AUGUST/SEPTEMBER ISSUE 2001

DATELINE LOS ALAMOS

U.S. DEPARTMENT OF ENERGY
UNIVERSITY OF CALIFORNIA

For the first time ever, a cross-section of nuclear materials scientists and technicians at the Chemistry and Metallurgy Research (CMR) facility has fashioned an eight-kilogram tungsten- and nickel-clad sphere of neptunium. The actinide metal sphere will be used in criticality safety and nuclear non-proliferation experiments at Technical Area 18, the critical experiments facility.

A MONTHLY PUBLICATION OF LOS ALAMOS NATIONAL LABORATORY

DATELINE: LOS ALAMOS

FROM THE DIRECTOR

As I read of our tremendous technical achievement of building the world' s first neptunium sphere – to be used in nonproliferation and criticality safety studies – I was struck by two thoughts expressed by the workers who created this breakthrough.

They noted that they applied the principles of Integrated Safety Management "to solve problems fast with worker safety at the forefront." In addition, they cited close coordination with the Department of Energy and cross-organizational communication as essential elements to success.

To me, this effort demonstrates how the precepts of integrated management can be a tool toward more efficient and effective operations.

We have learned in our interaction with DOE and the National Nuclear Security Administration the importance of coordination and communication. In becoming a unified, customer-focused laboratory, it is critical that there be clear understanding between us and our customer. It also is critical that we work together toward a common goal, as the technical and operational organizations did in this activity.

Just as one picture is worth a thousand words, one notable achievement that demonstrates the value of integrated management speaks volumes about how this principle can benefit the Laboratory.

About the Cover: Work on the neptunium sphere fabrication took place inside a hot cell where technicians performed the "hands off" casting and machining of the sphere using manipulator arms and special handling tools behind special radiation shielding and oil-filled lead glass.

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A MONTHLY PUBLICATION OF THE PUBLIC AFFAIRS OFFICE OF LOS ALAMOS NATIONAL LABORATORY

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DATELINE: LOS ALAMOS

LAB BUILDS WORLD'S FIRST NEPTUNIUM SPHERE

Continued from the cover

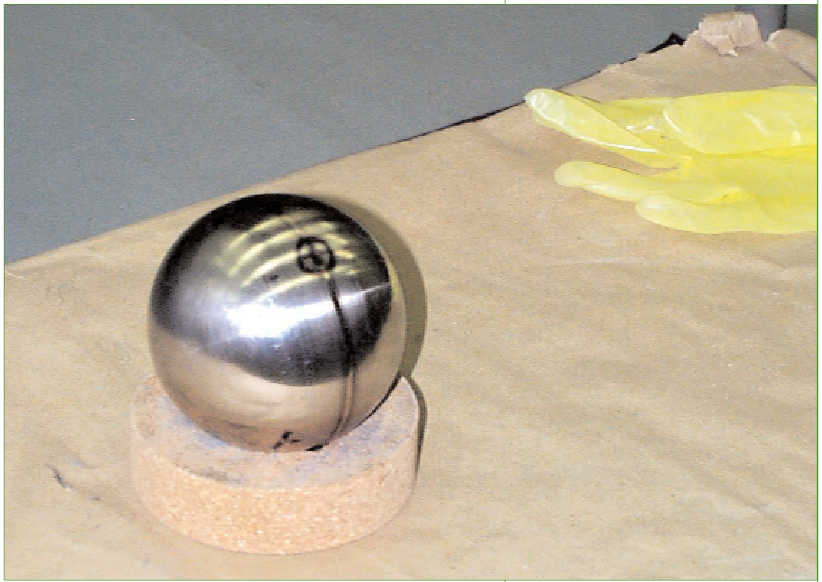
Not much is known about the properties of neptunium, a highly radioactive man-made material that is a byproduct of nuclear reactors, except that it emits alpha, beta and gamma radioactivity. The critical mass is not well known, with documented values covering a very wide range of masses.

