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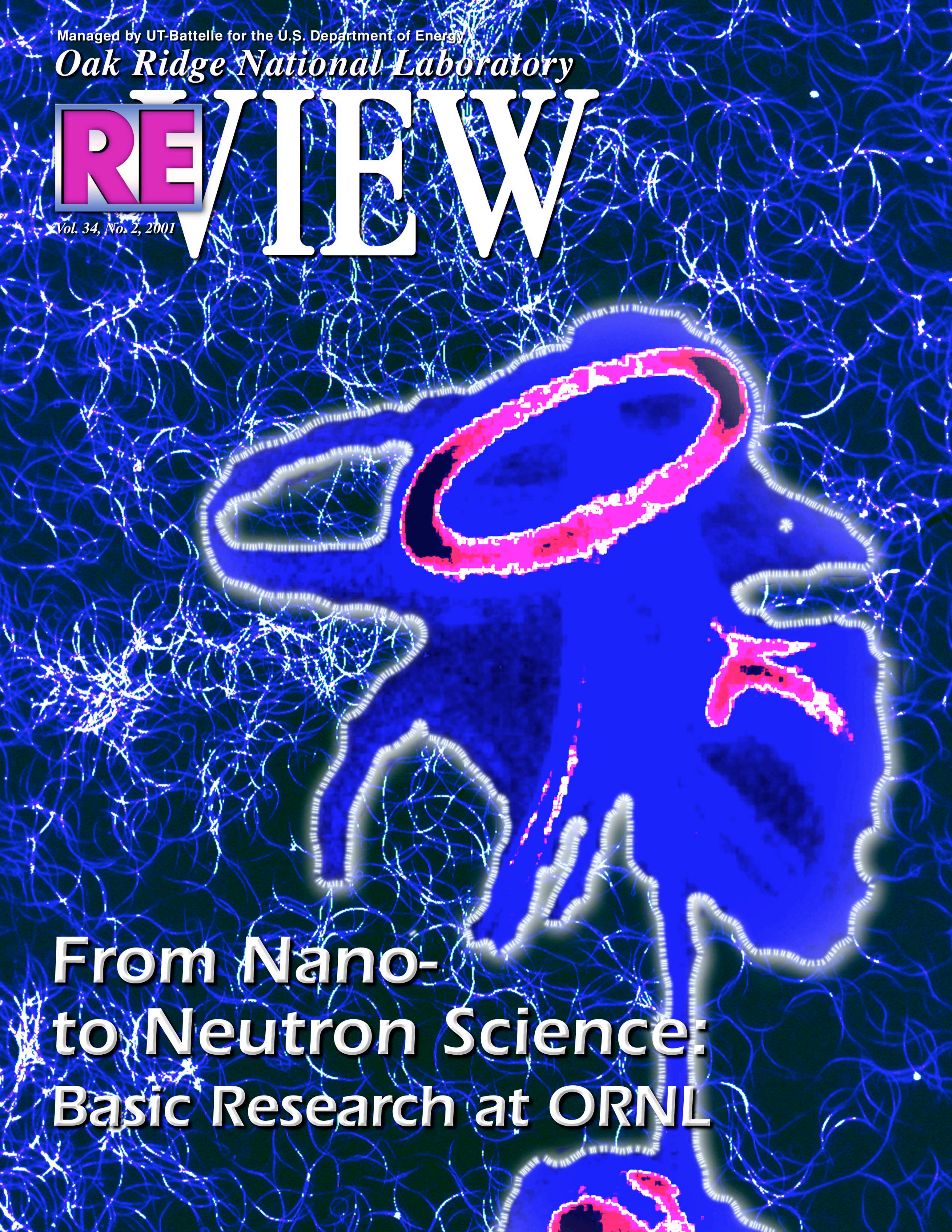
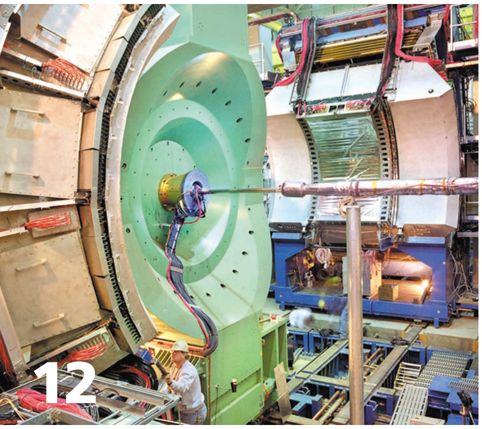
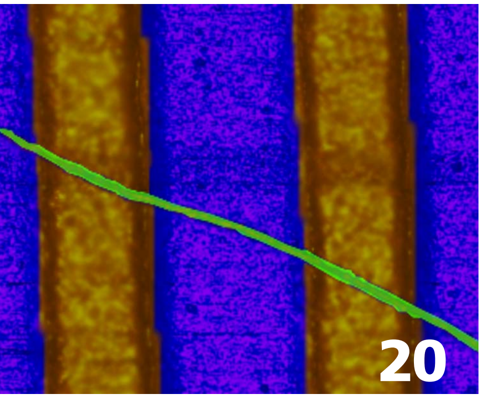
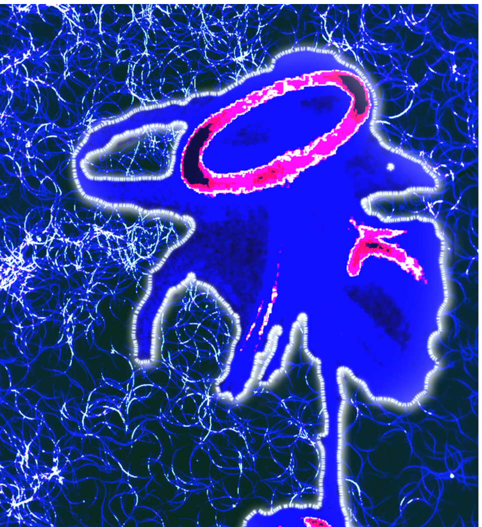


From Nano- to Neutron Science: Basic Research at ORNL







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Features

This issue provides highlights of basic research at ORNL, including research on producing, characterizing, and finding applications for carbon nanotubes produced at ORNL by several techniques. The cover shows single-wall carbon nanotubes created by laser vaporization (note pink laser plume), which were then chemically purified and spray-deposited onto a substrate. The image above the cover image shows a carbon nanotube on electrodes, a possible nanoscale replacement for today's microscale silicon transistors. See pp. 20-21 for a description of this and other nanoscale research. Images by Jason Fowlkes, Derek Austin, and Henrik Schittenhelm.

REVIEW

Editor and writer—Carolyn Krause
Assistant editor—Deborah Barnes
Editorial Board—Lee Riedinger (chair),
Fred Bertrand, Eli Greenbaum,
Russ Knapp, Reinhold Mann,
Stan Milora, Thomas Zacharia
Designer and illustrator—Jane Parrott
Photographer—Curtis Boles

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Editorial office address:
Building 4500-North, M.S. 6266,
Oak Ridge, TN 37831-2008
Telephone: (865) 574-7183;
FAX: (865) 241-6776;
Electronic mail: krausech@ornl.gov
ORNL *Review* Web address:
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Oak Ridge National Laboratory is a multiprogram, multipurpose laboratory that conducts research in energy production and end-use technologies; biological and environmental science and technology; advanced materials synthesis, processing, and characterization; and the physical sciences, including neutron-based science and technology.

Basic Research at ORNL: A Distinguished Past, An Exciting Future


Lee Riedinger


Jim Roberto

ORNL has a time-honored tradition of basic research accomplishments in physics, chemistry, biology, and the materials sciences. In 1951 ORNL researchers were the first to confirm that a neutron decays into a proton, electron, and electron antineutrino. ORNL biologists discovered the function of messenger RNA and the chromosomal basis for sex determination in mammals. This year the Department of Energy recognized three ORNL discoveries as among the top 23 of DOE national laboratories' scientific accomplishments. They are nickel and iron aluminides for high-temperature applications, ion beam techniques for making longer-lasting artificial hips and knees, and the Z-contrast electron microscopy technique, which produced the most detailed image of a crystal structure ever recorded in a microscope.

In December 2000, an ORNL physical chemist, the late Sheldon Datz, received DOE's prestigious Enrico Fermi Award for pioneering the use of crossed molecular beams to study the details of chemical reactions and for demonstrating ion channeling, in which charged atoms pass between a thin crystal's rows of atoms. (See p. 26.)

Our basic research tradition continues today, thanks largely to support from DOE's Office of Science. Much of the research, described in this issue, deals in a big way with very small features of matter ranging from quarks, electrons, photons, neutrons, and heavy ions to DNA and carbon nanotubes.

By studying the properties of short-lived nuclei and searching for rare isotopes, using the Holifield Radioactive Ion Beam Facility, ORNL nuclear physicists are gaining a better understanding of the origin of the elements and the mechanism of energy generation in stars. ORNL physicists and electronics experts have played a major role in developing electron and photon detectors and electronic components, to help search for evidence that the universe's beginning has been mimicked in DOE's Relativistic Heavy Ion Collider.

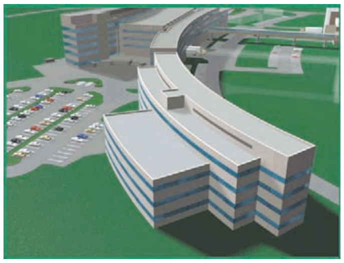
ORNL is well positioned to become the world's leading center in neutron science with the completion of our upgraded High Flux Isotope Reactor (HFIR) in 2003 and the Spallation Neutron Source (SNS) in 2006. Using neutron scattering at HFIR and elsewhere, ORNL researchers recently found evidence to support a leading theory for explaining high-temperature superconductivity. Neutron data from another ORNL neutron source, the Oak Ridge Electron Linear Accelerator, is helping computational astrophysicists improve their understanding of nuclear processes by which isotopes are synthesized in stars. The SNS may also be used for this purpose.

The SNS will enable advances in characterizing nanoscale materials, such as triblock copolymers. In other nanoscience efforts at ORNL, we are working toward fabricating nanofluidic lab-on-a-chip devices, conducting experiments with them, and predicting fluid behavior in them, as well. We are devising innovative ways to trick nanoscale bits of matter into assembling themselves into useful products, such as artificial membranes and electronic components. An ORNL team is designing a quantum-dot array that can be operated at room temperature to carry out innovative computations.

As disk drives and transistors are further downsized, today's materials will eventually reach limits in performance. We are addressing these issues through experimentation and computer simulation.

DOE's Office of Basic Energy Sciences has recommended construction funding in fiscal-year 2003 for a proposed Center for Nanophase Materials Sciences at the SNS. If Congress approves, the new center will integrate nanoscience research with our unique combination of capabilities in neutron scattering, synthesis of new materials, and theory and simulation, using supercomputers at DOE's Center for Computational Sciences at ORNL.

Among its many uses, the Lab's IBM supercomputer is being used to simulate a fusion heating and plasma control method involving radio waves, as well as to model a future fusion device that may be built here in a few years. This basic research is essential to developing fusion as a future energy source. To help make fossil fuel, nuclear, and geothermal energy sources more economical for producing power, our geochemists are performing important basic research.


Rendering by John Jordan

Artist's conception of the proposed Nanophase Materials Science Center.

In computer science, we perform basic research to enable computational researchers to get better results faster. Recently, an ORNL algorithm was shown to reduce and predict delays in data delivery over the Internet.

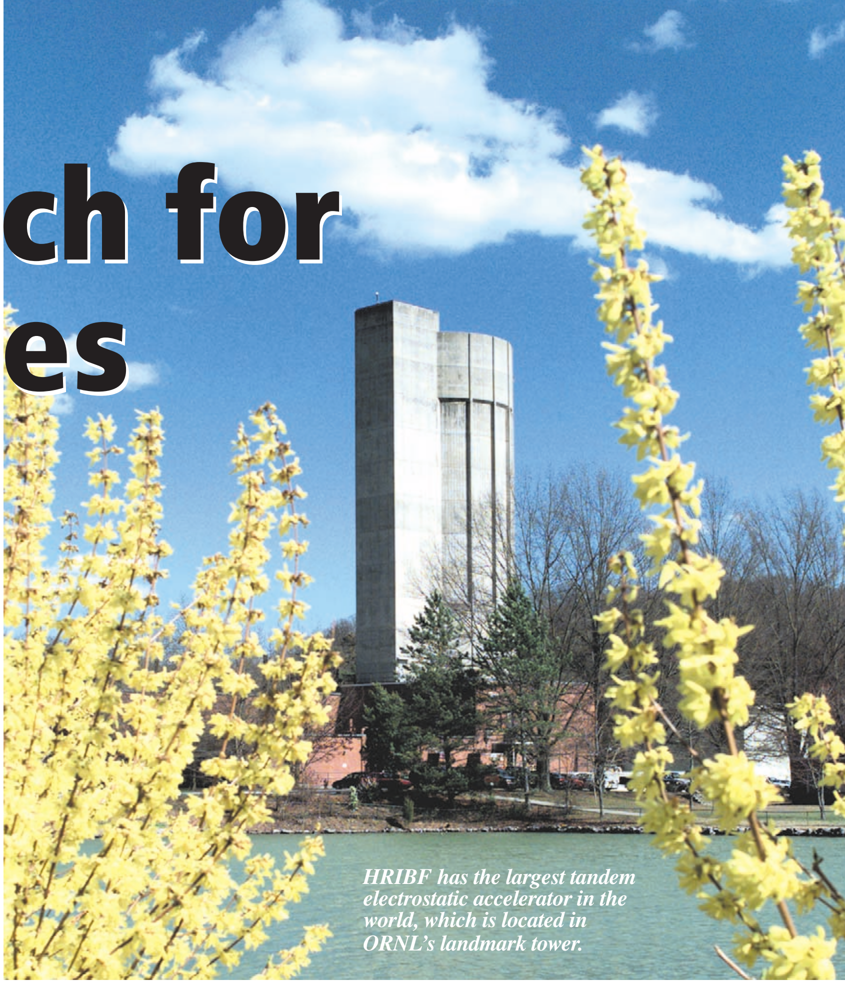
In the biological area, ORNL received a 2001 R&D 100 Award for its protein structure prediction tool. ORNL basic research involving mice and their DNA may shed light on why some humans are more susceptible than others to getting cancer after exposure to low doses of radiation or environmental chemicals. Research being conducted at ORNL and the University of Southern California suggests that a spinach protein might someday restore sight to the legally blind.

Basic research has been a pillar of our work. As ORNL gets new facilities this decade for neutron science, computer science, nanoscience, and biology, an even brighter future is in store for fundamental research at the Laboratory.

Lee J. Riedinger – Deputy Director for Science and Technology
James B. Roberto – Associate Laboratory Director for Physical Sciences

ORNL's Search for Rare Isotopes

ORNL researchers are taking advantage of HRIBF's special ability to make neutron-rich beams to allow studies of highly unstable nuclei not found on the earth. These studies may allow them to better understand the nature of nucleonic matter and the origin of elements in the cosmos.



HRIBF has the largest tandem electrostatic accelerator in the world, which is located in ORNL's landmark tower.

Jim Richmond

Our earth is home to 81 stable elements, including slightly fewer than 300 stable isotopes. Several other elements (e.g., thorium and uranium) and more than 130 unstable isotopes also exist on the earth, but all of them eventually decay. That is, the atomic nuclei of these isotopes eventually capture or emit electrons, positrons, or alpha particles, or they undergo spontaneous fission, making the isotopes radioactive. Many radioactive isotopes are quite useful in the diagnosis or treatment of diseases, biological and environmental studies, archeology, national security, and energy generation.

Each unstable isotope is characterized by its half-life—the time it takes for half of the sample to decay. Isotope half-lives range from less than a thousandth of a second to billions of years. Short-lived isotopes cannot be found naturally on the earth because they have long since decayed in that our planet was formed about 4 billion years ago. Yet, thousands of short-lived isotopes are continually created in the cosmos. Their existence may be fleeting, but they play a crucial role in the ongoing formation of the elements in the universe. In fact, synthesis of heavy elements involves unstable nuclei at every stage.

The properties of most rare isotopes are unknown and can be only inferred, with considerable uncertainty, from theoretical calculations. Nevertheless, at several laboratories around the world, including the Department of Energy's Holifield Radioactive Ion Beam Facility (HRIBF) at ORNL, it is possible to produce beams of some rapidly de-

ORNL Theorists and the Nuclear Shell Model

In 1997 ORNL physicist David Dean received the Presidential Early Career Award for Scientists and Engineers for his leadership role in developing the Quantum Shell Model Monte Carlo technique for solving the nuclear many-body problem. He performed this work with Steve Koonin and collaborators at the California Institute of Technology and has continued developing the technique during his time at ORNL. The techniques are particularly well suited to investigating thermal properties of nuclei such as phase transitions and critical temperature phenomena that can be induced by bombarding a nucleus with projectile ions and other particles.

The idea of independent neutrons and protons that make up a nucleus moving in a common potential, an attractive force created by the self-interaction of the nucleons that binds them into a nucleus, is central to the description of atoms, metals, and hadrons. It is also realized in nuclei and was first put on a firm theoretical basis in 1949 by Maria Goeppert-Mayer and Hans Jensen, who later shared a Nobel Prize for their work.

In contrast to other quantal systems cited above, the residual interaction between the protons and neutrons in a nucleus is strong and severely perturbs the naive picture of the nucleus as a collection of independent particles. This interaction mixes together many different independent-particle configurations, generating phenomena such as superfluidity (pairing), deformation (non-spherical ground-state shapes), and collective rotations and vibrations (where many neutrons and protons are involved in the motion) that are common properties of nuclei.

In the 1960s scientists developed one of the first shell model codes to solve the nuclear structure problem by diagonalization. This work—carried out by Bruce French (University of Rochester) and by Cheuk-Yin Wong, Joe McGrory, and Edith Halbert (all from ORNL), among others—was seminal in providing an understanding of nuclei with up to 30 nucleons (neutrons and protons). With advancing computational technology, a second generation of shell model codes was developed in the late 1970s and 1980s, using ideas of the U.K. theorist John Whitehead.

Currently, a Joint Institute for Heavy Ion Research postdoctoral fellow, Andrius Juodagalvis (from Lithuania), is working with Dean to develop a parallel implementation of the Whitehead scheme on modern parallel supercomputers.

Quantum Monte Carlo methods (pursued by Dean and collaborators) solve this same problem with path-integral techniques and are used to investigate both the ground-state and thermal properties of nuclei. These methods are based on a quantum Monte Carlo integration technique. This technique allows for the integration of very large, multidimensional integrals that naturally arise in the nuclear structure problem. The methods are also applied to other areas of science where the particles involved are quantum-mechanically strongly correlated. The differing approaches are complementary and, thus, allow a more complete picture of the nucleus to emerge.

Shell model diagonalization has recently been used to understand the structure of nickel-56 (^{56}Ni). This nucleus has 28 neutrons and 28 protons, so it is a doubly magic nucleus. In 2000 an ORNL/UT experimental group led by Cyrus Baktash—along with Dean, Witek Nazarewicz, and collaborators—published a scientific paper on ^{56}Ni entitled "Rotational Bands in the Doubly Magic Nucleus ^{56}Ni" in the 82nd volume of *Physical Review Letters* (1999). The paper won a Technical Achievement Award from UT-Battelle in 2000.

According to Dean, the nuclear shell model indicated both a spherical ground-state band and a highly deformed rotational band at higher excitation energies

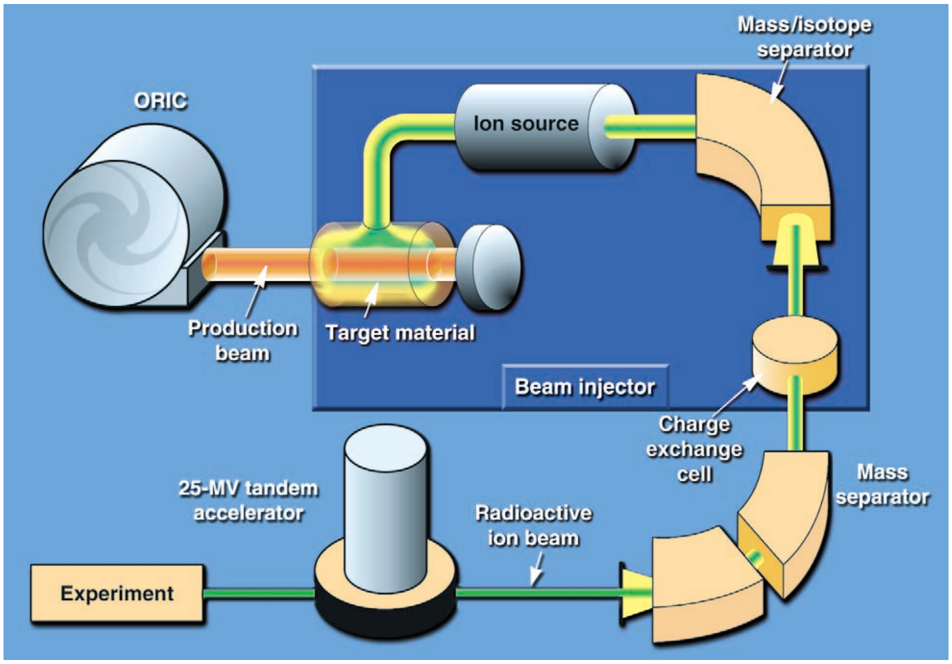


Illustration enhanced by LeJean Hardin

The Holifield Radioactive Ion Beam Facility (HRIBF) is an international user facility that produces beams of short-lived, unstable nuclei for research in nuclear structure physics and nuclear astrophysics. A production beam (e.g., hydrogen nuclei) from the Oak Ridge Isochronous Cyclotron (ORIC) strikes target material. Reaction products diffuse out of the target and into the positive ion source where they are ionized. The positively charged ions may be several different isotopes and atomic species, so they are separated in the mass/isotope separator. The ions are then converted to negatively charged ions in the charge exchange cell so they can be accelerated . The mass separator filters out the desired isotope for the radioactive ion beam, which is accelerated by the 25-MV tandem accelerator in the Holifield tower for use in experiments.

caying, rare-isotope nuclei that can be used to study properties of nuclei that are difficult to access.

NATURE OF THE NUCLEUS

The nucleus is the core of the atom, containing more than 99.9% of the atom's mass. Nuclei are composed of protons and neutrons, together called nucleons. The attractive force between nucleons is responsible for holding them together to form a nucleus. However, this force is to some extent counterbalanced by the electrostatic repulsion between the protons, which are positively charged. The binding energy that results from the combination of these forces determines the stability of nuclei—that is, which combinations of protons and neutrons are stable, which are not, and how unstable nuclei decay. One of the greatest challenges in nuclear physics is to understand the boundaries of nuclear existence, which are commonly depicted on a nuclear chart. (See nuclear chart and its caption on p. 4.)

One of the most recognized nuclear physics theorists in the United States is Witek Nazarewicz, a University of Tennessee physics professor and the deputy director for science at HRIBF. According to Nazarewicz, neutron-rich nuclei pose many fascinating questions. They have a "neutron skin" consisting of numerous neutrons with a greater radius than that of bound neutrons deep within the nucleus. The question of how many neutrons are too many for a given isotope is one of great interest to nuclear physicists. They talk about the "neutron drip line" beyond which the nucleus cannot exist as a bound system. If one neutron too many is added to a nucleus, a neutron will "drip out." It's similar to what happens when water is added with a medicine dropper to a full cup of water; one drop will cause the water to spill over, or drip out of, the cup.

"Our challenge is to find out where the drip line is for each neutron-rich nuclide," says Nazarewicz. "Knowing the drip line will help us better understand how well neutrons are bound to protons in a nuclear cluster—that is, the limits of nuclear existence for a given element. Helium-5 doesn't exist. If you add a neutron to helium-4, it flies away, but you can make helium-8. We know the limits of nuclear existence up to oxygen. It is possible to make oxygen-24, but not oxygen-25 or oxygen-26. Many more experiments are needed to find the limits of nuclear existence for heavier elements. It won't be easy."

and experimental and theoretical results agreed. At the time, these calculations were among the largest performed using the shell model diagonalization approach.

