experiment enters the computations; only the atomic numbers and mass numbers of the atoms in the system are required. The computational approach then solves the quantum-mechanical equations for the system, producing information about the exact location of the atoms and the electronic wave functions, from which various properties of the system can be derived. The development of new algorithms and the availability of larger computing resources have enabled investigations of systems of increasing size and degree of complexity.

The role of first-principles calculations has often been a supporting one. When experimental observations indicated novel or unexpected behavior or properties, computations subsequently provided consistent and comprehensive explanations. Recently, however, computational physics has assumed a more active role by actually predicting new materials with useful properties. A prime example is supplied by the work of Marvin Cohen of the University of California at Berkeley.

Cohen originally developed an empirical model for the bulk modulus of covalent solids. In the absence of defects in the crystal structure, the bulk modulus determines the hardness of the solid. In turn, the bulk modulus depends on the nature of the chemical bonding. It was found that two properties are needed to achieve a large bulk modulus: low ionicity and short bond length. (The ionicity of a material increases with increasing difference in electronegativity between the constituent elements.) Both properties are present in diamond, which has the largest bulk modulus and is the hardest known solid. On the basis of the empirical model, however, it was suggested that a covalent solid formed of atoms of carbon (C) and nitrogen (N) could have a larger bulk modulus than that of diamond, which is all carbon. The proposal was put on a stronger footing when Cohen and Amy Liu carried out first-principles calculations for a hypothetical covalent C-N solid, modeled after the known β-Si_3N_4 (silicon nitride) structure. The calculations showed that β-C_3N_4 is at least a metastable structure, with a moderately large cohesive energy and a bulk modulus comparable to that of diamond.

Stimulated by this prediction, Chumming Niu, Yuan Z. Lu, and Charles M. Lieber of Harvard University synthesized the material and verified the prediction about the hardness. Fragments from pulsed laser ablation of high-purity graphite and a beam of atomic nitrogen were used to form C-N films on a substrate. Electron diffraction data indicated the presence of β-C_3N_4 crystallites in the films, while photoelectron spectroscopy revealed that the C-N bond is covalent with relatively little charge transfer, in agreement with the theoretical predictions. While the bulk modulus and hardness of β-C_3N_4 remained to be measured, Niu and co-workers stated that their C-N films are "thermally robust and hard." The confirmation of theory implied by the experiments indicates that it is possible to use theory to design materials with predictable properties.

Isotopically controlled semiconductors. The elements in the periodic table are characterized by their atomic number, corresponding to the number of protons in the nucleus. For a given number of protons, the number of neutrons may vary, giving rise to isotopes with different masses. For instance, germanium (Ge), which has an atomic number of 32, has five stable isotopes: ^{70}Ge (20.5%), ^{72}Ge (27.4%), ^{73}Ge (7.8%), ^{74}Ge (36.5%), and ^{76}Ge (7.8%); the natural abundance of each isotope is indicated in parentheses. A germanium crystal would normally include a mixture of all these isotopes, in accordance with their natural abundance. Those properties of a solid that depend on the atomic mass therefore actually reflect some sort of average over these masses.

The advantages of being able to control the isotopic composition of a semiconductor have been known for some time. One example is the study of local vibrational modes (LVMs). When a light impurity is introduced in a semiconductor, vibrational modes appear that are localized on the impurity and that have specific frequencies, similar to molecular vibrations. Substituting with a different isotope of impurity atom leads to a predictable shift (inversely proportional to the mass of the impurity atoms) in the vibrational frequency and hence aids in the identification of the impurity. Isotope separation has traditionally been cumbersome and expensive, severely restricting the type and number of experiments that could be performed. Recently, however, isotopes for

various elements became more readily available owing to the opening of markets in the former Soviet Union. Eugene Haller and co-workers at the University of California at Berkeley took advantage of this opportunity to grow isotopically controlled crystals (mostly germanium), which in turn allowed unprecedented experiments.

One type of investigation concerns the LVMs mentioned above but involves substituting different isotopes for the host atoms. The masses of the atoms surrounding the impurity atom affect the vibrational frequency. With host crystals made of isotopes occurring in their natural abundance, a large number of peaks in the vibrational spectrum may be produced. On the other hand, isotopically controlled crystals offer a tremendous simplification of the spectrum, allowing a detailed understanding of the origin of lines and a more straightforward identification of the location of the impurity in the crystal lattice.