"We were starting from scratch when this project began back in 1997," said Stanley Bodenstein, who led the project in its early stages. "Nothing like this had been done before with neptunium. We were going to cast, machine and clad a sphere of material that is pyrophoric, meaning it can catch fire if exposed to oxygen, and so radioactive it must be handled remotely, completely hands-off."

The neptunium sphere team included Actinide Chemistry Research and Development (NMT-11), Materials Technology: Metallurgy (MST-6), CMR Facility Management (NMT-13), Experimental and Diagnostic Design (DX-5), Advanced Nuclear Technology (NIS-6), Security (S) Division, Environment Safety and Health (ESH) Division, and the Department of Energy's Los Alamos Area Office and Albuquerque Operations Office.

Before the creation of the 3.25-inch-diameter sphere, about the size of a baseball, the Laboratory's criticality safety and nonproliferation work dealt with neptunium in a variety of other shapes. "No direct measurements for neptunium critical mass have been done," said Rene Sanchez of NIS-6. "The Laboratory possessed some quantities of neptunium, but not the right amounts or shapes.

Starting from scratch, a team of Laboratory scientists and technicians have fashioned an 8-kilogram, tungsten- and nickel-clad sphere of neptunium. The sphere, about the size of a baseball, will be used in criticality safety and nuclear nonproliferation experiments.



With this new sphere we now have the capability to go beyond the current data that are only estimates."

Creating the sphere from scratch is no exaggeration. "We had to ramp-up the entire process from basically nothing," said Bodenstein. "The whole thing had to be done in an 'alpha box' placed inside a 'hot cell.' Special tools had to be designed, built and tested by the technicians so they could be used with remote manipulators, one-of-a-kind melting and molding equipment had to be created and then all of it had to go through a DOE readiness assessment."

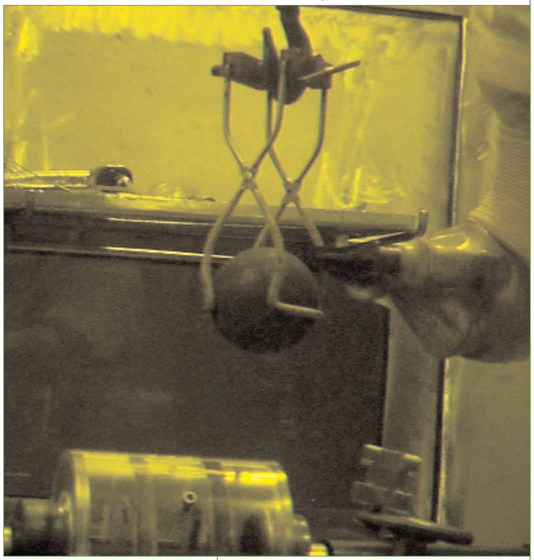
The alpha box and hot cell are equipment at the CMR building. An alpha box is a large, highly specialized containment vessel built for a specific job intended to prevent the spread of radioactive particulate inside the hot cell. The work was accomplished inside one of CMR's 16 hot cells, small rooms that are heavily shielded with three-foot-thick walls for radiation protection and outfitted with lead glass, oil-filled windows and remote handling arms.

"There were many challenges along the way," said Bob Romero, team leader at the hot cell facility. "We were in the midst of removing a lot of materials at CMR, we were influenced by an upgrade schedule that called for technical improvements to the hot cells and we were faced with changing security and safety requirements. We were interrupted several times because of funding, stand-downs, management changes, a division reorganization and of course, the Cerro Grande fire in May 2000."

And the team realistically had only one shot at getting it right. "All of the equipment, tooling, work instructions, hazard control plans, training, security plans, everything was prepared to give the team the highest reasonable probability to perform the task correctly and safely on the first attempt. Resource restrictions would have made a second attempt doubtful," said Bodenstein.