HRIBF offers physicists a unique capability for understanding both nuclear structure and certain astrophysical phenomena, using similar experimental techniques (see main story and other sidebar).

"We are using our quantum Monte Carlo techniques developed for nuclear structure studies to understand the microphysics of supernova explosions and other astrophysical phenomena," Dean says.

For example, electron capture on iron-group nuclei plays a key role in determining energy release and subsequent element production in supernova explosions. Understanding the underlying nuclear structure turns out to be quite important in obtaining reliable electron capture rates.

"Through electron capture by a nucleus, a proton can become a neutron, producing a more neutron-rich nucleus," Dean explains. "What happens is that an electron is absorbed onto a nucleus where it reacts with a proton to produce a neutron and neutrino. Emitted neutrinos can drive the supernova explosion and aid in the synthesis of elements. With our current shell-model technologies, we are modeling various aspects of these nuclear reactions."

Dean and his colleagues run the Quantum Shell Model Monte Carlo codes at the Department of Energy's National Energy Research Supercomputing Center in Berkeley, California, and on the IBM supercomputer at DOE's Center for Computational Sciences at ORNL. They recently received funding from DOE's Scientific Discovery through Advanced Computing (SciDAC) program to continue to develop the new parallel shell model diagonalization codes and quantum Monte Carlo algorithms.

These researchers have contributed to the theoretical understanding of the structure of the atomic nucleus and the microphysics of exploding stars.

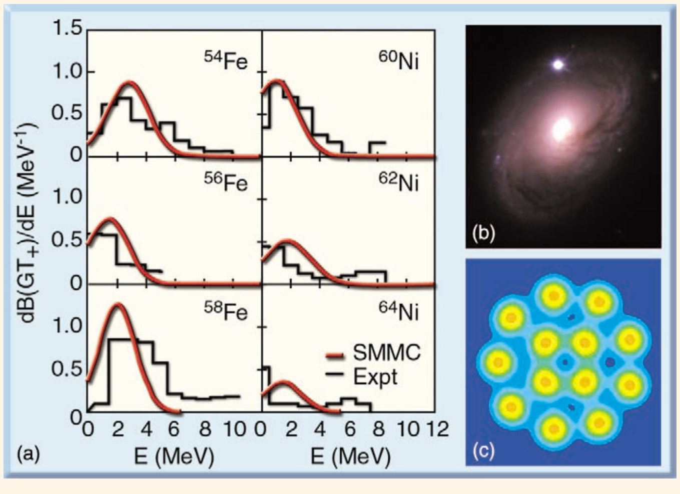


Illustration enhanced by LeJean Hardin

Understanding the nucleus and its interactions with other particles requires significant interplay between experimental and theoretical efforts. Shown are results of Shell Model Monte Carlo calculations of Gamow-Teller excitations within various iron-group nuclei compared to experiment (a). Low-energy electrons cause this excitation through their weak interaction with nucleons in the nucleus. The quality of these results required a significant investment in computational algorithm development and computer time. They have influenced our understanding of element production in supernovae. The bright dot at the top of the galaxy M98 is the supernova SN1997bu (b). Many of the tools of nuclear theory are common to other quantum-mechanical, many-body systems (clusters, quantum dots, atoms) in which the interacting particles are highly correlated (c).

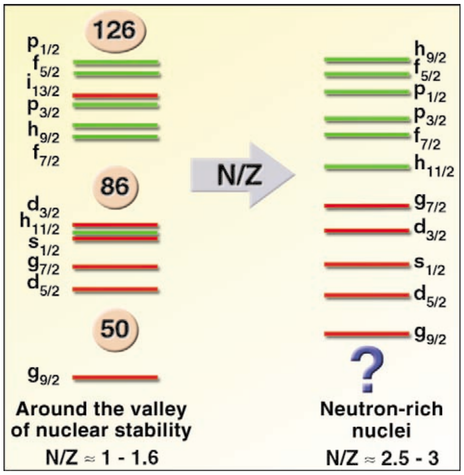


Illustration enhanced by LeJean Hardin

The cornerstone of nuclear structure for over half a century has been the shell model, in which each nucleon (neutron or proton) is assumed to move in average potential generated by its interactions with all of the other nucleons. This potential leads to the prediction that the quantum levels in a nucleus form shells within which nucleons reside. This picture of nucleon motion explains a host of phenomena, such as the existence of particularly stable "magic" nuclei corresponding to completely filled shells (corresponding to particle numbers 2, 8, 20, 28, 50, 82, and 126). The left-hand-side diagram shows the shell structure characteristic of nuclei close to the valley of stability. The right-hand-side diagram shows schematically the shell structure predicted in drip-line nuclei, which corresponds to a more uniform distribution of energy levels and the quenching of magic gaps. Radioactive ion beam facilities such as HRIBF offer unparalleled access to exotic nuclei where such predictions can be tested.

Nazarewicz cites the difficulty of finding the limit of nuclear existence for polonium, which has several neutron-rich isotopes (e.g., polonium-210 has 84 protons and 126 neutrons and has a lifetime of 138 days). "Polonium-218 was studied by Ernest Rutherford back in 1904," he says. "It took 94 years for scientists to find a way to add one neutron to polonium-218 to get polonium-219 and then 2 neutrons to make polonium-220. The work was done in 1998 in Darmstadt, Germany."

Are the basic properties of very neutron-rich nuclei much different from those of nuclei closer to the valley of stability that have been studied? According to Nazarewicz and his collaborators, who have performed some of the most important calculations in this field, the answer is, "Yes." Nuclei close to the drip line provide us with a new form of nuclear matter—something that resembles a dilute neutron gas with many new properties. One of the most tantalizing predictions is that the shell-like structure of atomic nuclei, introduced more than 50 years ago by Maria Goeppert-Mayer and Hans Jensen, may alter dramatically as we approach the neutron drip line. That is, the magic numbers* that by and large determine nuclear properties as we know them may be washed out or rearranged. (See sidebar on nuclear shell structure on pp. 2-3.) However, these predictions are based on experimental information obtained from nuclei that are not too far from stability. They need to be validated by studying unstable nuclei that are located much farther out. Understanding of these far-from-stability nuclei is also the key to understanding nuclear synthesis in the cosmos and origin of the elements.

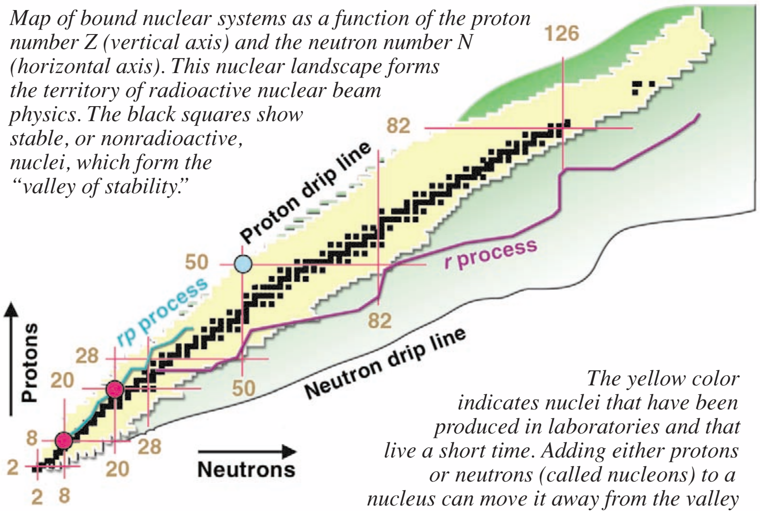


Illustration enhanced by LeJean Hardin

Map of bound nuclear systems as a function of the proton number Z (vertical axis) and the neutron number N (horizontal axis). This nuclear landscape forms the territory of radioactive nuclear beam physics. The black squares show stable, or nonradioactive, nuclei, which form the "valley of stability." The yellow color indicates nuclei that have been produced in laboratories and that live a short time. Adding either protons or neutrons (called nucleons) to a nucleus can move it away from the valley of stability, allowing it to reach the "drip line," where nuclear binding ends because the forces between neutrons and protons are no longer strong enough to hold these particles together. The nuclei beyond the drip lines are unbound to nucleon emission. Many thousands of exotic radioactive nuclei with very small or very large neutron-proton (N/Z) ratios are yet to be explored. In the (Z,N) landscape, they form the "terra incognita" indicated in green. The lines of astrophysics r and rp processes, which are responsible for the production of heavy elements in stars, are indicated. The red lines show the magic numbers known around the valley of stability. However, because the structure of nuclei is expected to change significantly as drip lines are approached, it is not known how the nuclear shell structure evolves at the extreme N/Z ratios. The doubly magic radioactive nuclei—neutron-poor tin-100 (50 protons and 50 neutrons) and neutron-rich tin-132 (50 protons and 82 neutrons)—are indicated by the red dots. Research at HRIBF addresses these unknowns.

Curtis Boles

David Radford adjusts a gamma-ray detector at HRIBF.

These experiments, however, are not easy; many of the most interesting nuclei cannot be produced from reactions involving beams of stable nuclei. Therefore, several nuclear physics laboratories around the world have developed, or are developing, new capabilities to produce beams of unstable nuclei that would extend their reach. HRIBF is the pioneering U.S. facility for producing and accelerating radioactive ion beams (RIBs) for nuclear physics and nuclear astrophysics studies.

THE BEAM IS THE TARGET

In the 1980s, the late Paul Stelson, former director of the Physics Division, led experiments at the Holifield Heavy Ion Research Facility in which uranium targets were bombarded with protons and alpha particles. Through these early Coulomb excitation experiments, they inferred that the uranium-238 nucleus is shaped like a diamond. Nearly 20 years later, ORNL researchers began producing neutron-rich radioactive ion beams by bombarding a uranium-238 (^{238}U) target with 40-million-electron-volt (MeV) protons from the Oak Ridge Isochronous Cyclotron (ORIC) and then extracting the fission-fragment nuclei out of the ion source to make beams. (See sidebar on p. 5 for more details.) This technique is referred to as isotope separation on-line (ISOL).

"We get more than 100 different RIBs from a three-dimensional matrix of carbon fibers with a thin layer of uranium carbide on the fiber surface," says Jim Beene, director of HRIBF. "These beams include atomic species ranging from gallium to lanthanum. The trick is to capture the fission fragments diffusing out of the target and to make them into an accelerated beam (which may be as weak as 1000 nuclei per second) before they decay."

(continued on p. 6)

** In the nuclear shell model, the constituent nucleons (protons and neutrons) move in nuclear-energy levels, or shells, that are filled, or closed, when the number of protons or neutrons equals 2, 8, 20, 28, 50, 82, or 126. These are the "magic numbers" because they indicate especially stable nuclei (e.g., helium-4 and tin-132).*

Beam Technologies Enable HRIBF Experiments

The principal developer of beam-production technologies that have brought praise and awards to experimentalists at ORNL's Holifield Radioactive Ion Beam Facility (HRIBF) is Gerald Alton, leader of the Advanced Concept R&D Group in the HRIBF Section of ORNL's Physics Division. He and current group members Yuan Liu, Sid Murray, Charles Reed, and Cecil Williams have been the unsung heroes in enabling world-class experiments in nuclear astrophysics and nuclear structure physics at ORNL. Dan Bardayan received the Publication of the Year Award from UT-Battelle and the American Physical Society's Dissertation of the Year Award for 2000 for one of these experiments. HRIBF operations staff members, including Dan Stracener and Paul Mueller, were vital allies in implementing and validating the ideas coming out of Alton's group.

The Advanced R&D Group's responsibilities include selection of target materials, design of high-release-efficiency targets and development of efficient sources for their ionization. Alton came up with the ideas that led to the production of the fluorine-17 (^{17}F) beam used by Bardayan, group leader Michael Smith, and their colleagues. Many radioactive beam scientists believed that a ^{17}F beam could never be produced at the needed intensity at ORNL, but the developments by Alton's group helped to produce this "impossible beam" and prove them wrong.

To make an ^{17}F beam, Alton had the idea of using highly permeable targets made from thin fibers of refractory oxides to allow fast diffusion of ^{17}F ions out of the target and fast transport to the ion source before they decay. The oxygen-16 in the oxide target is transmuted to ^{17}F by deuteron beams from the Oak Ridge Isochronous Cyclotron (ORIC). Oxide materials were selected by assessing their chemical equilibrium compositions and determining the highest temperature to which they could be heated. The best candidates proved to be aluminum, zirconium, and hafnium oxides (Al_2O_3, ZrO_2, and HfO_2). The preferred target material is Al_2O_3, because the release product is aluminum fluoride. On the other hand, both ZrO_2 and HfO_2 are more refractory than Al_2O_3, meaning that they can stand more beam-deposited heat. The speed of release strongly increases with temperature, so a hotter target can be important.

Dan Stracener and his HRIBF operations colleagues found that a combination of HfO_2 + Al_2O_3 target material gave the best results. The HfO_2 is the production target and absorbs the beam energy while the Al_2O_3 provides the Al for forming the aluminum fluoride molecules. These molecules are rapidly transported to a special ion source conceived by Alton, called the kinetic ejection negative ion source, which dissociates the molecules and negatively ionizes ^{17}F efficiently as required for direct acceleration with the tandem accelerator.

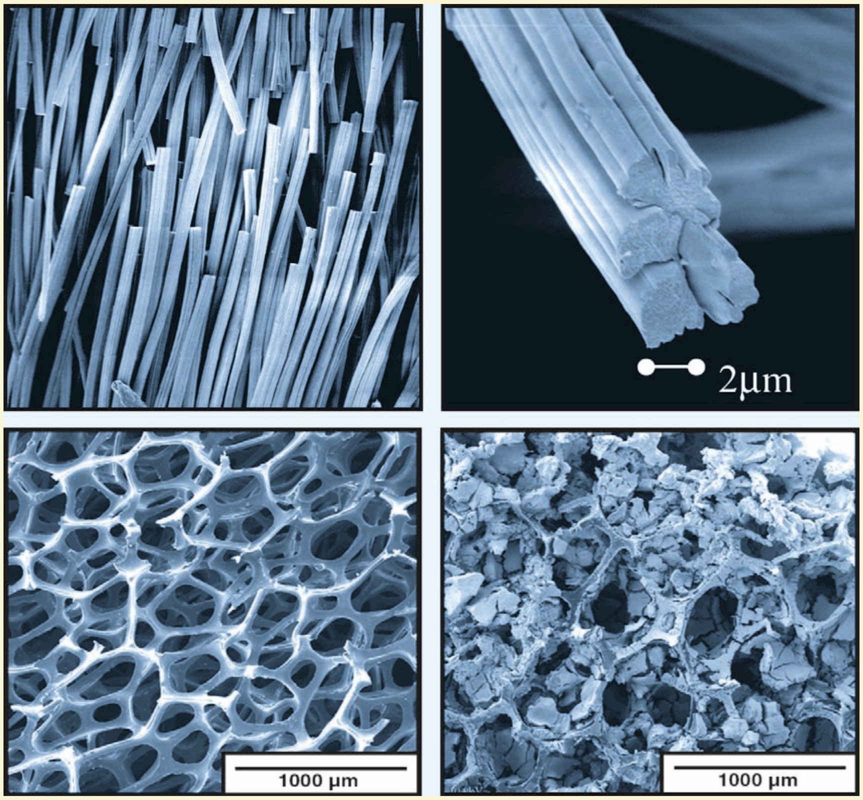
"The key to solving the target problems is the use of highly permeable fibrous or thin-layered composite materials with dimensions chosen so that the species of interest can diffuse from the material within its lifetime," Alton says. "We were the first to propose the use of custom-dimensioned target materials to optimize release from the target. We select refractory chemical compounds by performing thermal and chemical analyses and then format them with the dimensions appropriate for the fast release of short-lived species."

More recently, Alton's group developed a target for producing beams of neutron-rich nuclei for nuclear structure studies (see main article). This target consists of a stack of 12 to 14 carbon-fiber disks that are 2 millimeters thick and 15 millimeters in diameter. These carbon-fiber disks are coated with ~ 10 microns of depleted-uranium carbide, using a process developed for this purpose by McDermott Technology, Inc.

When a 40-MeV proton beam from ORIC bombards the uranium carbide coating of the disks, the uranium-238 fissions, forming a wide range of fission fragments. More than 132 radioactive isotopes from 28 elements have been extracted from this target so far. The energy of the fission products aids their diffusion from the target to the ion source. There an electron beam plasma ion source is used to knock off electrons from the fragments, making them positively charged. These positive ions are run through a cesium cell where they pick up a pair of electrons each, making a negative ion beam of 200 keV. The tandem accelerator can boost the energy of this beam to 350 or 400 MeV.

These target and ion source developments have enabled experiments to be done with, for example, tellurium-132 at intensity levels of up to 2×10^7 particles per second. The fibrous targets in combination with the kinetic ejection ion source produced beam intensities required to complete pioneering studies of reactions important in understanding element formation in stellar explosions.

"We have tried to move the state of the art in the technologies of both target and ion-source design from 'black art' toward science," Alton says. "These developments will have a strong impact on present and future radioactive ion beam facilities, based on the isotope separator on-line technique used at the HRIBF."



Gerald Alton's group developed target materials for producing radioactive ion beams. The above two scanning electron micrographs show hafnium oxide fibers for producing fluorine-17 beams. The bottom two micrographs show uncoated carbon fibers (left) and a carbon-fiber disk coated with depleted-uranium carbide, using a process developed for this purpose by McDermott Technology, Inc.

HRIBF is the first ISOL facility in the United States; it specializes in low-energy nuclear physics and nuclear astrophysics research. However, unlike other ISOL facilities, it can accelerate rare radioactive ions to energies sufficiently high to produce nuclear reactions.

"The Holifield facility is the only place in the United States where we can do preliminary experiments with accelerated ISOL beams," says Beene. "We have developed radioactive ion beams of fluorine-17 for nuclear astrophysics by making a novel target and ion source. We can now make neutron-rich nuclei by causing a uranium-238 target to fission after bombarding it with protons. Uranium-238 is itself neutron rich, having 92 protons and 146 neutrons, so its fission fragments are also rich in neutrons."

"Our special niche in this field," says Cyrus Baktash, head of the Radioactive Ion Beam Physics Section of ORNL's Physics Division, "is our ability to make neutron-rich beams to allow studies of nuclei far from stability. In addition, ORNL can accelerate beams of neutron-rich nuclei to high energies, whereas at CERN near Geneva, Switzerland, these nuclei can be produced only at low energies. At Holifield, we can accelerate these nuclei against a target to study nuclear excitations. We are now in a position to break the barrier to creating the next level of neutron-rich nuclides. This opens up a new area of experimental investigation."

"Besides being the only place where neutron-rich beams can be produced and accelerated for use in experimental physics studies, ORNL now has the best suite of detectors in the world for radioactive ion beams," Baktash continues. "ORNL staff members have developed sophisticated gamma-ray detectors and charged-particle detectors that can detect emission of particles and radiation following nuclear reactions, even though the background radioactivity is high and beam intensities are 10,000 to a million times weaker than stable beams. For example, a tellurium-136 beam is the weakest beam we have worked with. It has 20,000 particles per second, making it a million times weaker than the stable tellurium-128 beams we use for experiments."

David Radford and his colleagues in the Physics Division have used these experimental tools and the neutron-rich beams in several pioneering experiments to study nuclei close to the "doubly magic" tin-132. In the past, these nuclei could be studied only in a limited way via beta decays of their parents. The availability of accelerated neutron-rich beams at the HRIBF opens up many new and exciting possibilities. It is not easy to make an intense beam of tin-132, but a beam of tellurium-134 (^{134}Te) or tellurium-136 (^{136}Te) nuclei can be produced from the ^{238}U ion source at the HRIBF. "Because tellurium-134 is only two protons away from tin-132," Baktash says, "it teaches us a great deal about the magic proton number 50."

"David Radford and his colleagues have used reactions that range from 'gentle' Coulomb excitation to more energetic ones—like nucleon transfer and fusion. When energy is deposited in a nucleus by either bombarding it with a beam or scattering it off a target, the nucleus becomes excited. This excitation can take different forms. For example, the nucleus can vibrate, rotate, or simply rearrange the orbital motion of a few of its nucleons. This excitation, however, is short-lived. The nucleus gives up its excess energy by emitting particles or gamma rays."

"The Coulomb force, which causes the incoming beam to scatter off a target nucleus, such as carbon-12, also excites the projectile to a higher energy level," Beene says. "Upon de-excitation, the nucleus emits gamma rays. The angles and energies of these gamma rays are recorded by our sensitive gamma-ray detectors. We simultaneously detect carbon nuclei knocked out of the target to verify that the gamma rays we are detecting are the consequence of excitation in nuclei that have collided with the carbon target. This information allows us to determine how long it took the excited-beam nucleus to decay back to its ground state which, in turn, tells us about the nature of the excited state."

"In addition to being a unique facility now," says Nazarewicz, "the HRIBF will be a bridge to the DOE's proposed Rare Isotope Accelerator (RIA), which will be built somewhere in the United States in the next 10 years. Given the compelling physics that can be addressed with radioactive ion beams, the nuclear physics community in the United States has given construction of this facility its highest priority."

"Nazarewicz and his collaborators in nuclear physics theory group have played a leading role in predicting the properties of nuclides far from stability," Baktash says. "They have also developed a compelling physics case for RIA." The proposed RIA will make it possible to produce and study more than 1000 new rare isotopes in the laboratory. The primary accelerator at RIA would be capable of delivering intense beams of many elements from hydrogen to uranium, with beam power in excess of 100 kilowatts and beam energies per nucleon up to 400 MeV.

RIA will combine the two major techniques of rare isotope production: fragmentation or fission of the primary beam with in-flight separation of the reaction products, and target spallation or fission ISOL, followed by acceleration of the isotope of interest. The integration of both production techniques into a single, advanced rare-isotope research facility will allow use of the full arsenal of experimental techniques being developed worldwide. In the meantime, HRIBF will serve as an important facility where new physical phenomena will be explored using radioactive ion beams, the necessary teams of researchers will be trained, and new research tools and experimental techniques may be developed.

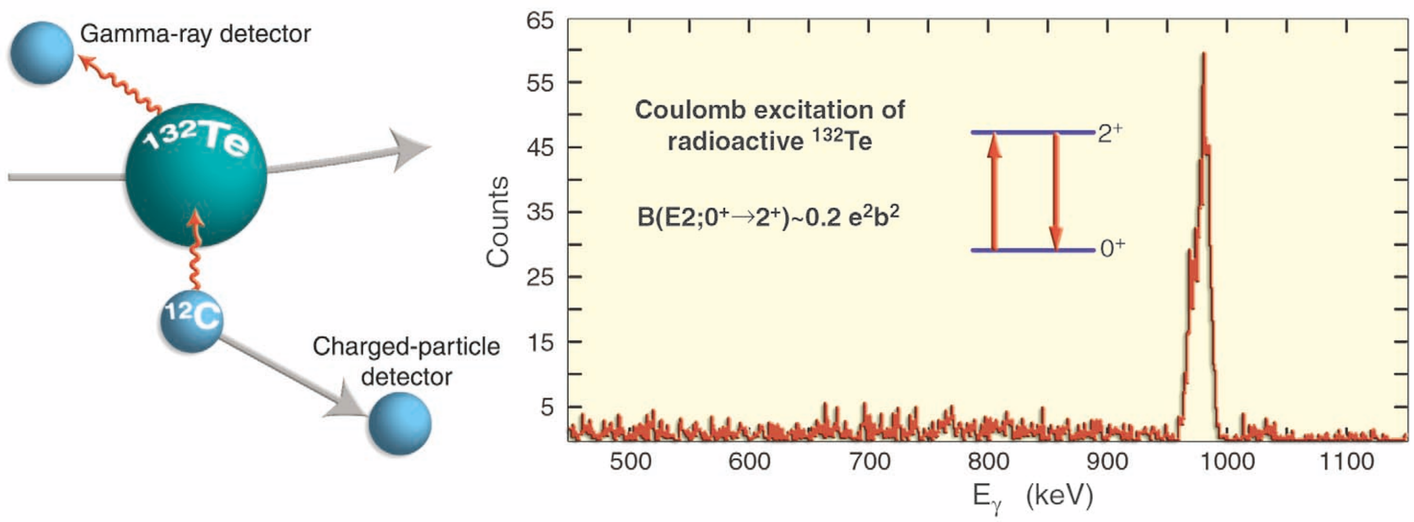


Illustration enhanced by LeJean Hardin

Coulomb excitation of neutron-rich nuclei is shown in this schematic in which a beam of tellurium-132 (^{132}Te) nuclei collides with a target containing carbon-12 (^{12}C) nuclei. Information about the shape of and charge distributions within a nucleus may be obtained from its electromagnetic properties. One of the best techniques for gleaning this information is to force an accelerated nucleus to collide with an appropriate target at energies just below the Coulomb barrier. Here, a ^{132}Te nucleus in a beam is excited to higher energy levels through collision with a ^{12}C nucleus. The excited ^{132}Te nucleus then releases this additional energy by emission of gamma rays. Simultaneous detection of charged particles (the scattered target ^{12}C nuclei) and gamma rays allows experimentalists to determine electromagnetic properties. In pioneering experiments at the HRIBF, this technique was used to investigate several radioactive isotopes of tin and tellurium for the first time.