The dependence of vibrational properties on atomic masses also affects the vibrational spectrum of the semiconductor; a group led by Manuel Cardona at the Max Planck Institute, Stuttgart, Germany, has been particularly active in this area. Various theoretical models, such as the coherent-potential approximation, have been used to take the distribution of atomic masses into account. The availability of isotopically controlled crystals now offers sensitive tests for such models. In germanium the mass differences are not large enough to produce localized modes, but resonances appear in the vibrational spectrum owing to the presence of specific isotopes.

Isotopic control can be applied not only to bulk solids but also to superlattice structures, artificial structures made of carefully controlled layers of atoms in which the atomic mass is varied from layer to layer. The periodic modulations of the isotopic mass in short-period superlattices can be used to investigate the vibrational properties of the bulk materials as well as the properties of the new, artificial structure. Such superlattices also allow the study of atomic motion through isotope disordering.

Isotopic control also leads to improved applications of neutron transmutation doping (NTD), a technique in which a semiconductor is bombarded with neutrons. Upon capturing a neutron, a nucleus may turn into another stable isotope of the same element or may be converted to another element, which can act as a dopant; *i.e.,* an impurity that modifies the electrical characteristics of the semiconductor. The technique produces an extremely homogeneous dopant distribution, which is important for applications such as radiation detectors or high-power rectifiers. Combining NTD with the ability to grow isotope superlattices enables the realization of novel device structures with sharp boundaries between different regions.

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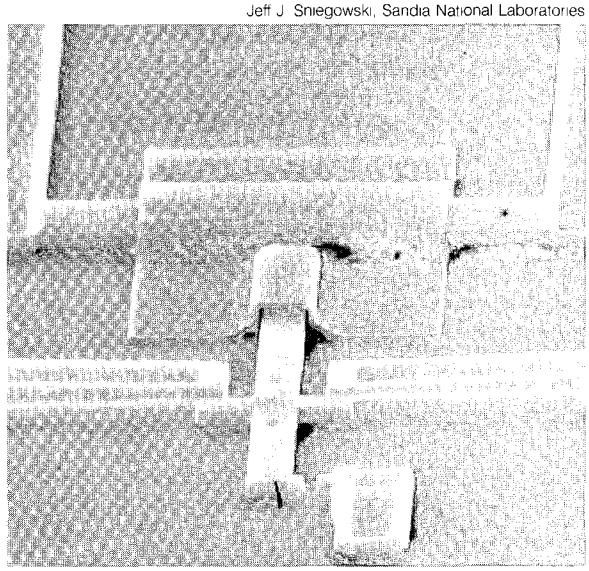

A microscopic steam engine built by physicists at Sandia National Laboratories, Albuquerque, N.M., is small enough to reside on a computer chip yet powerful enough to do useful work. Only micrometers in size, the engine consists of a piston that slides in and out of a silicon sleeve, propelled by a bubble of water vapor that expands on heating.

The availability of isotopes thus offers a wide range of scientific and technical opportunities. The increasing number of experiments carried out on "isotopically engineered" samples will continue to elucidate basic mechanisms as well as new physics.

High-temperature superconductivity. The record for the highest critical temperature in a superconductor, that is, the temperature below which the material loses all resistance to the flow of electricity, had been held by a thallium-bearing ceramic compound since 1988. That figure, 127 K (kelvins), was broken when a group from the Swiss Federal Institute of Technology, Zürich, reported a superconducting transition above 130 K in a compound of mercury, barium, calcium, copper, and oxygen. (To convert kelvins to degrees Celsius, subtract 273; thus, 127 K = −146° C. To convert Celsius to Fahrenheit, multiply by 1.8 and add 32.) In addition, the mercury-bearing material exhibits more favorable behavior in a magnetic field, and because of its simple structure it may offer some clues to the mechanism of superconductivity in the copper oxide ceramics, a consistent theoretical description of which is still lacking. A less firmly established result came from a group at the National Center for Scientific Research in Paris, who reported evidence for superconductivity at 250 K in a film containing copper and oxygen and built up layer by layer. Significantly more work will be needed to confirm this observation. (*See* Year in Review: CHEMISTRY: *Inorganic chemistry.*)

—Chris G. Van de Walle