Getting everything in place for the DOE Readiness Assessment (RA) was a major success, according to team members, but the real accomplishment was how the assessment and final fabrication processes were completed. "Often an RA and comment resolution process leading to the DOE approval of a project's 'readiness to proceed' takes about six months. Then the project itself typically takes many weeks to complete," said Bodenstein. "With close coordination between our team and the DOE RA team we were able to complete the RA in just nine days. Then, with total involvement from the whole team, we were able to deliver a finished product only four days later. Thirteen days, start to finish, this was unprecedented.

Technicians at the CMR facility improvised some of tools for handling the highly radioactive neptunium sphere during its fabrication and machining. Shown here is a grasping tool fashioned from a standard kitchen gadget normally used in canning. It was modified to securely hold the sphere so that it could not be accidently dropped when being moved.



As the team looks back on this major success they agree that communication is what made this project work. "Security was a major driver that required detailed planning and coordination," said Romero. "People worked weekends and evenings to prepare, sometimes into the wee hours of the night. It was a very intense effort. When problems occurred, we'd step back and evaluate what to do — we really used the five-step Integrated Safety Management process effectively to solve problems fast with worker safety at the forefront."

"There was total involvement across all organizations. Technicians were involved in development of the hazard control plan and procedures. MST personnel developed and supervised the melting and casting of the materials, and folks from DX-5 worked through the night machining the protective tungsten outer shell of the final casting," said Dave Yeamans, who led the project in its final stages. Sanchez added, "This was one of those projects that makes you very proud to be a Laboratory employee."

One technological advance was the fabrication of the one-of-a-kind, yttrium-oxide-coated graphite mold. The specialized design integrated several thermocouples, a highly sensitive type of thermometer, to help control the cooling process of the molten neptunium. "From a metallurgist's point of view, a sphere is the hardest shape to cast," said Sanchez. "From a physicist's point of view, it's the best shape for experimentation."

"We've already learned many things from this project about how neptunium reacts to melting and cooling, how hard the finished product becomes — it turns out to be harder than steel, something we did not expect — and how difficult it is to machine," said Yeamans.

"There is still so much more to learn and there is a lot of interest in neptunium," said Romero. "An internal Los Alamos Neptunium Working Group sponsored by the Glenn T. Seaborg Institute for Transactinum Science has already begun to think about new studies with neptunium."

The principal funding sources for the neptunium sphere project were DOE Defense Programs, Office of Emergency Response and DOE Nuclear Nonproliferation, Nonproliferation Research and Engineering.

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DATELINE: LOS ALAMOS

RESEARCHERS FIND HUMAN'S EARLIEST ANCESTOR YET

An international team of researchers has announced the discovery of fossil bones and teeth belonging to the earliest human ancestors yet discovered – a hominid who lived in what is now Ethiopia between 5.2 and 5.8 million years ago.

Hominid refers to the family of primates that includes all species on the "human" side of the evolutionary tree after the split from chimpanzees. Two reports on the extraordinary discovery appeared recently in the journal Nature.

Researchers found the fossil remains of several of the ancient individuals along the foothills of the western margin of the southern Afar Rift, located in Ethiopia's Middle Awash study area. The Middle Awash is located about 140 miles northeast of Addis Ababa, Ethiopia's capital city. The area also is located about 50 miles south of Hadar, where the 3.2 million-year-old "Lucy" fossils were discovered nearly 30 years ago.

➔ At right are hominid fossils belonging to Ardipithecus ramidus kadabba. The holotype mandible of the subspecies is at the upper left, the Amba toe bone is in the right upper row and the hand holds a fragment of collar bone. Inset above is a close-up of Lower canine tooth from the Saitune Dora site, collected beneath a lava flow dated to 5.54 million years ago. This is the most primitive hominid lower canine found to date.
(c) 1999 Tim D. White\ Brill Atlanta

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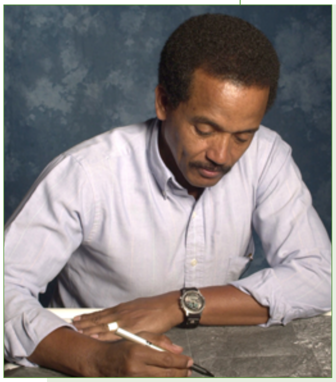

Giday WoldeGabriel, one of the lead authors of Nature articles on the discovery, is a geologist in the Lab's Hydrology, Geochemistry and Geology Group.