Neutrons, "Stripes," and Superconductivity

Using neutron scattering at HFIR and elsewhere, ORNL researchers have found evidence to support a leading theory that explains high-temperature superconductivity.

How electrons behave in high-temperature copper oxide superconductors is a mystery, but progress is being made in resolving that mystery on both theoretical and experimental fronts. One of the leading theories postulates that electronic matter organizes itself into fluctuating regions where the charge (holes) and the magnetism (spins) are separated in space in one-dimensional regions called stripes. These striped phases were predicted in theories developed by physicists at the Leiden Institute in the Netherlands, DOE's Brookhaven National Laboratory, and the University of California at Los Angeles.

Herbert A. Mook and Pencheng Dai, both of ORNL's Solid State Division, and colleagues from the University of Washington in Seattle have found evidence for this stripe theory in experiments on high-temperature superconducting materials such as yttrium-barium-copper oxide (YBCO). The results were obtained in neutron-scattering experiments on superconducting samples prepared by Rodney Hunt of ORNL's Chemical Technology Division.

Superconductivity in standard low-temperature materials is understood in terms of the theory developed by John Bardeen, Leon Cooper, and Robert Schrieffer (known as the BCS theory), who found a way to make superconductivity work by pairing up electrons of opposite spins. Normally, electrons bump into each other, impeding conductivity. However, the pairs glide through the superconductor like couples waltzing across a ballroom dance floor, completely unhindered by the other electron couples on the floor. The distance between the electrons in each pair is called the superconducting coherence length. Both electrons in each pair have a negative charge so that they repel each other, but the coherence length is long in the standard materials, so the electron partners are quite far apart and, in fact, have many other electron pairs dancing between them.

In the copper oxide superconductors, however, the coherence length is very short, so the paired electrons are dancing close together. This makes it very hard to find a pairing interaction strong enough to provide the glue to keep the pairs together.

"This is where stripes come in," Mook says. "Rather amazingly in one dimension, electrons can split in two parts with one of the parts carrying the charge and the other the spin. In this case, the spins can form superconducting pairs without their charges trying to keep them apart. The stripes provide the one-dimensional regions that make it possible for the electrons' spins to separate themselves from their charges."

Curtis Boles

Aerial view of the High Flux Isotope Reactor, where some of the neutron evidence was obtained to support a leading theory for explaining high-temperature superconductivity.

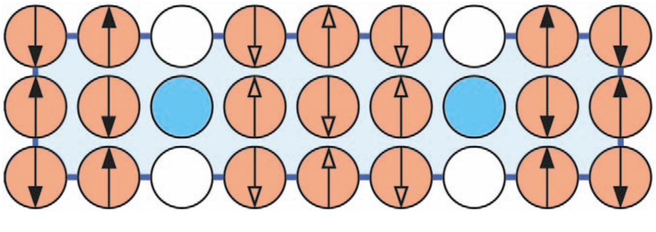
The neutron scattering results on stripes have been published in three papers in the prestigious journal *Nature*. The experiments led by Mook and Dai were performed between 1998 and 2000 at the Rutherford Appleton Laboratory's spallation neutron source at the ISIS Facility in the United Kingdom and at ORNL's High Flux Isotope Reactor (HFIR). Their first experiment at the ISIS spallation neutron source showed that the electron spins separated into distinct regions in the high-temperature, superconducting material.

"In our experiment at ISIS," Mook says, "we determined the spatial distribution of the electrons' spins, based on the neutron scattering pattern." These measurements provided the first direct evidence that striped phases occur in the YBCO superconductors.

A second set of experiments at the HFIR showed that the charge distribution was also consistent with stripes. "At HFIR we saw how the charges were distributed in crystals by measuring their effect on the lattice vibrations, which are called phonons," Mook says. "The changes in the phonons allowed us to see a periodicity in the pattern of these vibrations, which demonstrated that the charge part matched up with the spin part of a striped phase."

A third experiment, also conducted at HFIR, demonstrated that the spin distribution observed earlier was really one dimensional in nature. "This was a key issue in the stripes argument," Mook says. "We initially submitted the paper to *Nature* as a letter, but the head physical sciences editor wanted it expanded into a full article."

It will probably be some time before a consensus is reached on the mechanism behind high-temperature superconductivity. However, because of the neutron scattering experiments, the "stripe" theory is regarded as one of the leading theories for explaining high-temperature superconductivity.



Arrangement of the spins and charges in a striped phase. The circles represent the copper atoms in the copper-oxygen planes of the superconductor. The spin stripes are represented by the arrows while the open circles are the hole stripes. The shaded circle shows that the holes are not uniformly distributed on the hole stripe and may move along the stripe.

ORNL's Neutron Sources and Nuclear Astrophysics

Neutron data from ORELA and the SNS will help computational astrophysicists improve their modeling of the nuclear processes by which isotopes are synthesized in stars.

The Oak Ridge Electron Linear Accelerator (ORELA) at ORNL is the only U.S. facility that can provide much of the neutron data needed by computational astrophysicists modeling the nuclear processes by which isotopes are synthesized in red giant stars and supernovae. Measurements from ORELA are being used to improve computer models designed to enhance our understanding of the life and death of stars, the chemical evolution of our galaxy, and the formation of our solar system.

Almost all stable isotopes of the elements found on the earth and even some radioactive isotopes not naturally present on our planet were formed in stars as they burned fuel or exploded. "Almost all elements heavier than iron were made in stellar environments where neutrons play an important, if not dominant, role," says Paul Koehler, a nuclear physicist in ORNL's Physics Division. "Roughly half the isotopes of elements heavier than iron were synthesized in red giant stars. Through a complicated mixing process, newly synthesized elements were carried from inner regions of the star out to its atmosphere, where they are visible to astronomical observations. In fact, the observation of the radioactive element technetium in a red giant star's atmosphere provided the first direct proof that nucleosynthesis occurs in stars."

Intimately linked to the mixing process in a red giant (which our sun will become in a few billion years) is the synthesis of elements heavier than iron through a chain of nuclear reactions known as the slow neutron capture, or *s*, process. In the *s* process, free neutrons are produced as a by-product of nuclear reactions that generate the energy that powers the star. Heavier nuclei are synthesized when lighter nuclei capture one of these free neutrons. However, a typical stable nucleus can capture only a few neutrons before it becomes unstable. Through a process known as beta decay (whereby one of the neutrons in the nucleus disintegrates into a proton, an electron, and an antineutrino), the nucleus is transformed into the next heavier element. Starting from iron "seed" nuclei, this chain of neutron captures and beta decays continues all the way to elements as heavy as lead.

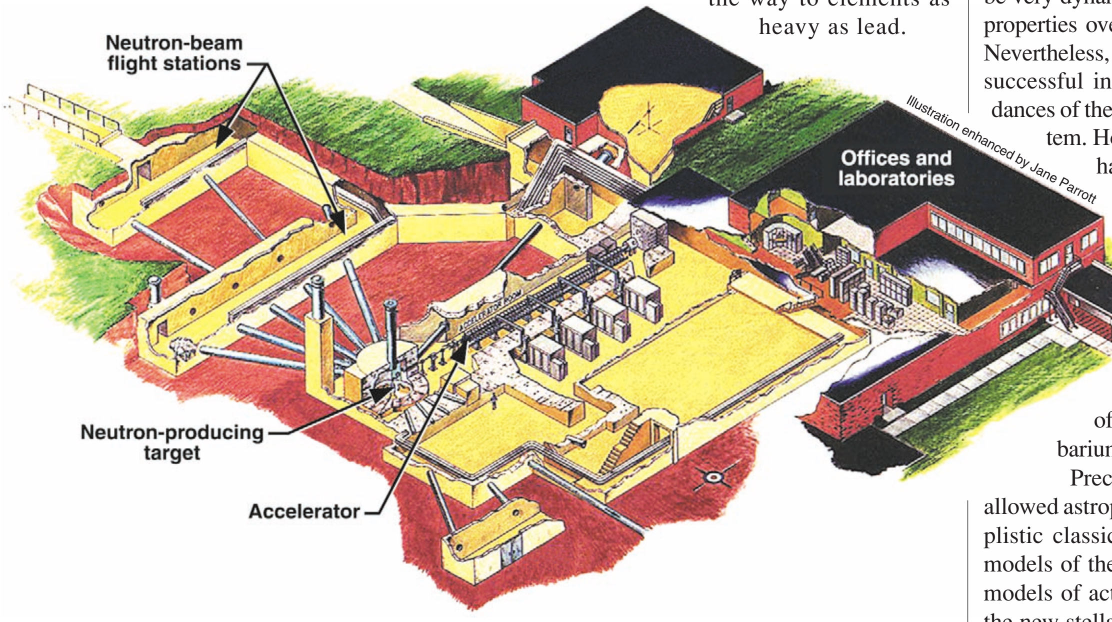


Illustration enhanced by Jane Parrott

A cutaway drawing of the Oak Ridge Electron Linear Accelerator facility showing the accelerator (center) for bombarding a tantalum target with electrons, causing the production of neutrons that travel through various beam lines for experiments. Researchers use these neutrons to bombard various targets to determine the probability that these neutrons will be absorbed by nuclei in the targets.

In the red giant stardust model, microscopic grains of refractory materials such as silicon carbide (SiC) form in the cooler outer regions of red giant stars, trapping within them trace amounts of the heavy elements made in the *s* process. Strong stellar winds from red giants disperse the products of the *s* process throughout the galaxy. Some of these grains have reached the earth aboard meteorites. The relative abundance of isotopes of many of the trace elements trapped within these stardust grains can be measured with exquisite precision by analyzing the content of stardust recovered from meteorites. These detailed, isotopic signatures provide a rich set of observational data with which to test astrophysical models of stars and of the chemical evolution of our galaxy.

The first, or "classical," model of the *s* process was proposed in 1957. In this simplified model, it is assumed that the temperature, neutron density, and matter density are constant during the helium-burning pulses in which the *s* process was thought to occur. In contrast, the *s*-process environment in real stars is thought to be very dynamic, with large changes in all these properties over relatively short periods of time. Nevertheless, the classical model has been very successful in reproducing the observed abundances of the *s*-process isotopes in our solar system. However, as the neutron capture data have become more precise, cracks in the classical model have begun to show. In the 1990s, precise new neutron-capture-reaction-rate measurements from ORELA and elsewhere showed that the classical model predicted incorrect abundances of several key *s*-process isotopes of barium, neodymium, and tin.

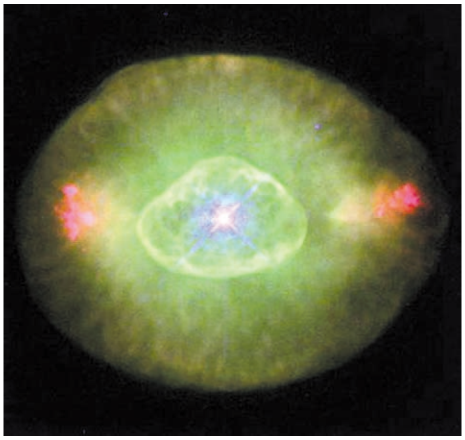
Precise, new neutron-capture data have allowed astrophysicists to move beyond the simplistic classical model and test more realistic models of the *s* process that are closely tied to models of actual stars. The first precise test of the new stellar models of the *s* process, including the red giant stardust model, was made possible recently by work at ORELA. There, ORNL physicists made the first precise measurements of the neutron-capture cross sections for two isotopes of neodymium, ^{142}Nd and ^{144}Nd. A cross section is a measure of the probability that a nuclear reaction occurs, such as the capture of a neutron by a nucleus.

Stellar *s*-process model calculations made using previously accepted cross sections for these isotopes were in serious disagreement with stardust data. The problem was that these calculations relied on neutron cross-section measurements made over too limited a range of energies, so they had to be extrapolated down to the lower temperatures predicted by the new stellar models. The new ORELA measurements, which were made with an improved apparatus and over the entire energy range needed by the new stellar models, showed that the old data were in error. With the new ORELA data, the agreement between the stellar model predictions and the measurements of neodymium isotopic abundances in stardust are excellent.

Five more measurements of this type have been made at ORELA through a collaboration led by Koehler, consisting of scientists from ORNL's Physics and Computational Physics and Engineering divisions and scientists from Denison University and Lawrence Livermore National Laboratory. In four out of five cases studied so far, Koehler says the precise ORELA data have demonstrated that extrapolations from previous measurements are in error by 2 to 3 times the estimated uncertainties.

"We are measuring neutron cross sections of isotopes thought to be produced solely by the *s* process (*s*-only isotopes) because they are the most important calibration points for testing the stellar models," says Koehler. "If an element's probability of capturing a neutron is very small, it is unlikely that it will be transmuted to another element, so its abundance will be high. If its cross section is very large, it more likely will be destroyed, so its abundance will be low. There are about 30 *s*-only isotopes. Cross sections at low energies have been measured for only 4 of these isotopes, using ORELA. Precise neutron-capture rates for the 26 other *s*-only isotopes could also be measured at this neutron source.

"This information also helps us better understand how the *s* process synthesizes elements, which of the heavier elements were formed first, and how the abundance of elements evolved over the lifetime of the galaxy," Koehler adds. "It allows us to predict how well materials in stars are mixed during the convection process, when heat from the star drives fluid flow. Convection and mixing are thought to play an important role in many astrophysical environments, such as in supernova explosions. But, because of their relative simplicity and because most of the important nuclear physics information can be measured in the lab on the earth, red giant stars offer perhaps the best hope for understanding convection and mixing in astrophysical environments. Precise new neutron-capture cross sections from ORELA and other facilities, as well as new stardust and other astronomical data, are helping theorists unravel the mysteries of complicated mixing processes."



Planetary nebulae from the death of a red giant star. The strong stellar winds responsible for planetary nebulae help to disperse elements synthesized (via neutron-capture reactions during the s *process) by red giant stars throughout the galaxy.*

Koehler and his colleagues recently received ORNL seed money to study the formation of proton-rich isotopes of elements heavier than iron during the *p* process. Some scientists believe that proton-rich isotopes, such as molybdenum-92 and ruthenium-96, are formed when high-energy photons produced late in the lives of massive stars or in supernova explosions knock out neutrons from nuclei. High-energy photons can knock out not only neutrons but also alpha particles, in gamma alpha reactions.

"Cross sections for gamma alpha reactions are next to impossible to measure for these heavier nuclei, but the nuclear statistical model should be able to predict them reliably enough for *p*-process calculations," Koehler says. "However, current models do a poor job of reproducing the few measurements that have been made. It turns out that by measuring the rate of neutron alpha reactions at ORELA, in which each nucleus captures a neutron and then ejects an alpha particle, we will be able to supply the best constraints for nuclear statistical models."

The neutron alpha measurements are still very difficult because of a background known as the gamma flash. At ORELA neutrons are produced in secondary reactions that occur when an electron beam strikes a tantalum target. The electrons first produce a very intense beam of photons that can blind detectors.

According to Koehler, "With the help of seed money and scientists from Russia and Poland, we were able to scale up a detector that had been pioneered at ORELA—called a compensated ionization chamber—that makes it possible to count the alpha particles in the presence of the very intense gamma-flash background. Surprisingly, we found that our first proof-of-principle neutron-alpha data, on samarium-147 and neodymium-143, are in reasonably good agreement with the older model from Caltech, but that the rates predicted by two very recent models are roughly a factor of three different from our data, but in opposite directions."

The high neutron flux at DOE's Spallation Neutron Source (SNS), which will be operating in 2006 at ORNL, will allow astrophysics measurements to be made using samples 10,000 times smaller than those currently studied at ORELA. The SNS should be especially useful for measurements of neutron-capture rates of radioactive isotopes, because only tiny amounts will be needed. The SNS could also be used to study very rare stable isotopes that are so expensive that only very small isotopically separated samples are affordable for research.

"The excellent time-of-flight resolution at ORELA makes it the only facility in the United States capable of measuring small, resonance-dominated neutron cross sections," Koehler says. "ORELA would also be an excellent facility for developing detectors for experiments at the SNS. ORELA and spallation sources such as the SNS are complementary facilities, both of which are essential to cover the wide range of measurements needed for nuclear astrophysics."

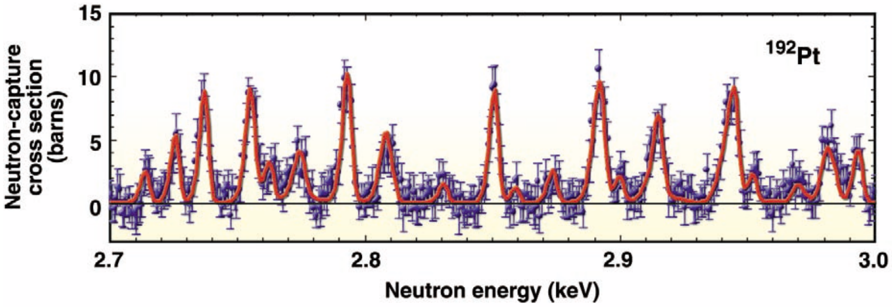


Illustration enhanced by LeJean Hardin

A very small portion of recent neutron-capture data from ORELA for isotopes of platinum. The entire data set spans the range from 0.02 to 500 kilo electron volts (keV). The excellent resolution of the ORELA facility makes it possible to discern the many peaks in the cross sections and thus determine the astrophysical rates for these neutron-capture reactions to high accuracy.

Modeling Magnetic Materials for Electronic Devices

As disk drives and transistors are further downsized, currently used materials will eventually reach fundamental limits in performance. ORNL researchers are addressing these issues.

Digital cameras, computer-game-playing stations, laptop computers, and portable devices that record music and play back television programs use magnetic disk drives as small as a fat credit card—taking up much less space than the shoebox-sized drives in desktop computers. The number of bits of information (1's and 0's) per square inch is doubling every year as magnetic disk drives shrink yet store and access more data in less time. But in its quest to make disk drives that are extremely fast and small, the magnetic recording industry will soon be hitting a wall. Currently used materials will eventually reach fundamental limits in performance as disk drives are further downsized.

ORNL and the Department of Energy's Brookhaven National Laboratory (BNL) are collaborating with industry to address the fundamental scientific problems confronted by the magnetic recording industry. The industrial partners in this Laboratory Technology Research (LTR) project, funded by DOE's Office of Science, are Seagate Recording Heads, Inc., the world's largest manufacturer of computer hard disk drives; the Almaden Research Laboratory of IBM, the inventor of the magnetic hard disk drive (in 1956) as a direct access storage device; and Imago Scientific, Inc., a startup company in Madison, Wisconsin, that can analyze magnetic materials using its patented local electrode atom probe (LEAP) technology. The ORNL researchers involved in this LTR project are Bill Butler, Malcolm Stocks, Mike Miller, and Balazs Ujfalussy, all of the Metals and Ceramics (M&C) Division; Thomas Schulthess of the Computer Science and Mathematics Division; and Xiaoguang Zhang of the Computational Physics and Engineering Division.

"Designers of the next generation of magnetic readers and magnetic media are working with badly blurred vision," Butler says. "They are unable to determine the structure of magnetic material at the necessary atomic scale. We plan to use atomic probe technology and computational simulation to better understand the limits of currently used magnetic disk drive materials and to identify new material structures and deposition processes that may overcome these limits."

To understand the problems, first it is necessary to understand how today's small magnetic disk drives work. Most of these drives read the stored data using giant magnetoresistive (GMR) read heads.

"The read head is like a jet flying at supersonic speeds a meter above a pasture and counting the grass blades pointed in two different directions," Schulthess says. "Think of each grass blade as a magnetic particle, or region of magnetization, pointing in one direction—or the opposite direction—like a compass needle. The directions, or magnetic moments, represent bits of information, either a 1 or 0."

The reader is a spin-valve device consisting partly of layers of nickel-iron and cobalt (separated by copper spacers). These layers are free to rotate, or spin, in response to an applied magnetic field. The total thickness of these free magnetic layers may be only 10 nanometers. Based on its orientation, the small magnetic field of each magnetic particle on the disk affects the electrical resistance of the read head.

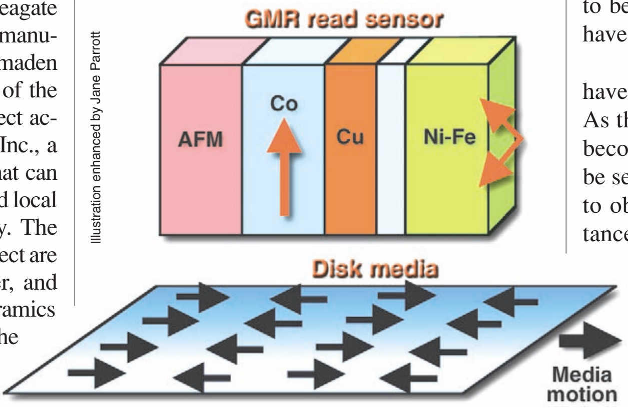


Illustration enhanced by Jane Parrott

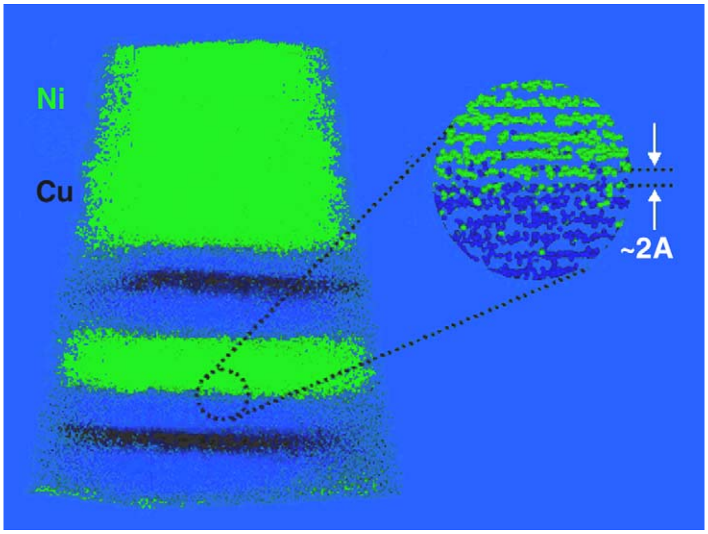
Schematic diagram of a GMR read sensor used in a disk drive. The sensor responds to the changing magnetic fields on the disk as it spins beneath it. The blocks indicate different layers of magnetic and nonmagnetic material, which may be only a few nanometers in thickness. A resistance change occurs when the magnetic fields from the bits on the disk cause a change in the relative orientation of the magnetic moments in the two magnetic layers.

In operation, the magnetic moments of one of the "pinned" magnetic layers are held fixed by an adjacent magnet, which has an internal magnetic field that does not destroy data on the magnetic media; it is made of an antiferromagnetic (AFM) material, such as a manganese alloy. A current is passed between the pinned and free magnetic layers. When the free layer senses a magnetic moment signifying "1," it stays or becomes parallel to the pinned layer; when it senses a "0," it adopts a position perpendicular to the pinned layer. In one position, the electrical resistance is high between the magnetic layers (because the magnetic moments of the free and pinned layers are not parallel), so the current passing through them is low; in the other position, the reverse is true. The shifting strengths of an electrical signal as a result of changes in resistivity allow the read head to copy stored data to a computer.