Yohannes Haile-Selassie, a doctoral candidate at the University of California, Berkeley, and Giday WoldeGabriel, a geologist with Los Alamos National Laboratory, are lead authors of the Nature articles associated with the discovery that appeared earlier this summer.

The team discovered the first fossils in 1997, with the latest one found this year. The fossil bones predate the oldest previously discovered human ancestor by more than a million years. The teeth and bone fragments apparently are from a hominid that emerged sometime after the split. The hominid is part of a newly named subspecies of early man called Ardipithecus.

While Ardipithecus ramidus kadabba is not the sought-after "Missing Link" – the yet-undiscovered creature that lived at the cusp of the evolutionary division between man and chimp – researcher Haile-Selassie said the hominid certainly is very close to the branching point.

Based on a toe bone discovered among other fossils, Haile-Selassie has determined that the new subspecies Ardipithecus ramidus kadabba almost certainly walked on two legs when on the ground. The creature's teeth share more characters with all later-discovered hominids than with the teeth of all fossil and modern apes. The relatively large back teeth and narrow front teeth indicate that Ardipithecus ramidus kadabba ate less fruit and more soft leaves and fibrous food than his chimpanzee contemporaries, who were specialized frugivores.

Haile-Selassie believes Ardipithecus ramidus kadabba was about the size of a modern-day chimpanzee and about 20 percent larger than the "Lucy" specimen. Because neither the skull nor intact limb bones of Ardipithecus ramidus kadabba have been found, however, an artists' rendering of the creature is impossible at this time.

But Ardipithecus ramidus kadabba no doubt was a hardy little soul. WoldeGabriel and his colleagues characterized the creature's environment during its life in the Miocene era (5 to 6 million years ago) in Africa. At that time, Ardipithecus ramidus kadabba lived in a forested environment – a far cry from the region's present day environment of harsh desert surroundings.

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The area where the hominid dwelled was as much as 1,500 feet higher in elevation than today and it was much cooler and wetter.

But the hominid lived at a time when Africa was in the throes of continental change. The area was peppered with active volcanoes and intense earthquakes related to the formation of the rift valley. The Awash region during Ardipithecus ramidus kadabbas' day was showered with pulses of thick, hot volcanic ash from nearby volcanoes.

"It's hard to imagine that life would go on under such hostile environmental conditions," WoldeGabriel said. "Ardipithecus and the other animals inhabiting the region were real survivors."

The researchers found that numerous animals lived during the time of Ardipithecus ramidus kadabba. The research team found more than 1,900 fossil specimens comprising the remains of more than 60 identified mammal species. The fossils included primitive elephants, horses, rhinos, rats and monkeys. Researchers found the remains of more than 20 primitive elephants together at one site.

The Middle Awash project initiated site management of this locality in 1997 when the first specimen of the Late Miocene hominid was found here by Yohannes Haile-Selassie. In this photograph he is standing in the foreground where the mandible was found, while geologists work on an exposed overlying volcanic ash on the hillside behind him. Beginning in the 1997 season, the project's paleontologists stripped the surface of the sediments of the overlying basalt boulders, facilitating erosion. This strategy has resulted in the discovery of many additional fossils, including hominid specimens.

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Finding the Ardipithecus ramidus kadabba specimens represented a tremendous challenge to the researchers. Lakes, forest areas, volcanic rocks and recent sediments cover about 87 percent of the present-day Middle Awash area. The remaining area contains patches of ancient sediments exposed by erosion, but less than 1 percent of the Middle Awash has windows of exposed ancient-sediment outcroppings that contain mammal fossils.