What are the problems that will result from downsizing disk drives made of currently used materials? According to Butler, "As the disk drive density gets higher, the magnetic particles representing each bit get smaller. So the read head must be shrunk to several hundred angstroms. Because Seagate wants the fixed AFM magnet to be much thinner, the material structure may have to be changed to make it work effectively.

"Secondly, the smaller read head must have a higher sensitivity to detect smaller bits. As the density of the regions of magnetization become smaller, the magnetic fields that must be sensed to read the data get weaker. We need to obtain the largest possible change in resistance for relatively small changes in the magnetic field. One solution may be to grow smooth films with the proper interfacial structure to optimize the magnetic performance of the device."

The third problem is that, as bits get smaller, the superparamagnetic limit is reached. "When magnetic particles become small enough, their magnetism may be affected by changes in temperature," Butler says. "These thermal fluctuations can upset a tiny magnetic particle's magnetization, causing loss of valuable data. To solve this problem, a magnetic disk could be made out of a magnetically hard material, such as neodymium iron boride. But that would create a new problem: You could not write new information on such a disk without using higher magnetic fields. To generate these higher magnetic fields, the write

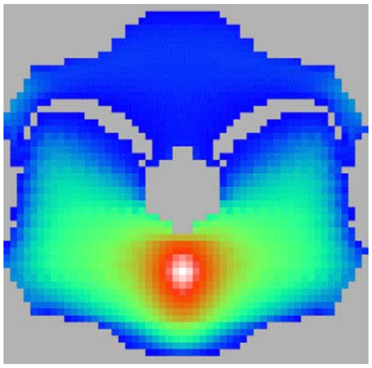


Atom probe image of a magnetic multilayer. The individual atomic planes can be clearly discerned.

head must be made of material that has a higher saturation magnetization."

Another LTR objective is to create a structured material that has a higher number of unpaired electron spins per unit volume, or a higher saturation (density) of magnetization. Iron has a magnetic moment of 2, or 2 unpaired spins per atom; manganese has a moment of 5 and some rare earths, 7, but their spins are often in the opposite rather than the same direction. Using computational simulation at the IBM supercomputer at DOE's Center for Computational Sciences at ORNL, Butler, Stocks, Schulthess, Ujfalussy, and Zhang hope to design artificial, layered structures for smaller read heads. These structures may contain iron, manganese, and rare-earth thin films that offer a higher magnetization saturation, as well as magnetic softness and corrosion resistance. Such structures may also be used for write heads for magnetic recording.

The LTR project also has an objective to use computational simulation to help enable atomic probe field ion microscope tools (such as those employed by Mike Miller of the M&C Division, as well as the LEAP technology developed by Imago Scientific) to better image metallic multilayers with atomic-scale resolution. Dave Larson, formerly of the M&C Division and now with Seagate, has already done atomic probe studies of a structure containing layers of nickel, cobalt, and copper. His images show some diffusion of nickel atoms into the cobalt layer and diffusion of cobalt atoms into the nickel layer. Such interdiffusion could make differences in resistivity impossible to detect.

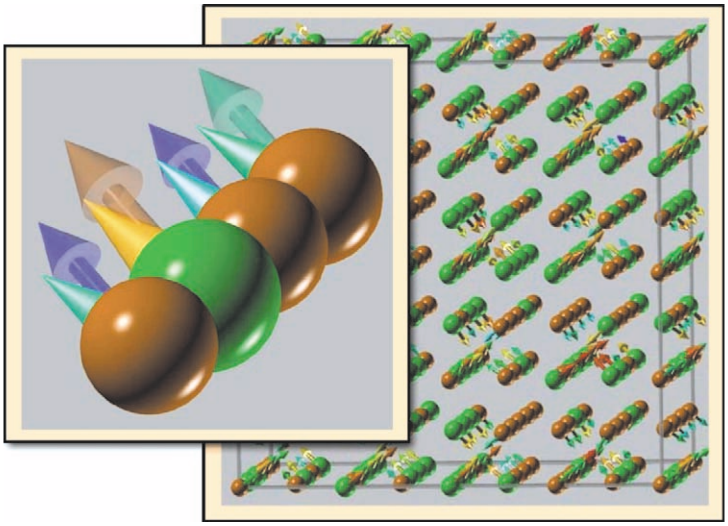


Plot of scattering intensity caused by cobalt impurities in copper.

"Atom probe information may allow us to compare deposition processes to determine which ones make thin-film structures that work best as read and write heads in very small disk drives," Butler says.

Using computer simulation at ORNL, Stocks and Schulthess recently obtained insights about antiferromagnetism in iron manganese (FeMn), an alloy used in the fixed AFM magnet of spin-valve GMR read heads. They studied the alloy's non-collinear magnetic structure, in which the magnetic moments point at angles to each other rather than up or down.

"We did calculations using constrained density functional theory and spin dynamics," Stocks says. "Our goal was to understand the alloy's noncollinear antiferromagnetic 3Q magnetic structure, which has the lowest known energy level for a system of atoms and electrons in a crystal, compared with the 1Q and 2Q structures. We predicted there is a more relaxed, even lower-energy-level magnetic state that we call 3QR in which R stands for relaxed. In this state, the magnetic moment orientations, shown as arrows, are pointed in a slightly different direction, according to our simulation. This insight could lead to a design of improved GMR devices."



Detailed magnetic structure of an iron manganese alloy showing small relaxations of the magnetic moment directions relative to the 3Q structure.

Stocks and his colleagues have also been involved in another problem in which a material currently being used in a basic electronic device will hit a wall as the device is downsized. As transistors are shrunk to increase a chip's computing power, the use of silicon dioxide to block or allow electron flow will limit transistor performance as an on-off switch, or memory unit, for storing a bit (1 or 0). When silicon dioxide becomes too thin, electrons will leak from it by quantum tunneling, making it useless as a gate electrode material.

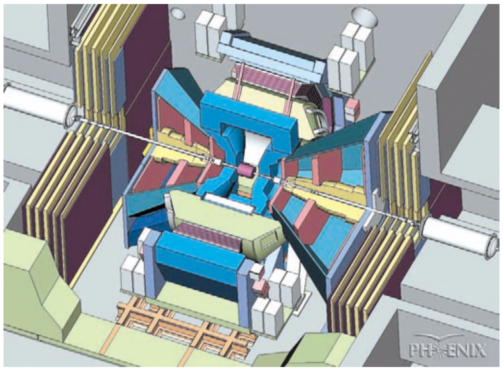
Rodney McKee of the M&C Division and his colleagues have shown that silicon dioxide can be replaced by certain crystalline oxides whose superior electrical properties will allow reduction in transistor size without loss of performance; more research is being done on this project by ORNL in collaboration with Motorola and DOE's Pacific Northwest Laboratory under a cooperative research and development agreement. Stocks and his colleagues are using the IBM supercomputer to model the interfaces between silicon and silicon dioxide and between layers on silicon. These layers consist of strontium disilicide, strontium oxide, titanium dioxide, and strontium titanate (to make the gate electrode ferroelectric).

"We are simulating the electronic structure of strontium disilicide and trying to determine how many layers of strontium oxide are needed to make it a good insulator," Stocks says. "Sometimes the experimental observations do not agree with our calculations because we find electrons diffusing between layers, while the observations suggest that the interfaces are clean." The simulations could aid the experimenters in improving their deposition processes to make a more effective thin-film structure as an advanced transistor gate material.

When a material's performance in an electronic device is about to hit a wall as the device gets very small, some ORNL materials scientists focus on designing advanced materials to allow the electronic industry to leap to the other side.

ORNL physicists and electronics experts have played a major role in developing detectors and electronic components to search for evidence that the beginning of the universe has been mimicked in DOE's Relativistic Heavy Ion Collider.

In Quest of a Quark: ORNL's Role in the PHENIX Particle Detector

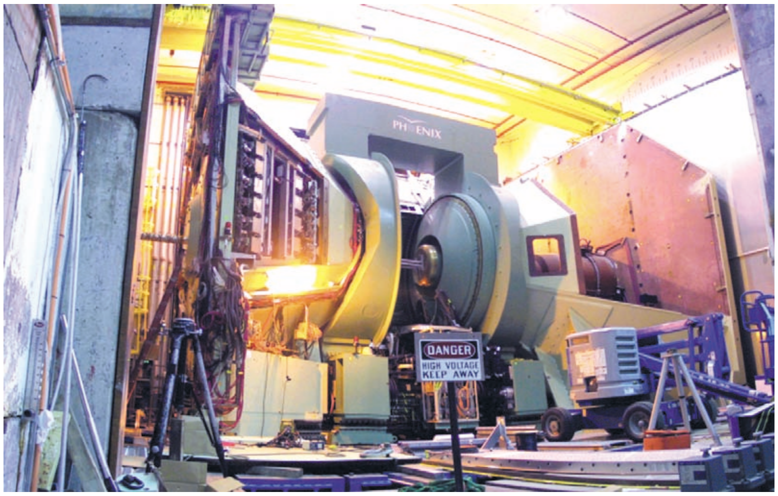


Courtesy of Brookhaven National Laboratory

Just as violent wars have liberated oppressed peoples, scientists are hoping that violent collisions between gold nuclei racing around a circular track in opposite directions will free the building blocks of some protons and neutrons that make up the atomic nucleus. These building blocks are quarks, which combine in groups of three to form individual protons or neutrons (both of which are called nucleons).

Quarks are held together to form nucleons by particles called gluons, the carriers of the strong nuclear force. No one has succeeded in knocking a quark loose and seeing it in isolation as a free quark. It is believed that if the nucleons of heavy nuclei are compressed and excited enough by colliding nuclear beams, the quarks and gluons may be liberated temporarily from their nucleon prisons. In this process, called deconfinement, these quarks and gluons would roam freely in a volume much larger than that of a nucleus, forming an extremely hot soup called a quark-gluon plasma. Such a soup is thought to have existed during the latter part of the first 10 microseconds of the Big Bang, the explosion of an extremely dense blob of energy that formed our universe.

Terry Awes, Vince Cianciolo, Yuri Efremenko, Frank Plasil, Ken Read, Soren Sorensen, Paul Stankus, Glenn Young, and other ORNL physicists have been searching for free quarks since 1986. That's when they first conducted experiments using oxygen beams at the Super Proton Synchrotron at the European Laboratory for Particle Physics (CERN) near Geneva, Switzerland; later, also at CERN, they performed experiments with sulfur (1987-1992) and lead (1994-1996). In 2000 many of the scientists conducting experiments at CERN claimed they had observed deconfinement. But other scientists called this announcement premature. According to Young, "We felt the announcement was premature and did not address several expected signals of deconfinement."



Courtesy of Brookhaven National Laboratory

View of all three PHENIX spectrometer magnets installed in the collision region. The long axis of the photograph spans some 50 feet. One of the central arm carriages has been retracted; the other can be glimpsed behind the central magnet. The octagonal magnets carry the muon spectrometers.

Now, the ORNL physicists and scientists all over the world are pinning their hopes of freeing quarks and gluons on gold beams colliding at nearly the speed of light (100 billion electron volts per nucleon) at the $600-million Relativistic Heavy Ion Collider (RHIC) at the Department of Energy's Brookhaven National Laboratory. RHIC's first gold-gold (Au-Au) collisions were observed on June 13, 2000. In January 2001, at a conference at the State University of New York at Stony Brook, physicists involved with RHIC announced that Au-Au collisions had produced the densest matter ever created in a laboratory—the first step toward making a quark-gluon plasma. Such a particle soup in a very small volume would have a temperature of 2 trillion degrees Kelvin, 100,000 times hotter than the sun.

The ORNL physicists from the Physics Division and researchers from ORNL's Instrumentation and Controls Division are involved in the 420-person PHENIX collaboration at RHIC. The $100-million PHENIX is one of two large arrays of particle detectors at RHIC; the other large detector is STAR.

On April 16, 2001, scientists in the PHENIX collaboration—including Awes, Cianciolo, Efremenko, Plasil, Read, Sorensen, Stankus, and Young—published a paper entitled "Centrality Dependence of Charged Particle Multiplicity in Au-Au Collisions," in the Volume 86, Number 16 issue of *Physical Review Letters*. According to Young, the paper provided evidence that the PHENIX detector works as planned and that 6000 particles are emitted per collision as predicted. "Most of these particles are produced by conversion of energy into matter during the collision," Young says. "These particles spraying in all directions are the result of smashing the 394 nucleons contained by two gold nuclei together at a total energy of 25 trillion electron volts."

ORNL physicists and engineers have developed two detectors and also electronic components for many of the 500,000 particle-detection channels of PHENIX. The goals of this work are to sort through the data on a selected subset of the 6000 particles emitted per Au-Au collision and to select the most meaningful collision events that are of greatest interest to the physicists. The STAR, on the other hand, is a gigantic digital camera, which has electronics for detecting and analyzing all 6000 particles emitted per collision.

"PHENIX is used to detect all the particles striking it, but the electronics decide which particle events should be stored in memory and analyzed in detail later by a parallel computer," Young says."Gold-nuclei collisions occur 1000 times a second. About 90% of the time the collisions are not interesting but 1 to 5% of the time they are very interesting.

"Of the 6000 subnuclear particles emitted after each collision event, which lasts only 10^{-22} second, about 90% are pions, which originally were thought to be the particles that hold the nucleus together. Our ORNL team is interested in studying mainly photons, electrons, and muons, a heavier partner of the electron." Pions are the lightest particles to feel the nuclear force and are thus most easily produced during the collision.

ORNL researchers have focused on the detector and electronics for two types of PHENIX detectors—a muon identifier and a calorimeter. The first detector detects muons and the second one detects electrons and photons. ORNL also produced electronics used in four other PHENIX detectors.

Muons are 210 times as massive as electrons. First discovered in cosmic rays by Nobel Laureate Carl Anderson, a muon is unstable; it decays in 2.2 microseconds into an electron plus two neutrinos (almost massless particles that can penetrate the earth). Of the 6000 particles emitted in a collision between two gold nuclei, only about 10 are muons. Even rarer is a muon pair (a positive muon paired with a negative muon), but if one is detected, it will be of interest to physicists.

This muon identifier is designed to spot a muon by screening out other particles, including pions, that cannot cleanly penetrate the detector's 600 tons of steel walls as well as muons can. Instead, pions usually strike iron nuclei in the steel, creating reactions that stop the pions or events that destroy the particles. A muon loses just a bit of energy as it flies through these walls and strikes proportional counters interleaved with steel plates containing an electrically conducting wire and a mixture of two gases—carbon dioxide (CO_2) and isobutane (C_4H_{10}) The muons knock electrons loose from the gas mixture, ionizing it. These free electrons are attracted in an avalanche to the electric field of the wire where they cause a pulse of detectable current that indicates a muon got through. A team consisting of Vince Cianciolo and I&C members Bobby Ray Whitus, Tim Gee, Steve Hicks, and Miljko Bobrek created custom electronics boards, logic chips, and firmware to detect these pulses and record them for later analysis.

A set of precision proportional chambers, which measure position to 100 microns, is placed just before the muon identifier and inside a large electromagnet. These chambers, which are used to measure the muons' momenta, were built by a consortium headed by DOE's Los Alamos National Laboratory. Chuck Britton and Mike Emery (and earlier, Mark Musrock) of the I&C Division developed a preamplifier that senses, adds up, and amplifies the charges induced by the pulse on the wire, signaling the presence of a muon. This development in low-noise electronics is essential to the detector's success in finding muons.

Courtesy of Brookhaven National Laboratory

View of the two PHENIX central arm carriages with their detector and electronics packages installed. The far one is in the process of being rolled into position. The cylindrical beam pipe threading the large central magnet (in green) is some 15 feet above floor level and carries the two counter-rotating beams of high-energy nuclei, be they protons, gold nuclei, or intermediate species.

To detect photons and electrons emitted by the Au-Au collisions at RHIC, a calorimeter was built for PHENIX by a team of researchers from ORNL, Russia's Kurchatov Institute in Moscow, and the University of Münster in Germany. This calorimeter measures the energy of the photons and electrons coming into PHENIX. It is made of leaded glass similar to what is found in cut glass. The glass is 55% lead oxide. Because of the index of refraction of the glass, when a particle enters it, Cerenkov light is emitted and picked up by one of 25,000 photomultiplier tubes. These tubes amplify the light flash and convert it to 6 billion electrons, which form a brief (15 nanoseconds) pulse of electrical current caught by the electronics. The pattern of the Cerenkov light and its energy and time of arrival indicate whether the particle is an electron or photon on the one hand, or a charged pion, kaon (another type of meson), or proton on the other. An ORNL I&C team led by Alan Wintenberg and including Mike Cutshaw, Mike Emery, Shane Frank, Don Hurst, Gentry Jackson, Mark Musrock, Mike Simpson, David Smith, and Jim Walker designed custom circuits, chips, firmware, and circuit boards to read out data from these photomultipliers. Physics Division staffers providing assistance were Stankus, Awes, Efremenko, Plasil, Young, and postdoctoral scientist Sergei Belikov.

ORNL also designed and built custom electronics for a novel proportional chamber readout with small "pixels," a project handled by Bill Bryan, Usha Jagadish, and Melissa Smith. Alan Wintenberg and Shane Frank developed electronics, similar to those for the calorimeter, to read out a gas-filled Cerenkov counter used in PHENIX to tag electrons. Chuck Britton, Tony Moore, and Nance Ericson built a system used to detect the tiny (4 femtocoulomb) signals induced on 100-micron-wide strips of silicon diode, a detector used to count the particles hitting PHENIX.

ORNL has developed "trigger electronics" to decide what information to keep. If the 25,000 photomultiplier tubes of the calorimeter detect an interesting amount of energy, the electronics raise a red flag and ask for this collision event to be saved for later analysis. Similarly, if the 7000 elements of the muon identifier spot the pattern characteristic of a muon passing through, the flag is again raised.

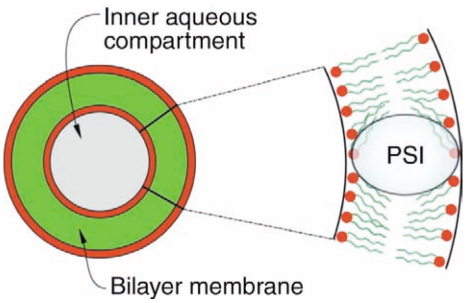
"We keep up to 10% of the raw information on collision events that comes through," says Young. "Our electronics take 4 millionths of a second to decide whether to store a particle event in memory for later analysis or to not store it. A global triggered decision is made by electronics built by Iowa State University/DOE's Ames Laboratory. If the decision is to keep the 500,000 bytes of information from one collision, the event is digitized, sent along an optical fiber to data collection electronics prepared by Columbia University, and thence along another fiber to a magnetic tape drive for storage. Later it is analyzed by a powerful parallel computer provided by BNL."

About 35 ORNL researchers and technicians and some 20 University of Tennessee graduate students were involved, especially between 1995 and 1998, in designing and testing 2200 electronic-circuit boards for PHENIX. Other researchers in the electronic development collaboration are from Iowa State University; Columbia University; SUNY at Stony Brook; Brookhaven and Los Alamos national laboratories; Lund University in Sweden; and the KEK Laboratory, plus the universities of Tokyo, Waseda, Hiroshima, and Nagasaki, all in Japan. Overall, some 200 persons worked on the electronics for PHENIX.

"Without such a diverse collaboration and an amazing collider," Young says, "we could never hope to mimic the beginning of the universe."

New Hope for the Blind from a Spinach Protein

Research at ORNL and the University of Southern California suggests that a spinach protein might someday restore sight to the legally blind.



Liposomes are tiny spheres that consist of a bilayer membrane and an inner aqueous compartment. Photosystem I (PSI) reaction centers have been inserted into the bilayer membrane to create PSI-proteoliposomes. The liposomes will be used as delivery vehicles for insertion of the PSI reaction centers into retina membranes, illustrated here.

Spinach may make Popeye the Sailor Man strong, but a protein from spinach may someday strengthen the vision of people who can barely see. Researchers at ORNL and the University of Southern California (USC) are investigating whether this chlorophyll-containing protein might be useful in restoring sight to the legally blind. The protein could replace a key, light-receiving part of the human eye that has lost its ability to function. People who suffer from age-related macular degeneration (AMD) or retinitis pigmentosa (RP), diseases that are the leading causes of blindness worldwide, may find hope in this research.

Although the neural wiring from eye to brain is intact in patients with these diseases, their eyes lack photoreceptor activity. Eli Greenbaum and his colleagues in ORNL's Chemical Technology Division (CTD) propose replacing these inactive photoreceptors with a spinach protein that gives off a small electrical voltage after capturing the energy of incoming photons of light. Called Photosystem I, or PSI (pronounced PS One), the main function of this "photosynthetic reaction center" protein is to perform photosynthesis, using the energy of the sun to make plant tissue.

Greenbaum made this proposal after meeting with Mark Humayun of the Doheny Retina Institute at USC. Humayun and his research team showed that if retinal tissue is stimulated electrically using pinhead-sized electrodes implanted in the eyes of legally blind patients, many of these people can perceive image patterns that mimic the effects of stimulation by light. Greenbaum suggested that it might be possible to use PSI proteins to restore photoreceptor activity. ORNL experiments showed that PSI proteins can capture photon energy and generate electric voltages (about 1 volt). The question is, can these voltages trigger neural events, allowing the brain to interpret images?

Currently, in the United States, degeneration of the retina—the light-sensitive layer of tissue at the back of the eye—has left 20,000 people totally blind and 500,000 people visually impaired. RP is an inherited condition of the retina in which specific photoreceptor cells, called rods, degenerate. The loss of function of these rod cells diminishes a person's ability to see in dim light and gradually can reduce peripheral vision, as well.

AMD is a disease that affects the center of vision; people rarely go blind from the disease but may have great difficulty reading, driving, and performing other activities that require fine, sharp, straight-ahead vision. AMD affects the macula, the center of the retina. When light is focused onto the macula, millions of cells change the light into an electrical current for the benefit of the neural wiring that tells the brain what the eye is seeing.

Using internal funds from the Laboratory Directed Research and Development Program at ORNL, Greenbaum, Tanya Kuritz, and James W. Lee, all of CTD; Frank W. Larimer of ORNL's Life Sciences Division; Ida Lee and Barry D. Bruce, both of the University of Tennessee; and Humayun and his team at the Doheny Retina Institute at USC are seeking a cure for AMD and RP. "We have assembled an outstanding interdisciplinary team of scientists, vitreo-retinal surgeons, ophthalmologists, and biomedical engineers, to attack this important problem," Greenbaum says.

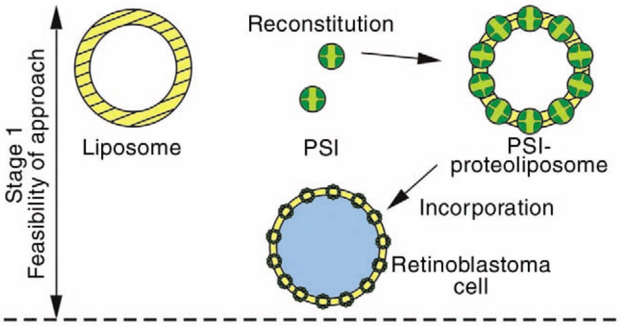
This project, he adds, is based on recent original discoveries in CTD. "Using the technique of Kelvin force microscopy, we have performed the first measurements of voltages induced by photons of light from single photosynthetic reaction centers. This work was published in 2000 in an issue of the *Journal of Physical Chemistry B*. The measured photovoltage values, typically 1 volt or more, are sufficiently large to trigger a neural response.

"We are proposing the insertion of purified PSI reaction centers into retinal cells to determine whether they will restore photoreceptor function in persons who have AMD or RP. Once we demonstrate this is possible, USC researchers will test the technique in the laboratory, and if feasible, later in humans in clinical trials."

In recent research, the collaborators showed that PSI reaction centers could be incorporated into a liposome, an artificial membrane made of lipids that mimics the composition of a membrane of a living cell. They also demonstrated that the PSI can be functional inside a liposome—that is, it produces the experimental equivalent of a voltage when light is shone on it. A liposome will likely be used to deliver PSI to a retinal cell.

Also, in work recently published in *Photochemistry and Photobiology* (June 2001), the collaborators have shown that isolated PSI reaction centers can photo-evolve hydrogen, indicating that PSI maintains its voltage-generating properties under conditions of current flow.