Discovering, correlating and searching these small windows to the past is a research challenge. The new Ardipithecus subspecies fossils were tiny nuggets in a huge landscape littered with pebbles and boulders. Finding the fossils truly was like finding the proverbial needle in a haystack.

To determine the age of the fossils and to understand the overall geology and ancient environment, geologists WoldeGabriel and Grant Heiken of Los Alamos, Paul Renne of Berkeley Geochronology Center and UC Berkeley's Department of Earth and Planetary Science, Bill Hart of Miami University of Ohio and Stanley Ambrose of University of Illinois at Urbana collected volcanic and sedimentary rocks that lay above, beneath and within the hominid-bearing sediments. The dates of the ash layers and lava flows bracket the age of the fossil remains.

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To determine the age of the volcanic layers, researchers measure the amount of argon gas contained in volcanic rocks in them. The gas is a radioactive decay product of naturally occurring potassium that was in the rock when it cooled. Argon accumulates at a known rate in rocks and minerals. By measuring the amount of argon in the volcanic crystals, researchers are able to precisely determine the age of the rocks – and the fossils as well.

The international team includes more than 45 scientists from 12 different countries. Institutions represented by team members include UC Berkeley, Los Alamos, Miami University of Ohio, University of Illinois at Urbana, the Cleveland Natural History Museum and the National Museum of Ethiopia.

The international research

Yohannes Haile-Selassie searches for fossils among the lava boulders. The fossils are eroding from beneath the horizontal black and white band, the Witti tuff (Afar for "Lizard"), which is made of volcanic ash that has been dated to 5.65 million years old.

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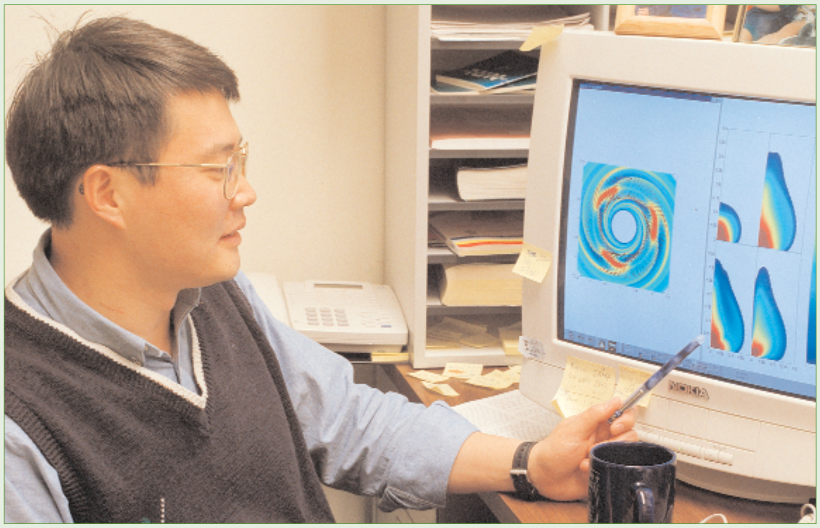
DATELINE: LOS ALAMOS

THE MAGNETIC UNIVERSE: WHERE DID THE BLACK HOLE ENERGY GO?

Researchers in Applied Physics and Theory Divisions have recently compiled a sample of nearly 100 giant radio galaxies powered by black holes.

A typical giant black hole forms when 100 million solar masses are packed into a region the size of the solar system, creating an extraordinary deep potential well. Researchers have estimated that a total gravitational energy equivalent to nearly ten billion supernovae is released during a typical formation, garnering the prize of being the largest energy production process in the present universe. Modern astronomical observations suggest that giant black holes were more active in the past, when the universe was only a fraction of its current age.

So where did all that black-hole energy go? Intense radiation, powerful winds and enigmatic magnetic fields are three of the most important channels for transporting this energy away from the black holes. Some models suggest that the radiation released when black-hole systems formed in the



Hui Li of The Laboratory's Plasma Physics Group and colleagues developed a comprehensive theory of the accretion process of energy flow in the universe.

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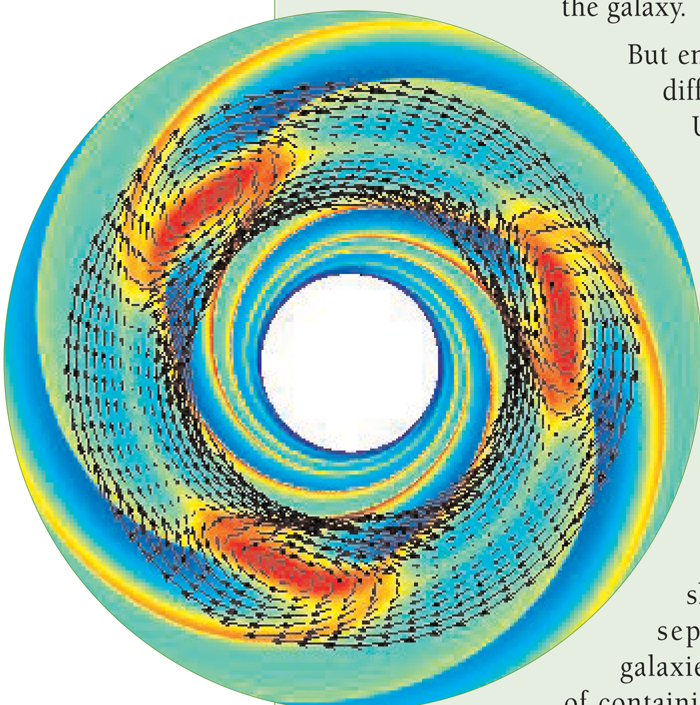
early universe is responsible for re-ionizing the universe after recombination. But to a large extent, radiation has very little dynamic impact once the matter becomes very dilute. Similarly, kinetic winds tend not to propagate very far before losing most of their energy within the galaxy.



The illustration shows the formation of large-scale vortices in an accretion disk around the black hole. Pressure is overlaid with velocity arrows. The vortices are anti-cylones enclosing the high-pressure region. Large-scale waves are also produced in connection with the vortices.

But enigmatic magnetic fields are a different story. Working with the University of Toronto, Hui Li of Plasma Physics and Stirling Colgate of the Theoretical Astrophysics group have accounted for a significant fraction of a black hole's energy in magnetic fields. The magnetic energy is carried away in the form of neatly lined-up columns of magnetic fields that propagated to a distance slightly larger than the average separation distance between galaxies. The field's unique nature of containing a large amount of energy while occupying a limited volume causes magnetic fields to remain dynamically important for a long time, perhaps as long as the age of the universe, according to Li.

Li and a team of other researchers, including Burt Wendroff of Mathematical Modeling and Analysis and John Finn of Plasma Theory, have developed a comprehensive theory of the accretion process – an increase in the mass of a celestial object by the collection of surrounding inter-stellar gases and objects by gravity – and have confirmed the theory by extensive hydrodynamic simulations.

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Li says that researchers are just beginning to understand the pieces of the picture and the results are encouraging. There is increasing evidence that we should view the evolution of the universe as a magnetohydrodynamic phenomenon rather than a process dominated only by gravity and hydrodynamics.