Greenbaum has long envisioned that his group's research in photosynthesis could have important impacts on humans in terms of energy production and biomolecular electronics. Now, he is especially excited that it also could lead to restoration of vision to the blind.



The PSI-proteoliposomes will fuse with deficient neural cells of the eye. If functional PSI reaction centers are inserted into a neural cell, sodium and potassium ions may be set in motion by the voltage generated by PSI reaction centers when stimulated by light. This ion motion can lead to the propagation of a voltage impulse along a neuron that transmits information to the brain. Figure by Tanya Kuritz.

Human Susceptibility and Mouse Biology

ORNL researchers are studying gene expression in mice to help find out why some persons are more likely than others to get certain diseases, even though their environmental exposures are similar.

Why does one person get cancer while other people do not, even though all have been exposed to approximately the same environment? Does genetic variability play a role in the susceptibility of each individual's cells to radiation damage, toxic chemical exposure, and possible cancer induction?

ORNL researchers are conducting studies with mice, which are genetically similar to humans, to help address these questions about human susceptibility. For example, the Department of Energy wants to know which parts of the human and mouse genomes cause individuals to differ in their responses to radiation. Which genes may be overexpressed (overactive in producing proteins) or underexpressed (turned down or off) in individuals whose DNA is more susceptible to radiation damage than others'?

Ed Michaud and his colleagues in ORNL's Life Sciences Division (LSD) are studying ORNL mouse mutants that are more susceptible to skin cancer. He is using gene microarrays to identify the networks of genes that are altered in mice that are more susceptible to skin cancer compared with normally resistant mice. "We are interested in determining which genes are involved in the normal development of the skin and its function as a barrier to protect our bodies from various environmental agents," Michaud says. "By determining the networks of genes that specify healthy skin, and how subtle changes in these genes make mice more susceptible to skin cancer following exposure to environmental stresses and toxins, we hope to gain a better understanding of the molecular mechanisms underlying human susceptibility to cancer and other diseases of the skin."

LSD's Gene Rinchik and his colleagues are beginning to study differences in the genetic responses of the skin, lymphoid, and reproductive tissues of mice from different strains as a result of exposure to low-level X rays. By studying in specific tissues the responses of many genes to low-dose radiation in different strains of mice, or in descendants of mice treated with a chemical mutagen, Rinchik hopes to identify individuals that differ in their cellular response to such low radiation doses. He and his colleagues can then study whether such variation is significant in the animals' susceptibility to various diseases, including cancer.

Using microarrays, they are looking at which genes are overexpressed or underexpressed in exposed versus nonexposed tissues in these different strains of mice. By looking at gene-expression ratios, they can identify variants in the response. Future genetic mapping and mutation-finding techniques (such as temperature-gradient capillary electrophoresis) can compare DNA from the mutant mouse with the draft sequence of the mouse genome, to identify mutant genes responsible for the differential response to radiation.

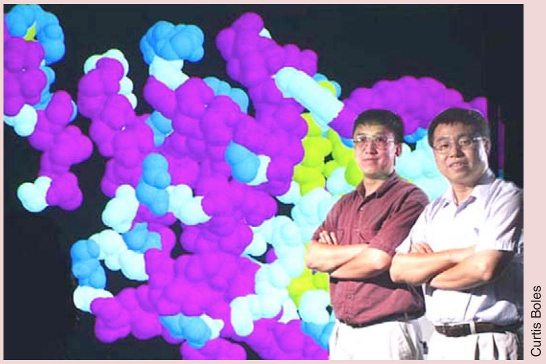
ORNL Corporate Fellow Liane Russell, shown here with ORNL Director Bill Madia, has found that the developmental stage at which parental reproductive cells are exposed is important to both the frequency and nature of transmitted genetic damages.

ORNL Corporate Fellow Liane Russell of LSD, in studying the risk of damage to a mouse's health from parental exposure to radiation or chemicals, has found that the developmental stage at which the parental reproductive cells are exposed is of paramount importance not only to the frequency but also to the nature of the transmitted genetic damages. Thus, the interval between exposure of an individual to a given mutagenic agent and the conception of offspring has a major influence on the likelihood that genetic damage will be inherited. While different environmental agents had been found to exert their maximum effects at various developmental stages, ranging from stem cells to mature sperm or ova, no chemical had been discovered to be especially active during stages critical for chromosome pairing and segregation. Recently, Russell found that the topoisomerase-II inhibitor "etoposide" not only induces mutations during that interval but also alters the frequency with which genes on homologous chromosomes recombine.

LSD's Bem Culiat is conducting a study to determine why some mice are more susceptible than others to DNA damage from toxic chemicals. Some 20 years ago retired biologist Walderico Generoso found evidence suggesting that eggs from some mouse strains can correct damage in sperm from male mice exposed to a toxic chemical, thereby reducing the percentage of embryo deaths. By using a combination of genetic, cytological, and gene expression studies in newly fertilized eggs, Culiat hopes to determine whether the egg repairs damaged DNA (Generoso's hypothesis) or whether the egg's extracellular coat can screen for normal sperm and keep damaged sperm out (an alternative Culiat hypothesizes). Early results have neither ruled out nor substantiated either hypothesis.

It thus appears that susceptibility to diseases or to exposures depends at least partly on multiple, genetically programmed internal responses of the body to external influences.

Award-winning Biology Feat



Ying Xu and Dong Xu, computational biologists at ORNL, received an R&D 100 Award from *R&D* magazine in 2001 for the product of their basic research—a protein structure prediction tool called PROSPECT.

Modeling a Fusion Plasma Heating Process and Stellarator

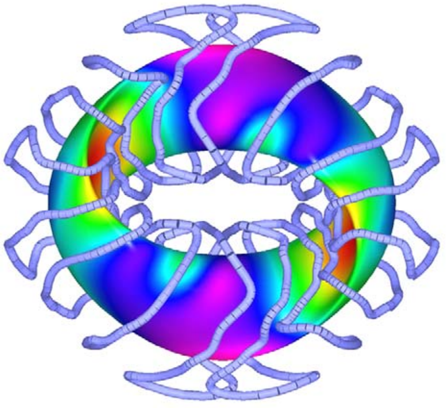
ORNL researchers are using a supercomputer to simulate a fusion heating method and future fusion device.

The wave of the future for controlling fusion energy—the process that powers the sun—may include more effective harnessing of a fusion device heating process, using electromagnetic, or radio, waves. An understanding of how to get "radio-controlled fusion" may come from calculations done using supercomputers at ORNL.

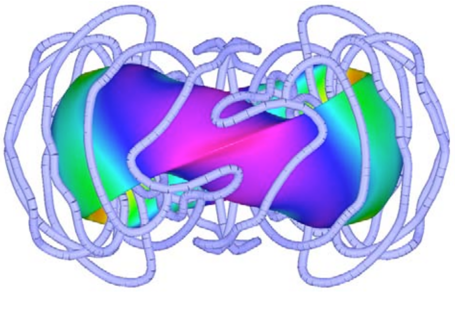
Controlled fusion energy, when achieved, could be a favored energy source someday. It would draw upon an unlimited source of fuel—hydrogen isotopes from seawater—and would produce no greenhouse gases that could adversely affect climate.

The first key to achieving fusion energy is to heat charged particles (nuclei of hydrogen isotopes) to very high temperatures such that the electrical repulsion of the nuclei is overcome during collisions, allowing nuclear fusion reactions to occur. At these temperatures, the electrons are completely stripped from the atomic nuclei, yielding an electrically conducting gas called plasma. The second key is to hold, or confine, the particles and their energy with magnetic fields long enough for many collisions and reactions to occur. Such fusion reactions would release enormous amounts of energy that can be converted to electricity.

In the quest for controlled fusion, scientists have attained several important milestones. They have achieved plasma temperatures as high as 520 million degrees, more than 20 times the temperature at the center of the sun. More than 16 million watts of fusion power have been produced in the laboratory. The unsolved problem is how to control fusion plasmas to get sustained fusion reactions. The goal is to prevent the loss of heat from the plasma center to the edge as a result of irregular fluctuations in plasma velocity and pressure (turbulence) brought on by the plasma current and other causes.



Above: Top view of the Quasi-Poloidal Stellarator (QPS), which is an optimized, low-aspect-ratio fusion stellarator device. The plasma shape (colors indicate magnetic field strength) and filamentary magnetic coils (light blue) are shown. Below: Side view of the QPS optimized low-aspect-ratio stellarator device. Visualizations here and on the back cover by Don Spong.



"Besides heating the plasma in the way that a microwave oven heats food, experiments show that radio waves can drive electric currents through the plasma and force the plasma fluid to flow," says Don Batchelor, head of the Plasma Theory Group in ORNL's Fusion Energy Division (FED). "These waves have even been seen to improve the ability of the applied magnetic field to hold the energetic particles and plasma energy inside the device."

"Radio waves give us the best 'knob' for precision control of the plasma," says Mark Carter of FED. "With radio waves we can control where the power goes, because these waves resonate with the motion of the plasma particles as they orbit around magnetic field lines. Unfortunately, because the orbiting plasma particles move at nearly the speed of light, it has been impossible to calculate how they will respond to radio waves and how much electric current they will produce."

To address this problem, Fred Jaeger and Lee Berry of FED, working with Ed D'Azevedo of ORNL's Computer Science and Mathematics Division, developed a computer program for the IBM supercomputer of the Department of Energy's Center for Computational Sciences at ORNL to compute plasma waves across the entire cross section of a fusion plasma. The program solves an enormous set of equations, providing the first two-dimensional (2D), high-definition picture of radio waves injected from an antenna into the plasma of a doughnut-shaped tokamak. Using 576 processors at speeds of up to 650 billion operations per second, the program shows that, at certain locations, the waves shift from a long-wavelength to a short-wavelength structure (mode conversion) and become rapidly absorbed by the plasma. The group has recently created a 3D code for this modeling that could lead to a method of fine tuning the injection of the waves to maximize control of the plasma.

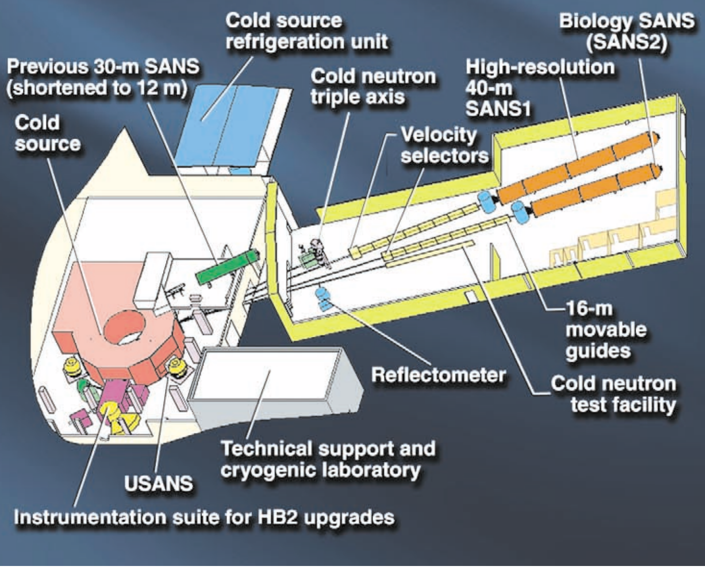
Another area in which FED scientists are using supercomputers to advance fusion research is in the analysis of very complex, nonsymmetric magnetic systems for plasma containment, called stellarators. These are shaped like a cruller wrapped with twisting magnetic coils. The ORNL supercomputers were used in the analysis and design of a new type of magnetic fusion device called the Quasi-Poloidal Stellarator (QPS). QPS will use a much smaller plasma current and rely more heavily on external coils to provide the needed magnetic fields for plasma confinement. This device may result in a much smaller and more economically attractive fusion reactor than existing stellarators and would eliminate the potentially damaging plasma disruptions that plague conventional research tokamaks. It is hoped that QPS will be built at ORNL, using DOE funds, starting in 2003.

"We are employing a Levenberg-Marquardt algorithm on the IBM supercomputer to calculate how to modify the plasma shape to optimize energy transport and plasma stability," says Don Spong of FED. "Once we have determined the best shape, then we will infer the design of external magnetic coils that can be engineered cost effectively to achieve that shape."

"We need supercomputers to model as many as 40 variables that interact with each other to describe the plasma," Batchelor says. "We are twiddling 40 knobs at the same time computationally to get six or more competing physical properties simultaneously as good as they can be."

The beauty of the new technique developed to study waves is that it can be extended to 3D plasmas such as those in stellarators. These are significantly more complicated in shape than the tokamak, the present state of the art for plasma wave computations.

With the help of ORNL's supercomputers and new funding from DOE's Scientific Discovery through Advanced Computation (SciDAC) initiative, fusion researchers at ORNL are likely to make waves in this important energy research field.



When ORNL becomes the world's leading center in neutron science, rapid advances in characterizing nanoscale materials will likely follow.

Neutron Sources and Nanoscale Science

When ORNL's new neutron sources go on-line in the next few years, researchers will have valuable tools for exploring the features of matter as small as a few billionths of a meter. That's one reason why many researchers involved in nanoscience and nanotechnology are excited by two ongoing initiatives at ORNL. One initiative is the upgrade of the High Flux Isotope Reactor (HFIR), which will offer in 2002 the world's highest thermal neutron intensities and in 2003 cold neutron fluxes comparable to the world's best. The other initiative is the construction of the Spallation Neutron Source (SNS), which by 2006 will provide 10 times the flux of any other pulsed (spallation) neutron source in the world.

"Reactor and spallation neutron sources are well matched to the nanoscale," states the 1999 *Nanotechnology Initiative Report* of the Department of Energy's Office of Basic Energy Sciences (BES). The report points out that neutrons, for example, "can be used not only to study nanoparticles themselves but also to examine protective coatings that are placed on the nanoparticles to prevent oxidation. Neutrons can also be used to study dispersants that disperse nanoparticles in a solvent or host medium."

Because nuclei of hydrogen and deuterium (heavy isotope of hydrogen) scatter neutrons differently, neutron scientists often selectively label organic material with deuterium or use deuterated solvents so they can highlight what they want to see and block out the rest. "Using this method," says George Wignall, a neutron scientist in ORNL's Solid State Division (SSD), "we can optimize the contrast between the nanoparticle and coating so we can study the structure and behavior of the organic material surrounding the nanoparticle."

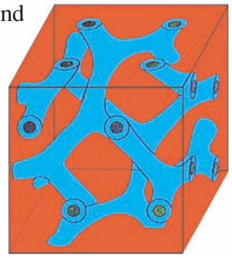
The use of organic materials, self-assembled organic structures, and organic hybrid materials is emerging as a route to producing functional nanoscale structures. Wignall is a principal investigator in a study of nanoscale-structured materials formed by self-assembly of triblock copolymers. Participants in the study, which is supported by internal funding from the Laboratory Directed Research and Development Program at ORNL, include Tony Habenschuss of ORNL's Chemical and Analytical Sciences Division (CASD) and polymer chemist Frank Bates and his colleagues at the University of Minnesota. Triblock copolymers synthesized by Bates have been studied by Wignall and Habenschuss using small-angle neutron scattering (SANS), X-ray scattering, atomic force microscopy, and electron microscopy. SANS will be especially useful for studying these fascinating materials at ORNL when the HFIR upgrade is complete.

In 2003, the cold neutron flux at HFIR will be comparable to that of the Institut Laue Langevin in Grenoble, France, which is the best research reactor in the world for neutron scattering research. "The upgrade will boost HFIR's cold neutron flux and detection efficiency," says Wignall. "Because our neutron detector will be two-and-a-half times larger than what we have now, we will be able to make simultaneous measurements over a much wider range of angles and perform time-resolved experiments. For example, we will be able to make real-time studies of materials as they are processed and observe the self-assembly of triblock copolymers."

Triblock copolymers are made by joining three chemically distinct polymer blocks (large molecules), each a linear series of identical monomers (small molecules).

"Because the three blocks linked together in a linear arrangement may be thermodynamically incompatible, they will try to separate from each other," Habenschuss says. "But since they are joined together, they can only form separate domains on a scale of the individual block sizes—that is, on a nanometer scale for typical block lengths. These separate domains self-assemble into complex ordered nanostructures."

Examples of these structures are rods or spheres of one material regularly arranged in the matrix of another. A particularly interesting morphology studied at ORNL is the continuous core-shell gyroid structure in which three-dimensionally continuous channels wind through a matrix.

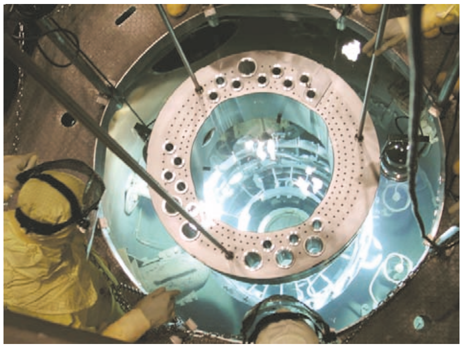

Core-shell gyroid structure.

"Previously we had used SANS to study diblock copolymers made of polystyrene and polybutadiene," Wignall says. "In the LDRD study we investigated triblock copolymers of polyisoprene, polystyrene, and polydimethylsiloxane."

Self-assembled triblock copolymers could create hundreds of new morphologies. Such materials could result in improved power-producing fuel cells and gas-separating membranes.

"A large fraction of potential users of the upgraded HFIR and the SNS have expressed interest in studying soft matter, such as proteins and polymers, using SANS, reflectometry, and other instruments," Wignall says. As noted in the *BES Nanotechnology Initiative Report*, "the potential impact of neutron sources for the elucidation of these nanostructures is tremendous."

According to Wignall, "We can expect studies of very small features in soft materials to get a big boost when ORNL becomes the world's leading center for neutron scattering research in the middle of this decade."


A new beryllium reflector (to redirect outflowing neutrons back into the reactor core) was recently installed as part of the HFIR upgrade.

Quantum-Dot Arrays for Computation

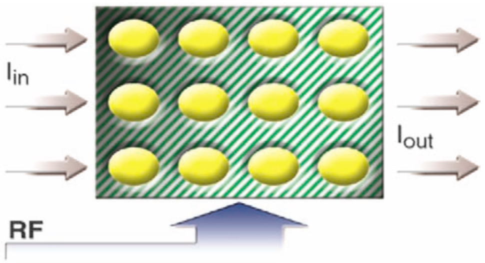


Illustration by LeJean Hardin

Two-dimensional quantum-dot array showing currents as input channels I_{in} and output channels I_{out}. A radiofrequency (RF) field is introduced to modulate the currents, providing the necessary degrees of freedom to perform pattern recognition.

An ORNL team is designing a quantum-dot array that will be used to carry out innovative computations at room temperature.

In recent years, considerable progress has been made in the development of advanced sensors, capable of detecting increasingly complex signal patterns. Hyperspectral imagers, for instance, that acquire data resolved not only in space but also spectrally (i.e., at many wavelengths), enable the extraction of unique characteristics, unobtainable by other means. For example, looking at a ball containing blueberries and grapes, one can, with the same sensor, not only distinguish each individual fruit, but also estimate the freshness of each or whether it has humidity on its surface. The ongoing trend toward sensor miniaturization (down to nanoscale sensors) provides a strong incentive to develop computational capabilities for processing the rich signal information at the sensor's scale. A major step toward developing computational "brain" power to speed up the processing of signal patterns is being taken by a multidisciplinary nanotechnology project at ORNL, supported partly by internal funding from the Laboratory Directed Research and Development Program. Researchers at the Laboratory are fabricating a nanoscale pattern-recognition device, using gold nanoparticles on a DNA template, which may eventually prove the feasibility of this concept.

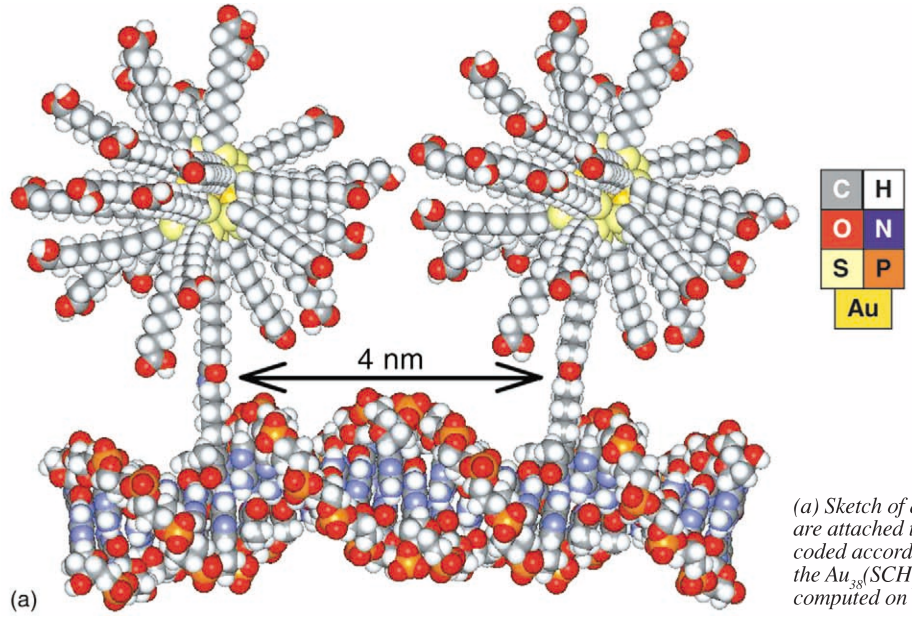
Specifically, the ORNL team is designing a quantum-dot array that can be operated at room temperature to carry out innovative computations. The construction and operation of this array, with the help of special algorithms, will constitute the world's first successful use of a nanoscale device to solve nontrivial computational problems such as signal discrimination. The advantage of embedding such a nanoscale computer into a micro- or nanosensor is that it avoids the need to send the signal from the sensor to a conventional computer a long "distance" away (both literally and figuratively in terms of scale). Information can be processed at the site of the sensor. An array of specially coated and closely placed gold nanoparticles, called quantum dots, may enable the operation of such "smart sensors" at room temperature.

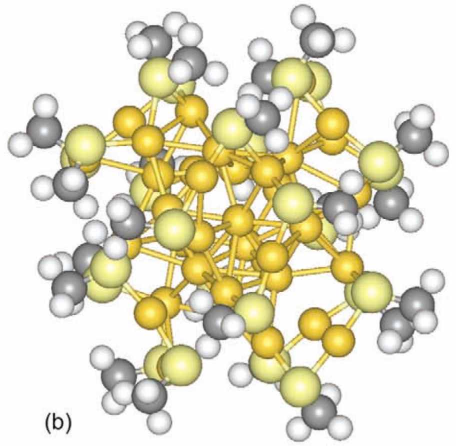
ORNL's first quantum-dot array, which will straddle gold electrodes, will receive a vector of input currents from a sensor and produce a vector of output currents. It will be "trained" to classify patterns into categories that characterize specific classes of properties to be detected by the sensor. The output currents will indicate the class of the observed pattern, to allow appropriate actions to be taken.

"Our goal is to demonstrate via a proof-of-principle experiment how to produce a nanoscale information-processing device for a sensor," says Jacob Barhen, director of ORNL's Center for Engineering Science Advanced Research (CESAR) and head of this project. Barhen, Yehuda Braiman, Vladimir Protopopescu, and Nageswara Rao, all from CESAR and ORNL's Computer Science and Mathematics Division (CSMD), are developing the methodology and algorithms needed to implement neuromorphic computations, which will allow the quantum-dot array to learn and retrieve information.

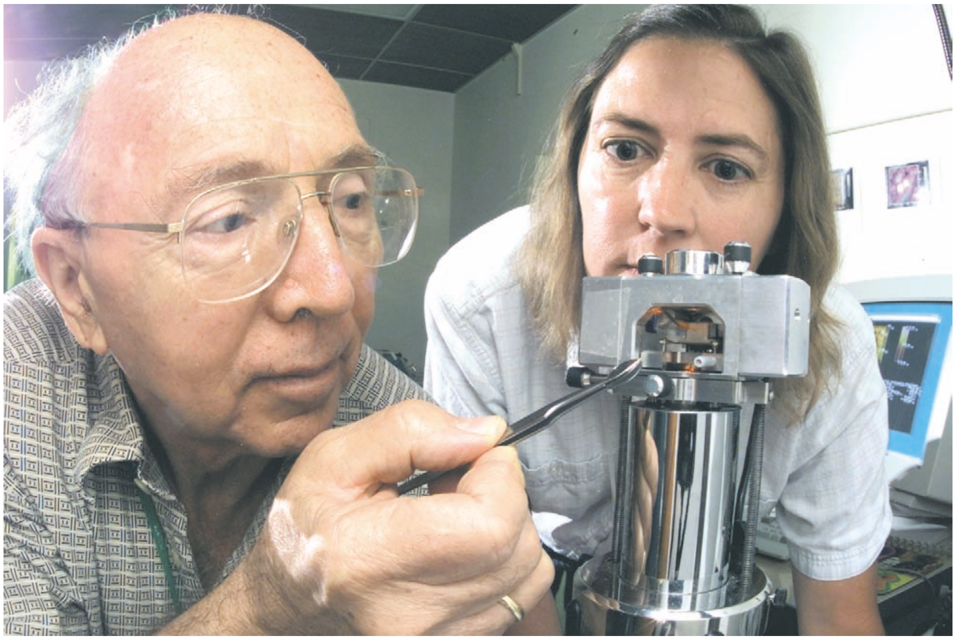
The practical goal of the ORNL team is to build a device that emulates a neural network. Instead of the neurons and connecting synapses found in the brain, the nanoscale computer will depend on electrically charged gold quantum dots connected by electrons that tunnel between them at different rates.

In a neural network, the learning process modifies the interconnection strengths (synapses) between neurons. In a quantum-dot circuit, the





(a) Sketch of a DNA-nanoparticle assembly. Functionalized gold clusters are attached to a DNA chain via peptide bonds. Atomic species are color-coded according to the table on the right. (b) An optimized structure of the $Au_{38}(SCH_3)_{24}$ cluster, obtained by quantum molecular dynamics computed on the IBM supercomputer at ORNL. See (a) for color coding.


Curtis Boles

Leon Maya (left) makes gold nanoparticles and coats them with alkylthial and carboxyl molecules. Karen Stevenson (right) will attach the coated particles to a DNA template.

inverse of a generalized capacitance matrix plays the role of the synaptic matrix. Unfortunately, once fabricated, the elements of this capacitance matrix are essentially fixed. Braiman suggested that exposing the array to an excitatory electromagnetic field would result in a modification of the tunneling rates of single electrons hopping between the quantum dots. By modifying the tunneling rate, the device will produce different output current patterns for the given input signals into the array. Using this phenomenon of photon-assisted tunneling, Barhen designed a neuromorphic learning algorithm, in which the amplitudes and frequencies of the polychromatic excitatory field are used as control parameters to achieve maximal discrimination between various classes of signals. Braiman and Protopopescu are focusing on issues related to the stability of the nonlinear dynamics underlying the device's operation, while Rao is exploring more advanced architectures for digital signal processing using nanodevices.

"The microwave field provides degrees of freedom and the ability to change electron pathways and rates of electrical conduction," Barhen says. "In this way, this device will mimic neurons in the brain. The pathways that the electrons take to minimize the discrepancy between a desired pattern class signature and one produced by the array under excitatory field illumination will enable the solution of the pattern classification problem. The array will consist of gold nanoparticles 1.5 nanometers (nm) in diameter that self-assemble by attaching to pre-selected locations about 3.5 nm apart on a specially engineered DNA template about 70 nm long. The nanoscale size of the particles and their regular placement in close proximity to one another is necessary for the array to function as a nanoscale computer at room temperature.

Because of gold's affinity to sulfur, the gold particles are coated and stabilized, or "passivated," by sulfur-containing molecules attached to gold molecules that connect into the DNA template. Specifically, the coating is a monolayer of alkylthiol organic molecules terminated with a carboxyl group (containing carbon, oxygen, and hydrogen) that binds to amino groups, attached to the DNA at specified locations. (Amino groups, which contain nitrogen and hydrogen, used in the coupling to gold, are external to the DNA, in contrast to amines involved in the pairing of bases between two strands of DNA to make it double stranded.)

The material's fabrication and assembly are being performed by CESAR's Leon Maya, a chemist in the Chemical and Analytical Sciences Division (he makes the gold nanoparticles and coats them with the alkylthiol and carboxyl molecules), as well as CESAR researchers Karen Stevenson, Muralidharan Govindarajan, and Thomas Thundat, all of ORNL's Life Sciences Division, who attach the coated gold particles to the DNA template. So far, some 20 gold nanoparticles have been attached along a DNA template. The plan is to attach the gold nanoparticles in a grid on a DNA scaffold, which will be fitted between the electrodes. If necessary, the DNA bases between the gold particles will be destroyed using ozone or ultraviolet light, leaving the gold particles on a substrate spanning the space between the electrodes.

A gold nanoparticle is a cluster of gold atoms bound together by mutual attraction. In a cluster, most electrons circulate around the gold nuclei, but some hop back and forth between the outer shells of the gold atoms. Using the IBM supercomputer at DOE's Center for Computational Sciences at ORNL, CESAR's Jack Wells (of CSMD), working with David Dean and Mike Strayer (both of the Physics Division), is simulating the electronic density of clusters of gold atoms in support of the design of the quantum-dot array.

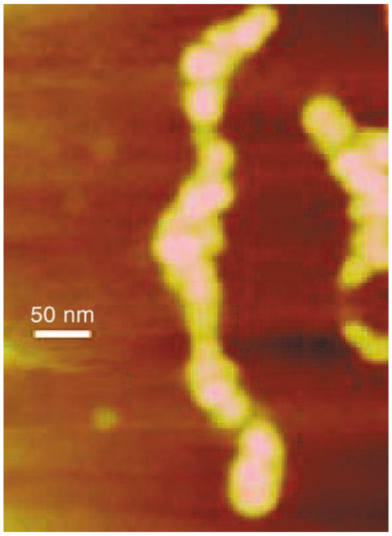
Understanding electron density in these clusters is important because the gold nanoparticles arranged every 10 or 11 DNA bases on a DNA scaffold will conduct electricity in the same way that water drips from a faucet rather than as a steady water flow. If the voltage is high enough, the electrons flow by single-electron tunneling, hopping between the weakly coupled nanoparticles and producing a very nonlinear relationship between the current and the voltage. A range of low voltages could produce no current, representing a "0," and higher voltages could produce a current spike that represents a "1" for use in information processing.

Employing a functional density code obtained from the IBM Research Division in Zurich, Wells, in collaboration with Wanda Andreoni of IBM, has modeled a bare cluster of 38 gold atoms, calculated their electronic structure (the locations of the electrons in shells and between outer shells of the atoms), and related the size of a cluster to the number of its electron charges. He has also simulated the energy effects of adding or removing an electron.

"This information is sufficient to predict the electrical capacitance of the nanocluster and to allow us to quantitatively analyze structures in nanoscale circuits," Wells says. "Such information is difficult to obtain from direct experimental observation."

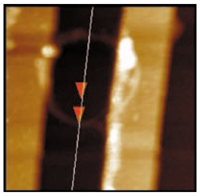
Wells modeled a passivated 38-atom gold cluster bound with 24 methylthiol groups (sulfur group plus a methyl group, or SCH_3). "I found the binding with the chemical group causes the reorganization or rearrangement of the gold atoms in the cluster, compared to the idealized case of the unpassivated cluster," he says. These calculations being done to find new properties in very small features require a large amount of computing capacity—about one-third of the IBM supercomputer's nodes.

The early research success in attaching gold nanoparticles to a DNA template has been submitted for publication. The researchers are now taking on bigger challenges as they attempt to build a world-class nanoscale device to solve global problems.



Atomic force microscope image of a gold nanoparticle attached to DNA.

Carbon Nanotubes and Nanofibers: The Self-Assembly Challenge



ORNL researchers are devising innovative methods that will trick nanoscale bits of matter into assembling themselves into useful products, such as artificial membranes, electronic components, and structural materials.

When Dave Geohegan and his colleagues in ORNL's Solid State Division (SSD) produce carbon nanotubes by laser ablation, they get a tangled mass of carbon that looks like black, fluffy felt to the naked eye and cooked spaghetti and meatballs in transmission electron microscopy images. By putting the material into a solvent and shaking it up using ultrasonic agitation, the carbon blobs disappear and the spaghetti-like tubes become less tangled. Some carbon nanotubes are pulled out of solution into a pipette and deposited on a spinning silica substrate where they naturally stick, partly because of static electricity. The problem with this manual technique is that it is slow, and only a small concentration of nanotubes is attached to the surface.

A dream shared by some researchers is to get nanotubes to assemble themselves into long rods, somewhat like uncooked spaghetti but far more flexible. Carbon nanotubes, which resemble rolled-up chicken wire because their carbon atoms are arranged in a hexagonal configuration, are only a few nanometers in diameter and up to hundreds of microns long. Their tensile strength is the highest in the world, some 100 times stronger than steel, with only one-sixth the weight. These materials may someday be linked together or incorporated as fibers in a polymer composite to form structural materials for aircraft, spacecraft, and suspension bridges.

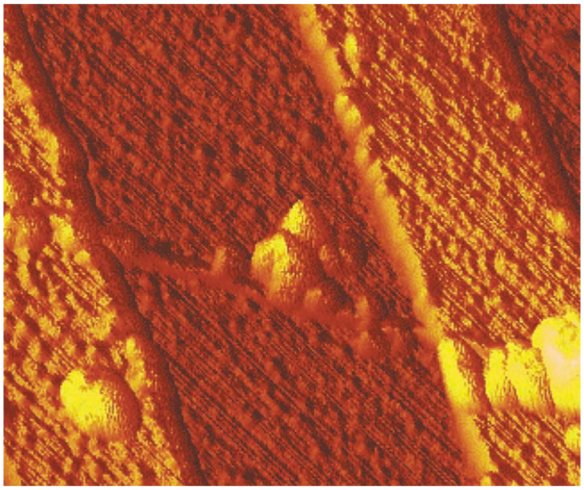
Carbon nanotubes also conduct electricity in different ways. In ORNL's Instrumentation and Controls (I&C) Division, Mike Simpson, Michael Guillorn, Derek Austin (University of Tennessee graduate student), and others have shown that the electronic properties of carbon nanotubes make them suitable to serve as miniaturized rectifiers (components that allow one-way flow of electrons) and replacements for silicon channels in field-effect transistors (FETs).

"How the carbon sheet is rolled up into a tube affects its electronic properties," Guillorn says. "Rolled one way, a carbon nanotube is a good electrical conductor and could be used as nanowires; rolled another way, it is a good semiconductor." In an FET, electrons flow through a silicon channel unless a gate electrode applies a voltage to a silicon dioxide film whose electric field pinches off the current by raising the resistance in the channel. In this way, a transistor can operate as an on-off switch or store a bit of information (1 or 0). This modulation of conductivity is possible because the silicon transistor is doped in a controlled manner with impurities that serve as charge carriers.

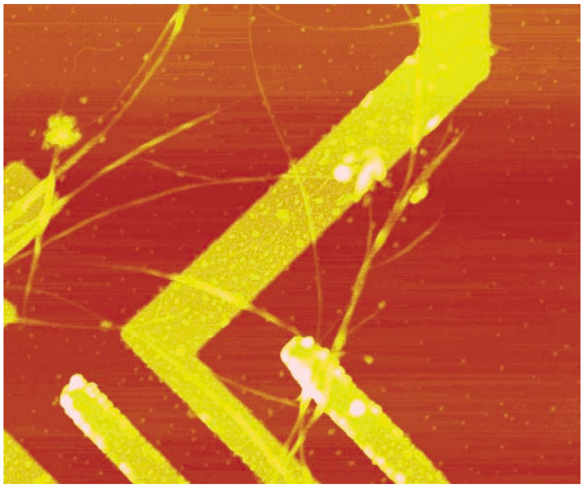
ORNL researchers have shown that a carbon nanotube supported on two electrodes on a silicon dioxide insulating layer can replace that channel and conduct electricity when a potential is placed on the silicon base. The conductivity of the nanotube is controlled by whether the electric field is turned on or off. Austin measured the change in current flow in a carbon nanotube that resulted when the voltage on a silicon gate electrode was changed.

"To get the right number of charge carriers, a certain concentration of dopants is needed in a silicon transistor," Guillorn says. "If the size of the transistor is reduced considerably, it could have virtually no dopants or charge carriers. That's why a device approaching the nanoscale may require a semiconducting carbon nanotube to replace the silicon channel."

Can individual carbon nanotubes a few microns long be interconnected chemically using molecular handles, incorporated as reinforcing fibers in a polymer matrix, or threaded through the helices of polymer molecules (e.g., polyphenylene)? Can a sheet of carbon nanotubes be grown using laser ablation? A major challenge in nanoscience is to trick tiny features of matter 50,000 times smaller than the period at the end of this sentence to assemble themselves into useful products, ranging from logic gates for nanoscale transistors, to structural materials for aircraft, to



An atomic force microscope (AFM) image of an ORNL-produced carbon nanotube bundle containing an impurity on a gold-palladium (AuPd) electrode structure.



An AFM image of single-walled carbon nanotubes deposited on a palladium electrode structure. These nanotubes were produced by laser ablation at ORNL.

(Opposite page) An AFM image of a circular carbon nanotube bundle on a AuPd electrode structure.

long cables for power transmission and suspension bridges.

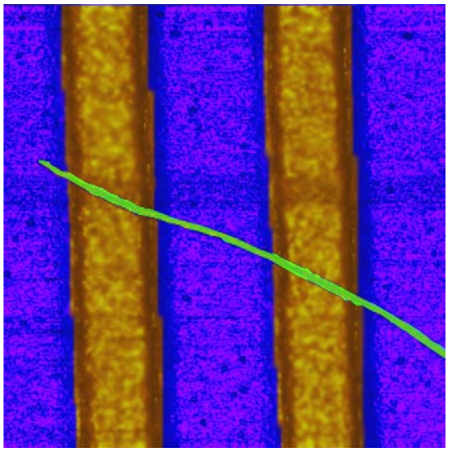
One approach being taken at ORNL is to link carbon nanotubes using strands of DNA. In double-stranded DNA, the chemical bases of either strand are paired with their complementary bases (A with T, C with G) in the other strand by hydrogen bonding. Because DNA can be terminally modified with primary amines, which can selectively react with carboxylic acids under certain reaction conditions, it may be possible to self-assemble carbon nanotubes by first linking them to DNA strands. The DNA strands could bring the nanotubes together; the DNA could be removed later by exposing it to high temperatures.

ORNL research showing early indications that carbon nanotubes can be connected chemically using DNA is part of the “Biomolecule-Assisted Self-Assembly of Three-Dimensional Carbon Nanotube Nanostructures” project at ORNL, which is supported by internal funding from the Laboratory Directed Research and Development (LDRD) Program. The project’s lead investigator is Mitch Doktycz of ORNL’s Life Sciences Division. Other participants are Doug Lowndes, Vladimir Merkulov, and David Geohegan, all of SSD; Simpson and Guillorn, both of the I&C Division; Phil Britt of ORNL’s Chemical and Analytical Sciences Division, and Anatoli Melechko, Lan Zhang, and Jim Fleming, all of the University of Tennessee.

“Our goal is to find ways to enable self-assembly of carbon nanotubes into nanoscale structures, systems, and devices by interfacing natural materials with artificial materials,” Doktycz says. “Self-assembly of nanosystems is recognized as one of the grand challenges facing nanotechnology. We believe a solution to many of these challenges lies in the use of natural systems such as DNA.”

The objectives of this LDRD project are to fabricate nanotubes and ordered arrays of nanofibers, attach biomolecules to carbon nanotubes and nanofibers, develop nanoscale characterization techniques, and design and build molecular assemblies. Nanoscale systems that could result from self-assembly could be nanoelectronic components and devices, sensors and biosensors, nanomachines, and materials that mimic the membranes enveloping living cells.

“Before attaching nanotubes to DNA, a raw mass of nanotubes must first be purified,” Britt says. “Single-walled carbon nanotubes produced by laser ablation at ORNL by Dave Geohegan and Alex Puretzky are digested in nitric acid to oxidize the carbonaceous impurities to make them soluble in water so they can be washed away. The material is then heated in air at 550°C to oxidize the remaining carbonaceous impurities. Hydrochloric acid is introduced to remove the remaining nickel-cobalt catalyst particles added during laser ablation to induce the growth of carbon nanotubes. During these purification steps, carboxylic acids are formed at the nanotube ends, giving us a chemical handle for attaching carbon nanotubes to DNA. Carboxylic acids bond selectively with the terminal amines that are added to DNA strands.”

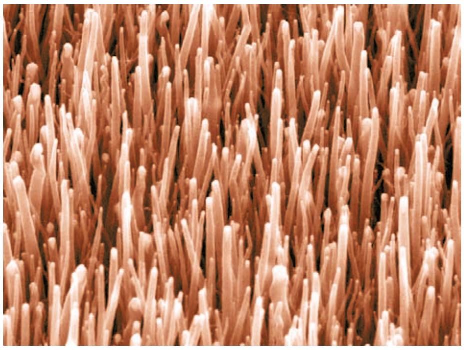


ORNL researchers have shown that a carbon nanotube supported on two electrodes could replace a silicon channel in a field-effect transistor.

Britt notes that ORNL researchers cannot confirm whether they have succeeded in attaching nanotubes to DNA through the formation of chemical bonds without using advanced characterization tools such as Raman spectroscopy, Fourier transform infrared spectroscopy, and near-infrared spectroscopy. “We also need to characterize ORNL-made nanotubes to determine the nature of their defects,” Britt says. “We may even find that the defects are good because they may provide handles for attaching the tubes chemically to another material.”

An earlier success in self-assembly at ORNL is the growth of a patterned carpet of carbon nanofibers on a silicon base. Using plasma-enhanced chemical vapor deposition (PECVD), ORNL researchers Merkulov, Anatoli Meleshko, Lowndes, Yayi Wei, and Gyula Eres, all of SSD, have demonstrated that they can grow vertically aligned carbon nanofibers in a desired pattern on the substrate. They can choose the diameters of the fibers, their positions, and the spacing between individual fibers.

Fiber sizes and locations are determined by depositing nickel dots and lines on a substrate, using electron beam lithography. The substrate is then placed in a furnace containing acetylene gas, the source of carbon that grows as crystalline fibers on nickel, which catalyzes fiber synthesis. One carbon nanofiber grows on each nickel dot. Plasma-enhanced CVD is used because the plasma creates an electric field perpendicular to the surface, causing the fibers to grow upwards on it. The patterned growth of vertically aligned carbon nanofibers using PECVD is an example of controlled self-assembly of a material at the nanoscale.



“Forest” of randomly placed, vertically aligned carbon nanofibers grown by ORNL’s Vladimir Merkulov and Doug Lowndes, using plasma-enhanced chemical vapor deposition. Note the nickel-catalyst nanoparticles at the tips of the nanofibers.

A carpet of closely spaced nanofibers could be used to create an artificial membrane that allows tiny molecules or small particles to diffuse through while keeping out unwanted large molecules or big particles. Such a creation might mimic the membrane covering a living cell that allows signal proteins to enter its pores and activate cellular machinery. Carbon nanofibers could also be used to make electron probes that characterize the electrochemical behavior of living cells and monitor intracellular phenomena.

Guillorn, Simpson, and others are experimenting with using carbon nanofibers as massively parallel electron guns—sources of precise electron beams that could create patterns of circuits that range from 10 to 100 nm across. If nanocircuits could be produced by electron beam lithography using computer-controlled, carbon-nanotube-tipped field emitters, the resulting chips would be closer to the semiconductor industry’s 2004 goal: production chips with circuits 8 times denser and 16 times faster than chips of the same size currently being etched by optical lithography. The electron beam approach is needed to reach this goal because the wavelength of an electron is much shorter than that of a photon of light.

Recent studies have shown that electrons are emitted from carbon nanotubes at relatively low electric field intensities of a few volts per micrometer. Thus, nanotube electron emitters should operate at the low voltages needed for nanoscale circuitry.

“We demonstrated that a carbon nanofiber inside a well can emit electrons,” Guillorn says. “When we placed a field on the fiber, an electron was emitted. The field allows electrons to escape from the tip.”

A carbon nanofiber could be used to make a higher-resolution electron microscope because it would focus the microscope’s electron beam on a smaller spot.

Research is under way to develop less expensive, more reliable, and energy-efficient flat-panel displays to replace bulky, power-hungry computer monitors. Because carbon nanofibers are inert, they could be more stable and practical than metallic (silicon) and inorganic electron sources for stimulating the emission of colored light in flat-panel displays. “All types of electron emitters work under ultrahigh vacuum,” Guillorn says. “But at the higher pressures that may occur in real-world devices, residual gases are ionized, and the resulting ions bombard the tip of a metallic or inorganic emitter, sputtering it off so it is less effective as an electron emitter. Carbon nanofibers resist this type of damage, so they should last much longer in advanced flat-panel displays.”

Carbon nanotubes and nanofibers are incredibly small, but their potential for creating advanced materials is huge.

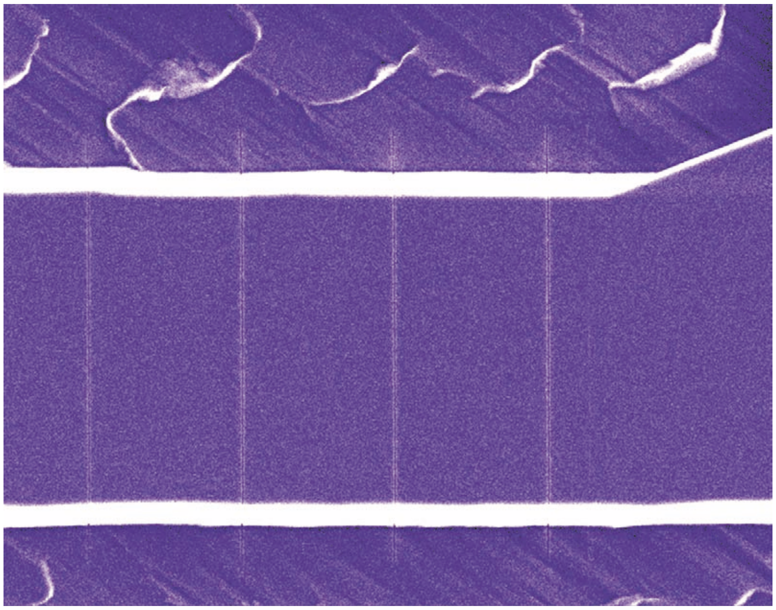
Incredible Shrinking Labs: Weighing a Move to the Nanoscale

ORNL researchers are showing they can fabricate nanofluidic lab-on-a-chip devices, do experiments with them, and predict fluid behavior within them, as well.

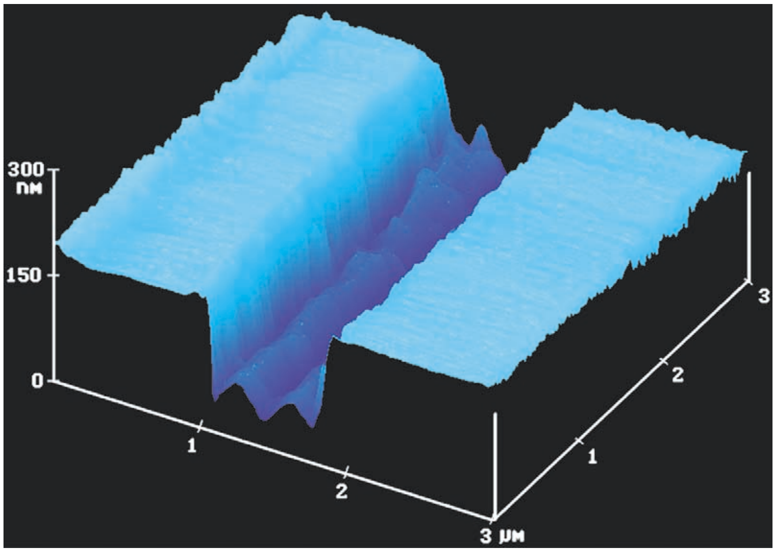
Imagine a device the size of a deck of cards that could help a physician quickly determine why you are feeling so sick and tired. By rapid analysis of the DNA and proteins in a drop of your blood, a "nanofluidic lab on a chip" could indicate to your doctor a million to a billion times faster than current devices whether a bacterium, virus, or a cancerous tumor is making you ill. At least, that's one application seen by scientists involved in the new field of nanofluidics: the active transport of material through a channel or conduit whose diameter is less than 100 nanometers (nm). A nanometer is a billionth of a meter.