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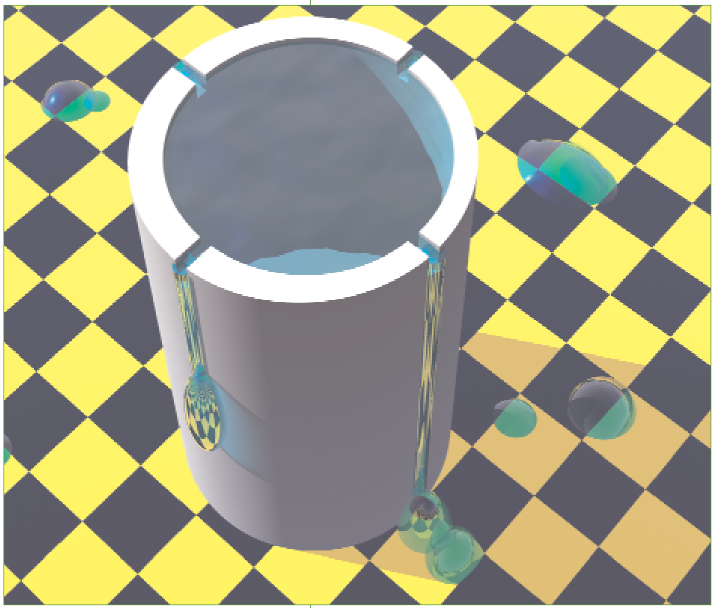
DATELINE: LOS ALAMOS

RIDING THE D-WAVE – LOS ALAMOS THEORY VALIDATED BY UC BERKELEY WORK

A paper appearing in a recent issue of the journal Nature has helped validate a theory on the enigmatic nature of superconducting materials that was first advanced by Los Alamos National Laboratory researcher Alexander Balatsky and his colleagues five years ago. The confirmation of the theory is another step in solving the enigma of superconductivity.

In 1986, certain compounds containing copper-oxide layers were discovered to be superconducting at relatively high temperatures. Researchers believed that in conventional superconductors electricity flowed with no resistance while being carried by pairs of electrons in which each pair formed a sphere-like configuration called an s-wave. As a result, an energy gap separating paired and unpaired electrons was the same in all directions. Despite substantial skepticism from the superconductivity research community, Balatsky and his collaborators suspected that the conducting electrons in superconductor materials might be paired differently, perhaps in a star-like configuration known as a d-wave, and that the energy gap would vary with direction.



↑ To picture the energy gap of the high-temperature superconductor, one could imagine four notches carved into the rim of a cup nearly filled with water. Water added to the cup would leak out through this cross-like shape. Similarly, electrons in the impurity state leak out where the energy gap is zero.

Balatsky theorized that replacing copper atoms with impurity atoms, zinc or nickel atoms, for example, would validate his hypothesis. He predicted that the impurities would interfere with the mechanism that creates the superconductivity and would create, in the area of the impurity, a localized state that would help reveal the nature of the superconductivity.

Yet to prove this theory, researchers would need to use a scanning tunneling microscope to image, on the atomic scale, the localized state

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created by the presence of the impurities. At the time Balatsky and his colleagues proposed the theory, the capabilities to do the work did not exist. The world would have to wait to see the hypothesis proven.

Proof came recently when a University of California, Berkeley, team lead by Seamus Davis created the impure state predicted by Balatsky and company and then used a scanning tunneling microscope to capture the images necessary to confirm the prediction. The resulting scanning tunneling microscope image, which records the probability that electrons will tunnel across the energy gap, shows the predicted cross image.

The success story, however, does not end there. According to Balatsky, adding impurities to determine the nature of the superconductivity is very much like destroying a toy to see how it works. He theorizes that the use of defects to deliberately destroy the correlated state could be quite useful as a means to learn more about material states. The use of impurity as an analysis of the correlated state might be used in analyzing carbon nanotubes, strontium ruthenate superconductors and other similar materials.

Research in the area of high-temperature superconductivity has implications in many critical areas of the economy. One of the most valuable applications is in the possibility of creating power transmission lines in which the flow of current through wires with virtually no resistance would dramatically lower the natural power losses caused by resistance. Given the current power shortages in densely populated urban areas like California the potential for this kind of highly efficient power transmission is enormous.