Basic research in nanofluidics is being conducted by ORNL and University of Tennessee (UT) researchers, using internal funding from the Laboratory Directed Research and Development (LDRD) Program at ORNL. The LDRD project is headed by Mike Ramsey, an ORNL corporate fellow in the Laboratory's Chemical and Analytical Sciences Division and the inventor of the lab on a chip.

The lab on a chip is a microfluidic structure first built by Ramsey 10 years ago to demonstrate the separation of chemicals in very small volumes. Six years ago, this technology was licensed to Caliper Technologies, Inc. Ramsey and his group in CASD are conducting considerable research on developing improved lab-on-a-chip technologies for biological, environmental, forensic, and defense applications. The lab on a chip has been honored by *R&D* magazine as one of the 40 top innovations it has recognized since beginning its R&D 100 competition in 1963. Additionally, a panel of citizens has named the lab on a chip one of the top 23 technologies developed using Department of Energy funding.



Above: Scanning electron microscope image of four nanotrenches vertically connecting two microtrenches. The nanotrenches are only 100 x 100 nm^2 in cross section but more than 40 microns long. Below: Perspective of a 900 x 80 nm^2 trench cut in silicon for nanofluidic studies at ORNL. The trench was created using a focused ion beam at Vanderbilt University and imaged with an atomic force microscope at ORNL.

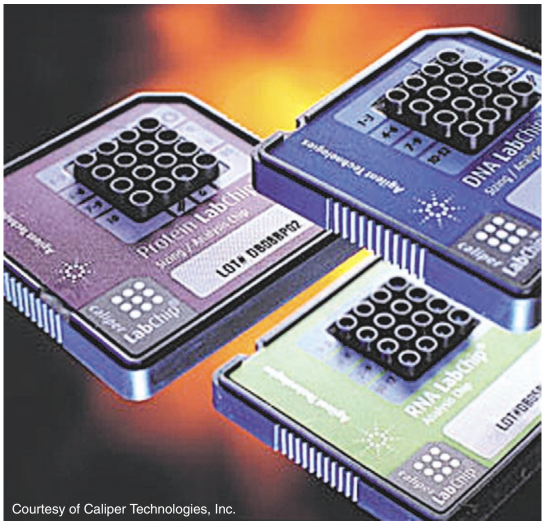


In a lab on a chip, several channels, each the size of a hair in width and one-fifth of a hair in depth, connect reservoirs containing chemicals. The channels and reservoirs are carved, or etched, in a glass chip (such as a microscope slide) using microfabrication techniques. Liquids are "pumped" through each channel, using electric fields or pressure differences, at a rate of one millionth of a drop per second.

"In a nanofluidic device," says Ramsey, "the typical channel would be 1000 to 10,000 times smaller than a hair. We expect that the interactions between the material in the channel and the channel walls—what we call solid-liquid interactions—will be much more dominant in a nanofluidic device from those in a microfluidic device. We expect fluids to change their behavior as we shrink the sizes of the channels through which they flow."

In the first nanofluidic experiment conducted at ORNL by Ramsey, Steve Jacobson, and Chris Culbertson, it was observed that electrokinetic transport is reduced as dimensions are scaled down from the micrometer range to less than 100 nm. These results are the first experimental verification of statistical mechanical theories developed more than 30 years ago for electrically driven fluid transport through small channels. "We fabricated an 80-nanometer channel that is 20 microns wide and 80 nanometers deep," Ramsey says. "We forced an electrolyte—a sodium tetraboride buffer solution—through it. We confirmed the theory that the fluid velocity would be reduced in such a small channel."

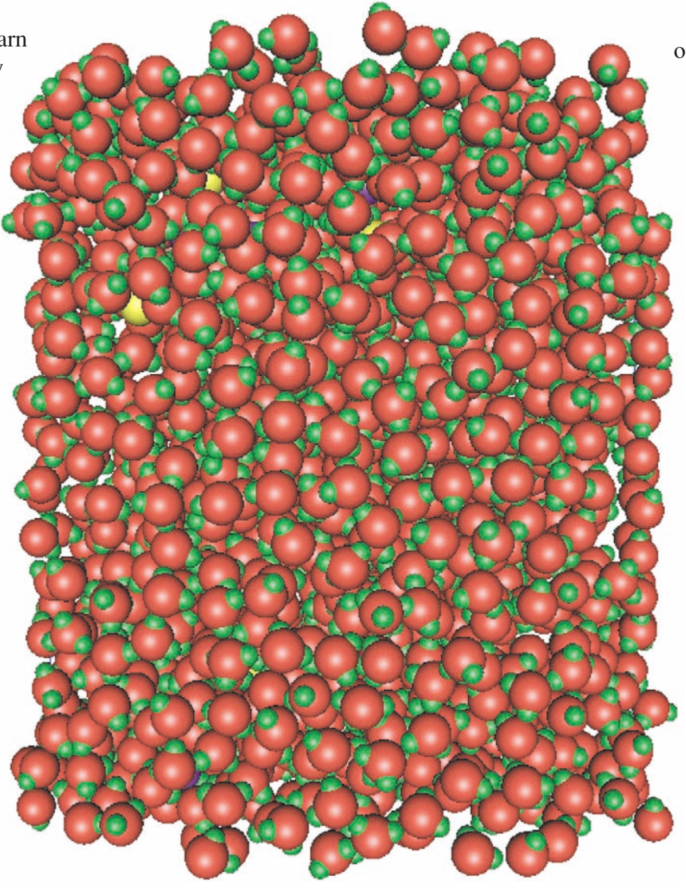
The reduction in fluid velocity at these small scales is related to the fact that the channel dimensions are similar to the electrical double-layer dimensions. The electrical double layer is the region of fluid near the solid-liquid interface where positive and negative charges may be separated so that the solution is not electrically neutral at a given location, giving rise to electrically driven fluid transport. As the channel approaches the double-layer thickness, the "pumping regions" begin to overlap and become less efficient in imparting momentum to the fluid.


Courtesy of Caliper Technologies, Inc.

These commercialized versions of ORNL's lab on a chip are products of Caliper Technologies, Inc., and Agilent Technologies, Inc.

"In our LDRD project," Ramsey says, "we are trying to show that we have the ability to fabricate nanofluidics devices with nanoscale features, that we can do experiments with them, and that we can understand their fluid transport characteristics experimentally and theoretically, using computational simulation.

"The ability to fabricate fluidic structures with dimensions at the molecular scale will allow fundamental studies of fluid transport at the smallest possible dimensions. In addition, practical tools for the analysis of biopolymer molecules, such as DNA and proteins, could well result from nanofluidic studies."



A snapshot from a molecular dynamics simulation of sodium chloride aqueous solution in a 4-nm cylindrical pore: red (oxygen); green (hydrogen); yellow (sodium); and purple (chloride). Some of the sodium and chloride ions are hidden from view. ORNL and UT researchers are simulating the behavior and transport of water containing salt and DNA or proteins in ultra-small channels (e.g., through a 4-nm pore) subjected to electric fields.

Ramsey's group is trying to learn how to fabricate nanoscale channels by shrinking the width and depth of channels etched in glass slides for microfluidic lab-on-a-chip devices. In ORNL's Solid State Division, Dave Zehner, Tony Haynes, and Arthur Baddorf are working with Len Feldman and his colleagues at Vanderbilt University to apply thin-film and ion-milling technologies to creating nanoscale channels for nanofluidic devices.

Sorting proteins by size and sequencing DNA a million to a billion times faster than current technologies are possible, practical applications of nanofluidic devices. But first, proof-of-principle experiments must be done. Ramsey's group plans to do some of these experiments.

One problem in using a lab on a chip to separate DNA molecules and proteins by size is that a sieving polymer must be added. When DNA molecules and proteins flow through this chemical sieve, the smaller biopolymers move faster than the larger ones, thus causing the separation.

"But it's a nuisance to get sieving polymer into a lab on a chip," Ramsey says. "It takes time and adds to the cost of making the chip."

Ramsey's group plans to do an experiment with a one-dimensional nanoscale channel to determine if biomolecules such as proteins or DNA strands can be separated by size, based on their mobility through the channel. "We believe that the larger molecules will move faster than the smaller ones as a result of hydrodynamic effects," Ramsey says. "The bigger molecules flowing along at the center of the fluid won't get as close to the channel wall as the little ones. Thus, the larger molecules experience, on average, a greater velocity and travel through a molecular-size channel faster. This is speculation, but we will do experiments to determine whether this hypothesis is valid."

Another experiment the ORNL group hopes to do is to show that a two-dimensional nanoscale channel structure can sequence a single strand of DNA by obtaining its electrical signature. Evidence obtained at Harvard University and theory done there by Dan Branton and colleagues suggest that each of four types of DNA bases—adenine (A), cytosine (C), guanine (G), and thymine (T)—can produce its own distinctive electrical conductivity through a nanoscale channel.

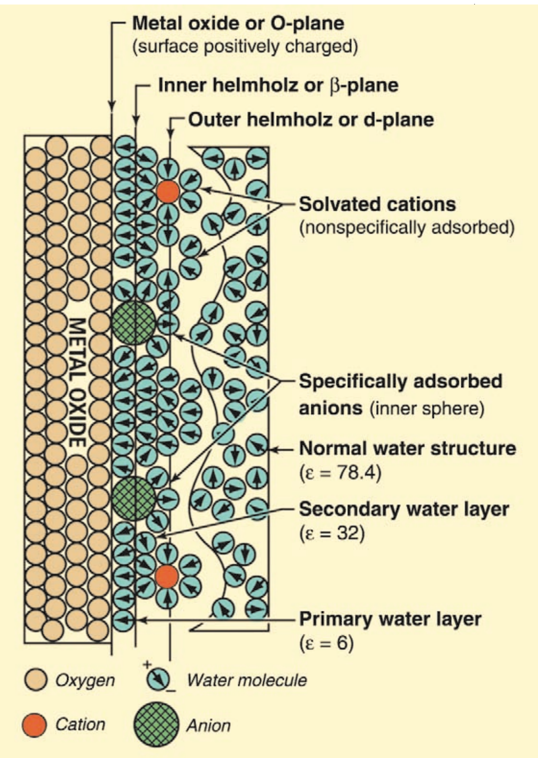
"If we could send a strand of DNA bases single file along a nanoscale channel with electrodes at each end," Ramsey says, "we might be able to interrogate the strand by measuring a current. The current variations indicate the order of bases in the DNA strand."

To help guide and interpret the results of experiments by Ramsey's group, Hank Cochran of the Chemical Technology Division and Shengteng Cui of UT are using computational molecular simulation. They are modeling the movements of individual atoms and molecules in fluids confined in nanoscale channels. They are also simulating the behavior and transport of water containing salt and DNA or proteins in ultra-small channels (e.g., through a 4-nm pore) subjected to electric fields. In employing these models, they take into account the electric-field and surface forces that extend through the liquid tightly confined inside a nanoscale channel. Modeling fluids in nanoscale channels under experimental conditions is challenging because the number of atoms or molecules simulated must be larger than is currently feasible by molecular methods, yet the models from continuum fluid dynamics become inaccurate at the nanoscale. Cui and Cochran are developing a new methodology that uses continuum equations, with local fluid properties determined from molecular simulation. This new approach should enable an understanding of the results of nanofluidic experiments and guide the design of nanofluidic devices.

In time, nanofluidics research could lead to very small devices that may have a very large impact.

Basic Geochemical Research Supports Energy Industries

Basic research by chemists and geochemists could help boost the economics of energy production.



This schematic model depicts the electrical double layer (EDL) at the interface between a positively charged metal oxide surface and an aqueous solution containing dissolved cations and anions. In this illustration, adapted from a drawing by Gordon Brown (Stanford University), negatively charged anions are adsorbed directly onto the positively charged metal oxide surface. Note the difference in orientation of water molecules (blue) around anions (green) compared with cations (red). Illustration by LeJean Hardin.

Water is the key ingredient that promotes and facilitates the transfer of mass and heat from one reservoir to another. The interaction between water and solid phases, whether those phases are natural minerals or metals in pipes, can typically lead to the release of metals and the formation of secondary corrosion or alteration phases. The solutions can range from dilute solutions of a single solute in water to complex systems containing high concentrations of more than 10 dissolved species. These solutions play a crucial role in such geochemical and technological processes as, for example, hydrothermal formation of mineral deposits, hydrothermal crystal growth and materials synthesis, and high-temperature electrochemical processes. Hot, aqueous solutions and mineral deposits can also respectively corrode and clog pipes, leading to inefficient heat transfer in geothermal power systems and reducing the operating capacity and potential lifetime of water desalination plants, boilers, power plants, and nuclear reactor cooling systems.

Chemists and geochemists in ORNL's Chemical and Analytical Sciences Division (CASD) and their collaborators have carried out pioneering studies of the consequences of water interaction with both natural and industrial materials. These studies range from those that address problems of water-solid interactions at the molecular level to more coarse-scaled studies of natural geological systems.

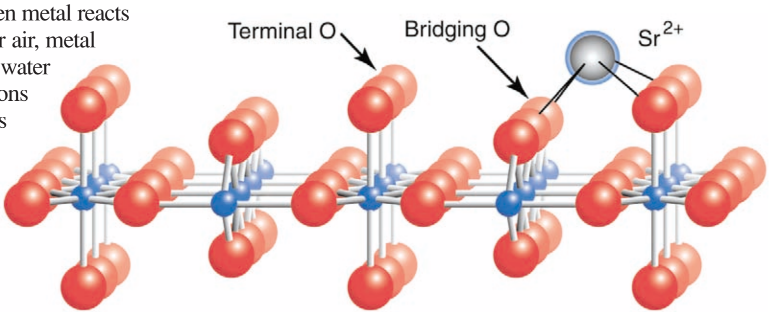
For example, chemists and geochemists in CASD are engaged in a major interdisciplinary research project, funded by the Department of Energy's Office of Basic Energy Sciences under the Complex and Collective Phenomena initiative, to quantify behavior at the oxide-water interface. What happens at the interface when water and its contaminants interact with metals and minerals is of great interest to the energy industry.

"Most of our world—from industrial materials to minerals in the earth—consists of metal oxides," says ORNL's Dave Wesolowski, the project's principal investigator. "When metal reacts with water or air, metal oxides form. When water and the dissolved ions it contains—such as chlorine, calcium, iron, lithium, potassium, sodium, strontium, and zinc—come in contact with these oxides, considerable reaction takes place at the interface. Secondary minerals can be formed there, plugging up pipes. Corrosion can result in the failure of pressurized pipes. Metal-oxide nanoparticles can spall off from the surface through contact with circulating water at high pressures and temperatures."

According to Wesolowski, when a metal-oxide surface reacts with water molecules and accompanying ions, an electric charge develops on the surface. If the surface charge is positive and if the ions in solution are negatively charged, the ions will deposit on the metal surface to which they are attracted, causing the buildup of corrosion products.

"Particles can be adsorbed onto the metal-oxide surface or can be released from the surface, depending on pH, temperature, and the chemical composition and concentrations of ions in the water," Wesolowski says. "When water reacts with the oxygen atoms bonded to atoms at the surface, hydrogen and hydroxide ions from the water cause the surface to be charged up. This surface charge is the principal driving force for both the adsorption of contaminant ions in subsurface aquifers and the formation and transport of colloidal particles in steam generator systems. It is this molecular behavior at surfaces we are focusing on in this project, through the use of sophisticated tools such as neutron reflectometry, standing-wave X rays (with partners at Argonne National Laboratory), molecular dynamic simulations, and high-temperature pH cells."

In fact, CASD researchers Wesolowski, Don Palmer, and Pascale Benezeth-Gisquet, in collaboration with a group of visiting researchers, including Mike Machesky (Illinois State Water Survey) and Moira Ridley (Texas Tech), have pioneered the study of the chemical prop-



A representative portion of a rutile titanium oxide (TiO_2) surface is shown interacting with a strontium cation (Sr^{2+}). In situ X-ray reflectivity is used to measure the atomic-scale positions of ions such as Sr^{2+}, rubidium (Rb^+) and bromine (Br^-) in aqueous solutions adjacent to the oxide surface. This work involving ORNL researchers is conducted in collaboration with scientists at the Advanced Photon Source at DOE's Argonne National Laboratory. Illustration by LeJean Hardin.

erties of oxides and other minerals as they exist in states from ambient conditions (10 to 50°C) to the extreme temperatures and pressures encountered in geothermal systems and commercial power plants (350°C, 150 atmospheres). These researchers have—for the first time–directly measured the sorption of ions on the surfaces of minerals that form naturally in geological environments, as well as the corrosion products that form in steam generators and other industrial settings, at temperatures exceeding 100°C.

The participants in this study of metal-oxide surface chemistry at high temperatures include Wesolowski, Palmer, Ariel Chialvo, Lawrence Anovitz and Bénézeth-Gisquet, all of CASD; Baohua Gu and Liyuan Liang, both of ORNL's Environmental Sciences Division; Bill Hamilton of ORNL's Solid State Division; Peter Cummings of the University of Tennessee at Knoxville (UTK); Jim Kubicki and Serguei Lvov, both with Penn State University; Paul Fenter and Neil Sturchio (ANL); and Machesky and Ridley.

The Geochemistry Group in CASD's Physical and Materials Chemistry Section has made its mark in other areas, as well. One such area is in the determination of the effects of temperature, pressure, and chemical composition on the redistribution of ratios of stable isotopes (rare over common) of light elements, such as oxygen ($^{18}O/^{16}O$), carbon ($^{13}C/^{12}C$), hydrogen (D/H), nitrogen ($^{15}N/^{14}N$), and sulfur ($^{34}S/^{32}S$) in fluids and rocks. Water (H_2O) in fluids deep within the earth has a stable isotope signature that can be very different from that of water in a river, lake, or the ocean. This is also true for gases such as carbon dioxide (CO_2) and methane (CH_4).

CASD's David Cole, Juske Horita, and Lee Riciputi are using sensitive techniques, including gas source isotope ratio mass spectrometry and secondary ionization mass spectrometry (ion microprobe) to determine shifts in isotopic signatures (isotope redistribution) that occur during the interaction of water with minerals, as a function of changes in temperature, pressure, and different concentrations of dissolved salts. Naturally occurring isotopes of O, H, C, S, and N provide built-in tracers for monitoring the interaction of fluids and solids in both natural and industrial settings.

In 1999, Juske Horita, postdoctoral fellow Thomas Driesner (now at Eidgenossische Technische Hochschule in Zurich, Switzerland), and Cole published a paper in *Science* magazine that refuted one fundamental assumption of stable isotope geochemistry. For decades it was believed that temperature, not pressure, had a dominant effect on the hydrogen-isotopic composition of hydrous minerals (e.g., brucite, or magnesium hydroxide) in the presence of water. Theoretical calculations performed by Driesner indicated that this might not be the case. So, the group set out to investigate experimentally the effect of pressure on hydrogen-isotope redistribution (changed D/H ratios) between brucite and pure water at elevated temperatures. They found that equilibrium D/H partitioning between brucite and water systematically increases by 1.24% as pressure increases from 15 to 800 MPa at 380°C. "We concluded that increasing pressure sometimes has more impact than increasing temperature on hydrogen-isotope ratio shifts," Cole says.

Also in 1999, ORNL's Horita and Michael Berndt (University of Minnesota) published a paper in *Science* magazine that explored the underground formation of methane, the earth's most abundant natural gas. Most methane is formed either by the digestion of organic compounds by microorganisms or by the thermal decomposition of organic matter. However, there is also evidence that some "abiogenic" methane is formed from inorganic matter in the earth's crust. In laboratory experiments, Horita and Berndt found that abiogenic methane can be produced rapidly from dissolved CO_2 in the presence of a naturally occurring nickel-iron alloy under hydrothermal conditions similar to those present in a mid-ocean ridge.

"We found that abiogenic methane can be formed rapidly under reducing conditions encountered in the earth's crust and that the ratio of carbon-13 and carbon-12 isotopes is not a clear-cut criterion for distinguishing biogenic from abiogenic methane," Horita says. "An important implication is that abiogenic methane could be far more widespread in nature than currently thought, especially in crystalline rocks on land and on ocean floors, including in gas hydrates."

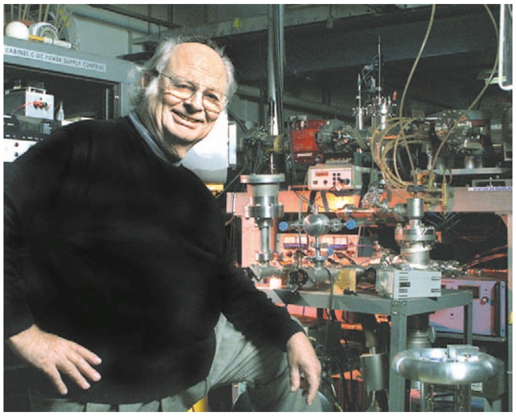
Curtis Boles, enhanced by LeJean Hardin

Lee Riciputi shows an obsidian souvenir depicting a native Mexican god of thunder and lightning and an obsidian sample that he analyzed using the ion microprobe (secondary ionization mass spectrometer). The analysis casts doubt on the validity of a traditional method for dating glassy artifacts.

Isotopic distributions can be determined in situ in minerals, using the microbeam capability of CASD's Cameca 4f ion microprobe. A tiny beam of ions (such as Cs^+ or O^-) is delivered to the mineral surface, liberating a cloud of secondary ions that is then accelerated down the flight tube of a mass spectrometer. This technology, expanded and refined by CASD's Lee Riciputi, allows determination of the concentrations and isotopic distributions of most elements in the periodic table, both laterally and vertically (depth profiling), for spot sizes on the order of a few microns, in phases such as oxides, sulfides, silicates, and glasses. In one application, Riciputi and Cole, along with Larry Anovitz and Mike Elam of UTK, debunked the long-standing industry practice used to date ancient glassy artifacts, such as prehistoric arrowheads, knives, and spear points made of obsidian (volcanic glass). Traditionally, these artifacts have been dated by observing through an optical microscope how far water from air and soil has migrated into the glass. Research using ORNL's ion microprobe demonstrated that the true position of the hydration front (penetration of hydrogen atoms in the absorbed moisture) was not at all coincident with the optical front (refracted light thought to represent the hydration front), as was originally assumed. Armed with experimental diffusion data on water in glass, which determines the rate of water migration into the glass, as well as measurements of water's true distribution in the glass, a new, more reliable dating method was proposed that capitalizes on the sensitivity of the ion probe.

Using a one-of-a-kind, vibrating-tube densimeter (VTD), CASD's Jim Blencoe is investigating the thermophysical properties (e.g., density and volume) of volatile species such as CO_2 and CH_4 at subsurface conditions. The VTD measures the density of an individual gas or gas mixture (e.g. CO_2-CH_4, CO_2-H_2O) at unprecedented precision and accuracy at a given temperature (up to 500°C) and pressure (up to 100 MPa). This activity is supplying a new body of the pressure-volume-temperature data for high temperatures and high pressures that is crucial to the development of equations of state (EOS) for geologically and industrially important fluids. These EOS are used to predict fluid behavior in a diverse range of environments, such as oil, gas, and geothermal reservoirs; volcanic systems; pipelines; the high-temperature treatment of wastes (supercritical oxidation processes); and CO_2 disposal in geological formations, such as depleted oil and gas reservoirs and coal beds. The results Blencoe obtains are directly relevant to the use of CO_2 to displace CH_4 from unmineable coal seams, a value-added technology that is being seriously considered by DOE for both producing an energy-rich gas and sequestering a greenhouse gas.

Fermi Award Winner Opened New Fields In Atomic Physics



Curtis Boles

Sheldon Datz was chair of the Local Organizing Committee of the International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC), held July 18-24, 2001, in Santa Fe, New Mexico. ORNL and Los Alamos National Laboratory physicists and support personnel organized and ran the conference.

Sheldon Datz's seminal research in colliding beam chemistry and ion channeling helped him win two prestigious prizes.

Editor's note: This article is based on a June 21, 2001, interview with Sheldon Datz, who died August 15, 2001.

Sheldon Datz, ORNL's recent winner of the Department of Energy's Enrico Fermi Award and a senior corporate fellow, was a strong believer in curiosity-driven science. Throughout his remarkable career, he planted seeds in different places and recruited collaborators to help the seeds grow and bear fruit, opening up several new fields in atomic physics.

In 1951, after earning an advanced degree in physical chemistry from Columbia University, Datz came to ORNL. He was hired by Ellison Taylor, then director of ORNL's Chemistry Division and his former supervisor at Columbia's Manhattan Project labs.

Datz and Taylor were interested in finding out what happens at the molecular level during a chemical reaction. The proposed approach was to make a beam of one type of gaseous molecule and shoot it at a beam of another type of molecule. It was believed that measurements made where the two beams cross would shed light on the details of gaseous chemical reactions. In 1955, Datz and Taylor first demonstrated the use of crossed molecular beams in studying the mechanisms of chemical reactions. They crossed beams of potassium and hydrogen bromide, and the resulting reaction yielded potassium bromide and hydrogen.

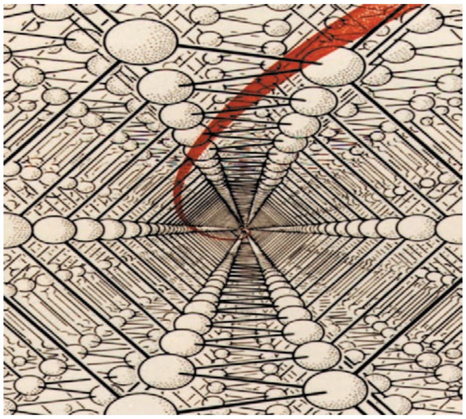
Asked why he chose to work in Oak Ridge, Datz responded that because only extremely small amounts of product could be expected from crossed-beam experiments, the Oak Ridge Graphite Reactor could be used to perform neutron activation analysis on the deposited potassium bromide. After a few less-than-successful efforts to use this difficult technique, Datz invented a new method, "differential surface ionization," in which two thin, heated wires—one of tungsten and one of platinum—could be rotated in the reaction plane and electrically record the elastic and reactive scattered product. The method greatly simplified the experiment.

This pioneering work opened up the new field of molecular beam chemistry. Much of our detailed understanding of chemical reaction dynamics has emerged from this new field of research. The ORNL work also laid the foundation for the research recognized by the 1986 Nobel Prize in Chemistry. Dudley R. Herschbach (Harvard University), Yuan T. Lee (University of California at Berkeley), and John C. Polanyi (University of Toronto) received the 1986 Nobel Prize "for their contributions concerning the dynamics of chemical elementary processes."

After receiving a Fulbright Senior Research Fellowship, Datz went to the Netherlands in 1962 and worked as a guest scientist at the FOM Institute for Atomic and Molecular Physics in Amsterdam. There he and Cornelis Snoek discovered that, at low energies, an argon ion could be bounced off, or scattered from, a copper atom on a solid surface. In 1964 they reported the discovery of collisions between an ion and a single metal atom, a process known as ion-surface scattering. Other groups soon used this method to analyze the elemental composition and structure of surfaces.

While in Amsterdam, Datz proposed shooting the ion beam at a single crystal target at a small angle, with respect to the rows of atoms, to reduce interference from ions backscattered from atoms below the surface. "The experiment worked and, surprisingly," said Datz, "the entrance angle could be made much wider than theoretically predicted. The cause? Channeling." Upon his return, he immediately joined a small meeting at Chalk River Laboratory in Canada where others reported effects that could be explained by channeling.

"This remarkable effect had actually been 'discovered' in computer 'experiments' at ORNL," said Datz. Because of concern about neutron-induced radiation damage in nuclear reactors, in 1962 Mark Robinson and Dean Oen, two researchers in ORNL's Solid State Division (SSD), attempted to model the effects of an energetic copper projectile ion on a copper crystal lattice. "They wanted to know how far a copper ion goes before it stops," Datz said. "They let their Monte Carlo computer program run for a long time, but they sometimes couldn't find where the particle went. They changed the code and their simulation showed that the copper atom



In 1962 ion channeling was discovered on a computer at ORNL. Sheldon Datz and his colleagues conducted the first energetic ion channeling experiments using Laboratory accelerators.

often came out the other side of the lattice." Their 1963 modeling led to their prediction that ions can travel through a crystal in the space, or channel, between rows of atoms and planes in the lattice—hence the term, ion channeling.

In 1964, then SSD director Doug Billington asked Datz to start a program on particle-solid interactions with emphasis on channeling. "We needed energetic heavy ions," Datz said. "Charlie Moak in the Physics Division produced them on the EN Tandem Van de Graaff accelerator. We also needed very thin crystals. Tom Noggle, an SSD expert in radiation damage in thin crystals, produced perfect gold crystals 300 atoms thick. We chose iodine-127 and bromine-79 ions at energies of 50 to 100 million electron volts because they could be viewed as synthetic fission fragments similar to what is produced in reactors."

In 1965 Datz, Moak, and Noggle demonstrated experimentally the phenomenon of energetic ion channeling in solids. They found that the ions moving along the channels of gold single crystals lost only about half the energy they would yield if they traveled through the same volume in a random direction. The explanation: Penetrating ions lose energy mainly through collisions with electrons, but the collective attractive action of nuclei in the planes gently pushes the positively charged ions away from the high concentration of electrons in the atomic cores.

In 1978 Datz and his collaborators reported the discovery of resonant coherent excitation of channeled ions. In this phenomenon, an ion with only one electron is raised to an excited state by traveling at the right velocity (and frequency) past the local electric fields of a "picket fence" of atoms, along a channel in a crystal. Work in this area is currently ongoing in Japan.

In 1979, Datz and collaborators in California (Lawrence Livermore National Laboratory and Stanford University) published two papers on their discovery of channeling radiation. They observed experimentally that ultra-relativistic electrons or positrons entering a channel oscillate in response to the string of atoms' local electric fields, resulting in the release of strongly forward-directed, high-energy X-ray radiation.

The study of atomic collisions in solids was initiated largely in response to problems related to radiation damage. The physics learned from these studies has numerous applications, including development of ion implantation, a technique widely used in the fabrication of computer chips.

In the late 1970s John Clarke, then director of ORNL's Fusion Energy Division (FED), suggested to Datz that his group should look into some interesting atomic collision problems affecting fusion plasmas. Datz chose dielectronic recombination, which was at that time a little known but nonetheless important area, especially for highly charged ions. In a plasma, excited electrons may break free of nuclei (ionization) and free electrons may recombine with ions that have lost electrons (recombination). Datz and ORNL's Pete Dittner pioneered the study of electron-ion recombination, using merged beams of electrons and ions. They were the first to make recombination measurements on multiply charged ions.

An FED group led by Clarence Barnett merged with Datz's Atomic and Molecular Physics Section in ORNL's Physics Division to perform basic fusion energy research. In the mid-1980s, this group (which is today led by Fred Meyer) built the Electron Cyclotron Resonance Multicharged Ion Source (ECR), which is used to obtain fundamental data on plasma–wall interactions of interest to fusion energy researchers. The ECR produces positively charged ions by using highly energetic electrons, heated by microwave radiation and confined by magnetic fields, to strip electrons from atoms of a specific element. Recently, DOE asked researchers in the Atomic Physics Section to focus on research using ions from an upgraded ECR.

On December 18, 2000, Sheldon Datz received DOE's Enrico Fermi Award from President Clinton. Other Fermi Award winners from ORNL are Liane Russell (1994), Richard Setlow (1988), Alexander Hollaender (1983), Alvin Weinberg (1980), William Russell (1976), and Nobel Laureate Eugene Wigner (1958).

DOE's investment in high-energy nuclear and particle physics is considerable. In the Large Hadron Collider being built at CERN near Geneva, Switzerland, lead ions will collide in a storage ring at speeds very close to the speed of light. It is expected that atomic physics processes will occur with much greater likelihood than the desired nuclear events, thus interfering with these experiments. A prime concern here is the loss of stored beam.

"In the collision region, a bare lead ion captures an electron that it has created as part of an electron-positron pair," Datz explained. The results of theoretical predictions differed widely in the early 1990s. Accordingly, Datz initiated a program to study atomic collision physics at ultra-relativistic energies, using 33-TeV lead ions from the Super Proton Synchrotron at CERN. This multinational effort included Randy Vane, Herb Krause, and Dittner from ORNL and collaborators from Sweden, Denmark, Germany, Switzerland, and South Africa. "The results, aside from quantifying expected phenomena," said Datz, "disclosed some new, totally unanticipated findings, which, in addition to their intrinsic interest, can be of use in designing very expensive particle physics experiments."

During his tenure as guest professor in Stockholm in 1990, Datz devised a method for using heavy-ion storage rings to study low-energy collisions between molecular ions and electrons. One result of these collisions is "dissociative recombination," in which molecular ions recombine and break up into neutral fragments. This process is of great importance to low-temperature plasma studies, astrochemistry, and aeronomy. Considerable work in this area is now being conducted at a number of storage rings around the world.

Although Datz did not win the Nobel Prize for pioneering the crossed molecular beam technique, his successes in opening up new fields of study in atomic physics brought him two other prestigious awards. In 1998 Datz received the American Physical Society's Davisson-Germer Prize in Atomic or Surface Physics for his research into atomic interactions with ions, electrons, and photons. On November 9, 2000, President Bill Clinton named Datz a co-winner of DOE's Enrico Fermi Award, one of the nation's highest prizes in science. On December 18, 2000, Datz received this award for his pioneering research in atomic and chemical physics.

Reflecting on DOE's decision to focus ORNL's atomic physics research on the ECR in light of his career, Datz said, "DOE thinks that we do too many things, that we should work on one or two projects. That is hard for us because we have developed many interests and capabilities. I contributed to a lot of different areas, all of which related in some way to DOE missions. To be sure, the main efforts at ORNL should be directed at larger projects, but I think it's vital to the Laboratory's health to also encourage more speculative, curiosity-oriented research."

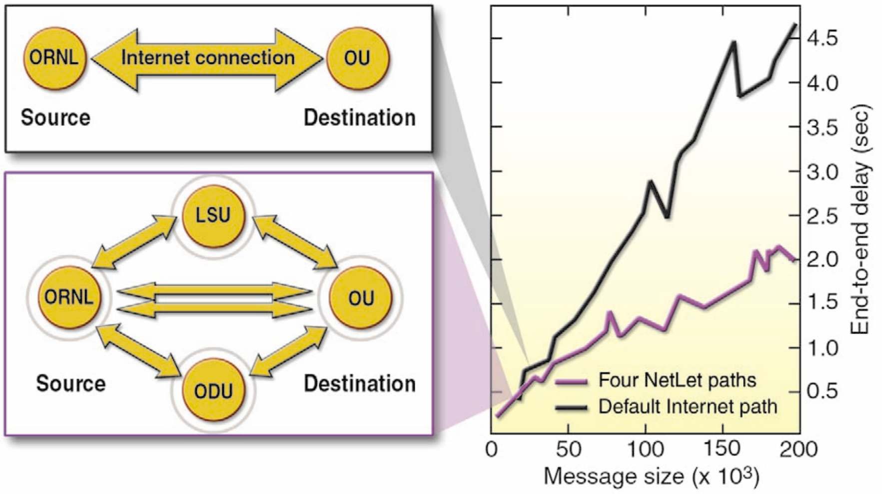
Improving the Internet's Quality of Service

An ORNL algorithm has been shown to reduce and predict delays in data delivery over the Internet.

If a physician wants to send a critically ill patient's X ray over the Internet to a radiologist who specializes in cancer diagnosis, should that X ray be delayed by transmissions of data between computer game players? Who should decide who gets needed data the fastest or who should get a message delivered first when there is considerable traffic on the network? Should only people willing to pay for service-delivery agreements receive messages faster than others who do not pay or who pay less?

Whether the desired performance in delivering messages and huge data files can be provided is an issue facing people concerned about the "quality of service" (QOS) of networks. QOS is all about being able to guarantee that data will be received by a certain time, at a certain rate, or with some other desired quality. "It is analogous to next-day-air delivery by Federal Express versus delivery by U.S. mail," says Al Geist, head of the High-Performance Computing Research Section in ORNL's Computer Science and Mathematics Division (CSMD). "If your Internet file absolutely has to be there by a certain time, then you need QOS. Unfortunately, the Internet does not have any delivery guarantees, but researchers at CSMD are trying to change that."

When a data file is sent over the Internet, it is sliced into pieces, or data packets. Computers called routers direct these packets along different paths over the network. The packets are then reassembled at their destination. One problem is that with today's Internet a router is allowed to throw away data packets in response to traffic conditions and priorities assigned by the service providers. In response, the lost packet must be resent, and there is no guarantee that this packet will not also be lost. The net effect is that delivery of the complete data file can be delayed for an unknown amount of time.



The ORNL-developed NetLet algorithm reduces by 40% end-to-end delays in transmitting data files over the network, with no support from Internet routers. In one set of tests in which the algorithm was used part of the time, the data files were sent between ORNL and the University of Oklahoma (OU) over the Internet. In another set of tests, the data files were transmitted from ORNL to OU via computers at Old Dominion University (ODU) and Louisiana State University (LSU).

Illustration enhanced by LeJean Hardin

A delayed response can be costly for a lot of reasons. Beyond the example of the physician and the patient's X ray, there are also examples in science. Say, for instance, a million-dollar supercomputer is waiting for the data it needs to perform certain calculations. If an unanticipated delay occurs in the transmission of the data, that million-dollar supercomputer could remain idle. A delay in relaying a complete message could also cause a chaotic response in a robot being operated remotely over a network, say, to run an experiment. "Just as a drunk driver may cause a traffic collision because of a delayed response, a robotic arm could behave wildly because of a delay in delivering the complete set of commands," says Geist.

To reduce and predict delays in data delivery, CSMD's Nageswara Rao has developed a computer program called NetLet that is currently being tested on a small subset of the Internet. "NetLet allows computers to talk with each other and determine whether a complete message got there and what the delay is in getting the dropped packet to the receiver," Rao says. "This algorithm enables the computers to measure connection speeds and the delays of alternate pathways and then identify the best combination of pathways to get the information delivered efficiently in the time or rate guaranteed."

Demonstrations of NetLet have shown that the algorithm has improved the speed of data delivery by about 40%, without any additional support from Internet routers. "Some of our data files used to take 10 seconds to get from our computer to a destination computer," Rao says. "Those same data files can now get there in 6 seconds. That means that a huge data file that takes 10 hours to arrive at a destination computer can now get there in 6 hours."

NetLet could be useful for speeding up the delivery of large data files from neutron scattering experiments performed at the Spallation Neutron Source (SNS) when it becomes operational in 2006 at ORNL. "We need to find ways to rapidly transfer hundreds of gigabytes or terabytes of data from the SNS across the country to scientists requesting the information," Geist says. "And our climate scientists are needing this capability today."

It takes about 2 hours to send 500 megabytes of climate data (calculated results of simulations of future climate) from DOE's Center for Computational Sciences at ORNL to the National Energy Research Supercomputing Center at DOE's Lawrence Berkeley National Laboratory in California. These data files are sent across DOE's new Energy Sciences Network (ESnet), a semiprivate part of the Internet.

Today, if high-energy physicists wish to transfer hundreds of terabytes of data from DOE's Stanford Linear Accelerator Center in California to the European Laboratory for Particle Physics (CERN) near Geneva, Switzerland, they don't use ESnet, because it would take a month to transmit all the data within these huge files. Instead, they deliver the information in a week by copying it onto tapes and transporting the tapes to CERN by Federal Express. The goal is to further develop NetLet and other approaches so that huge files of data from high-energy physics facilities and the SNS can be delivered in one to two days.

If NetLet is eventually incorporated into Internet routers, more users may feel they are sending and receiving their information by express.

QOS for Wireless Communication

According to Nageswara Rao (shown here), connectivity-through-time protocol enables robots to communicate with each other without network infrastructure and dynamic connectivity.

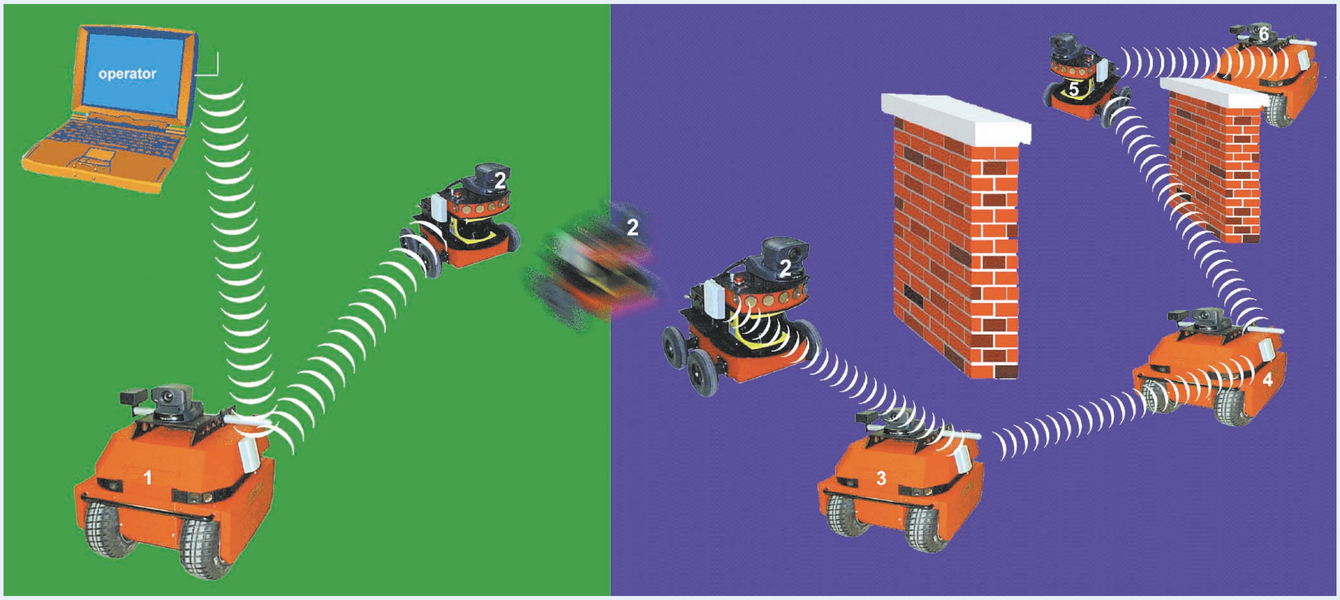
Curtis Boles, enhanced by LeJean Hardin

A team of mobile robots carrying radiation detectors in a remote building or at a waste burial site has a mission: Autonomously build a map of radiation levels in the area suspected of contamination. Through wireless communication the robots coordinate their activities to ensure a complete radiation profile of the building or waste site.

In such areas, the infrastructure for conventional wireless networks is lacking, and the wireless connectivity can be quite unpredictable. For example, in a typical building, a robot mapping one room for radiation cannot communicate directly by radio with a robot in another room because radio waves cannot pass through the thick walls separating the rooms. A possible solution to this problem has been devised at ORNL. To foster robust communication between robots and more generally mobile nodes, ORNL's Nageswara Rao has developed the "connectivity-through-time" protocol and implemented a system using NetLet software in which a robot serves as a "router."

In a recent demonstration at ORNL, a "mail" robot mapped the hall connecting two rooms, each of which was being mapped by robots not in direct wireless contact. As the robot in the hall moved past the entrance to each room, it communicated, by radio, with the robot mapping the room, keeping track of its progress in generating the radiation profile and the location and amount of building space that remained to be mapped.

The mail robot picked up a message from a robot in one room and delivered the message to a robot in the other room, thus allowing these robots to communicate with each other. Though never before possible, with this new system for improving quality of service in wireless communication, robots can exchange messages under conditions of highly unpredictable, wireless connectivity.



The connectivity-through-time protocol developed at ORNL exploits the motion of one robot to deliver messages to and from robots separated by walls, allowing wireless communication among all robots in a dynamic network.

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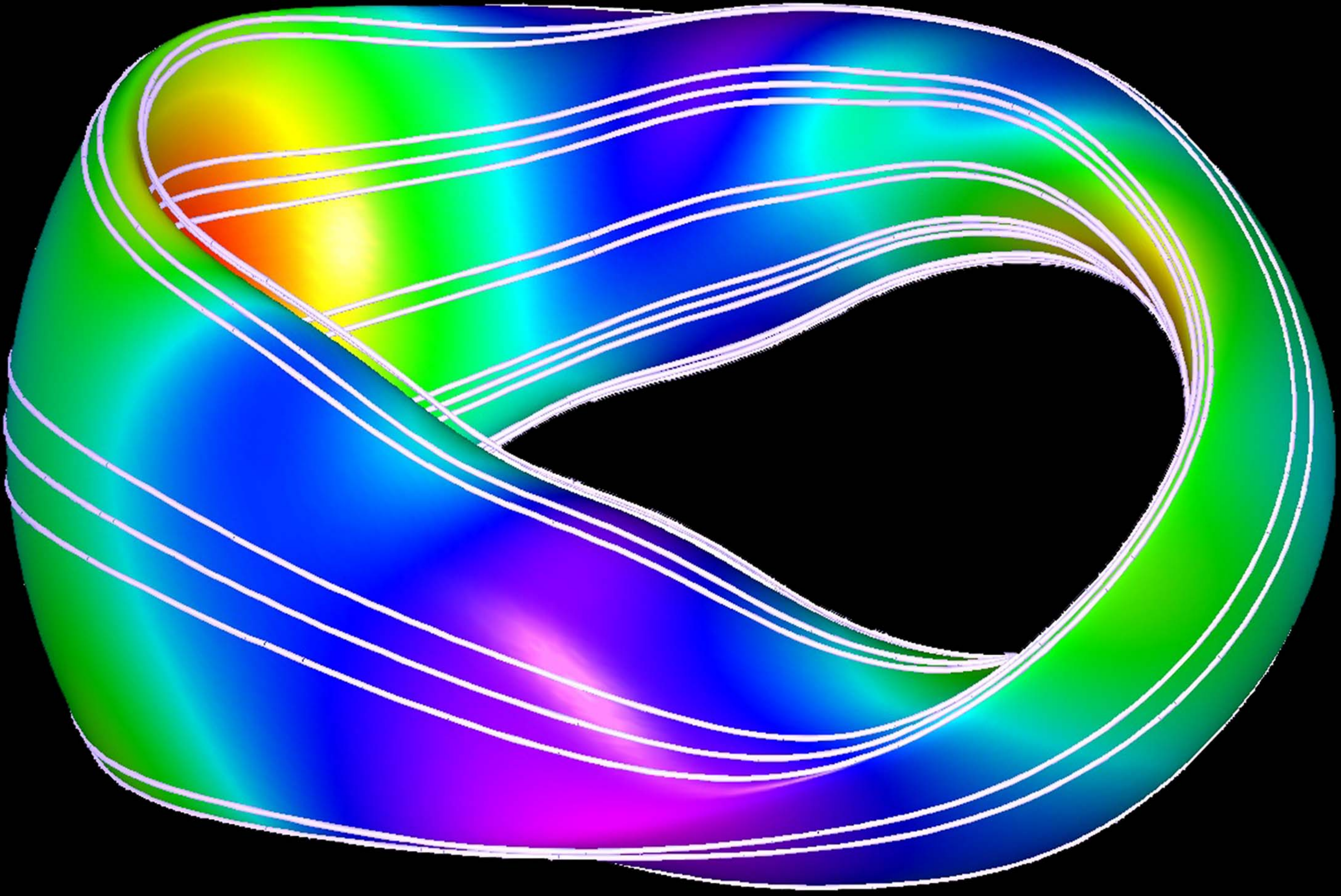

A fusion research device called the Quasi-Poloidal Stellarator may be built by 2006 at ORNL. It is being designed by ORNL fusion theorists with the help of the IBM supercomputer at DOE's Center for Computational Sciences in Oak Ridge. The above visualization by ORNL's Don Spong shows a QPS-optimized stellarator plasma surface with a magnetic field line (white) superimposed. (See article on p. 16.)