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DATELINE: LOS ALAMOS

LAB RESEARCHER'S TEAM SHINES IN PROTEIN FOLDING PREDICTIONS

The protein folding puzzle – determining the3-D structure of a protein given the sequence of its amino acids – is one of the major unsolved problems in molecular biology. A Los Alamos National Laboratory scientist along with a colleague and his students were recently recognized as the most successful team in an annual worldwide assessment of progress in protein structure prediction.

Charlie Strauss of the Lab's Bioscience Division and his colleague, Professor David Baker from the University of Washington, participated in the experiment during the fourth Critical Assessment of Techniques for Protein Structure Prediction (CASP4).

"This annual experiment is a delightful and terrifying phenomena for any protein scientist working on predicting protein structure," Strauss said. "Participants in the experiment are sent a list of proteins whose structures have been solved but not made public. They are invited to stick their necks out and predict the structure of a true unknown. Then they and their peers go to the conference and find out the answer. They are assigned grades, just like in school."

The computational technique, co-authored by the Strauss and Baker group, is known as Rosetta. The software is based upon the assumption that local sequence biases, but does not uniquely determine, the final structure. Predicted proteins are assembled from short fragments taken from a database of known structures with similar local sequences. Rosetta showed remarkable success in predicting the structure of folded proteins from its the linear sequence of amino acids.

"Some people call protein structure the second half of the genome project," Strauss said. "Genes code for proteins, and a unique property of proteins is that they derive their function from their structure. Structures begin to tell us what proteins do, and how they do it, and we are developing ways to predict a protein's approximate structure from its sequence. Billions of dollars are being spent worldwide on measuring protein structure, so doing it computationally is obviously very desirable."

There are between 10,000 and 100,000 important protein structures, but only a few thousand of these are currently known. Strauss specializes in predicting novel structures, ones that have not previously been seen.

"Nature recycles her structural designs," Strauss said. "Once we know all the important structures, any new proteins will probably have structures similar to these, but so far we've only begun to get a sampling from direct measurement. So getting ahead of the experimentalist and predicting the structure of proteins with previously unseen designs -- the novel folds – is a high value objective, not to mention the most fun and challenging. Predictions aren't nearly as good as measurements, and assessing prediction success is a relative kind of thing."

"We're fascinated with the idea of tinkering with proteins," Strauss said. "It's designing crescent wrenches at the molecular level."

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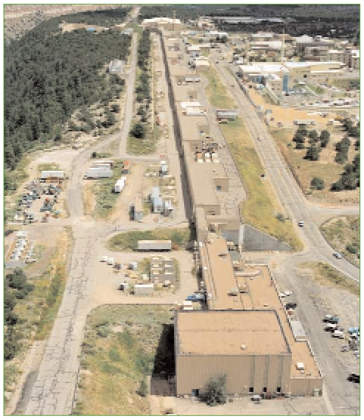
AUGUST/SEPTEMBER ISSUE 2001

DATELINE: LOS ALAMOS

BRIEFLY . . .

LANSCE PROVIDING BEAM TO USERS

The Los Alamos Neutron Science Center at Los Alamos National Laboratory is now up and running. LANSCE has begun beam delivery at both the Weapons Neutron Research Facility and the Manuel Lujan Jr. Neutron Scattering Center.



Above is an aerial view of the LANSCE beam line.

During the 2001 run cycle at the Lujan Center, ore than 100 experiments are scheduled to run on six user-program instruments. Experiments, which range from studies of new materials to biological protein studies, typically run from two to 10 days and often involve teams of researchers. In this year's cycle, 30 percent of Lujan Center users are from divisions across the Laboratory, and the remaining 70 percent are drawn from external experimental teams.

The external teams represent approximately 35 U.S. academic institutions, five national laboratories, seven foreign academic institutions, two members of industry and two U.S. government agencies. International users come from as far away as Germany, Slovenia and Japan. The Lujan Center expects to host approximately 150 unique users over the five-and-a-half-month run cycle that ends in mid December.

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