ARGONNE NATIONAL LABORATORY

UPDATE

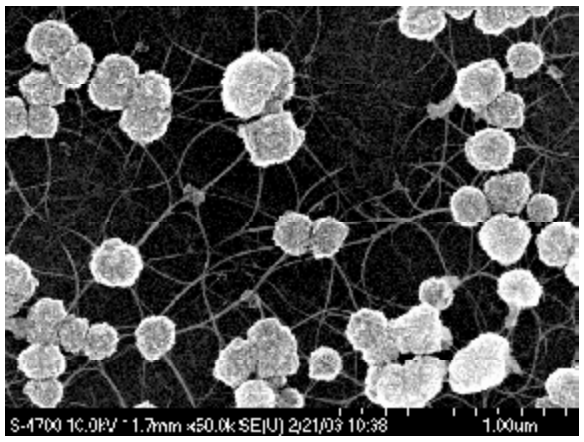
The community newsletter of Argonne National Laboratory
Fall 2005

Hardest, strongest materials combined

By Catherine Foster

Argonne researchers have combined the world's hardest known material, diamond, with the world's strongest structural form, carbon nanotubes. This new process for "growing" diamond and carbon nanotubes together opens the way for its use in a number of energy-related applications.

The technique is the first successful synthesis of a diamond-nanotube nanocomposite, which means for the first time this specialized material has been produced at the nanometer size — thousands of times smaller than the period at the end of this sentence.



Argonne scientists have achieved the first successful synthesis of a diamond-nanotube nanocomposite, setting the stage for several fundamental advances in the field of nanostructured carbon materials.

The result established for the first time a process for making these materials a reality, setting the stage for several fundamental advances in the field of nanostructured carbon materials.

The resulting material has potential for use in low-friction, wear-resistant coatings, catalyst supports for fuel cells, high-voltage electronics, low-power, high-bandwidth radio frequency microelectromechanical/nanoelectromechanical systems, thermionic energy generation, flat-panel displays and hydrogen storage.

"Diamond is hard because of its dense atomic structure and the strength of the bonds between atoms," said Argonne's John Carlisle, one of the developers of the new material. However, diamond is brittle and normally not electrically conducting. Nanotubes, on the other hand, are incredibly strong and great electrical conductors, but harnessing these attributes into useful materials has proved elusive.

The new material combines the properties of both diamond and nanotubes.

The next step is to develop patterning techniques to control the relative position and orientation of the ultrananocrystalline diamond and carbon nanotubes within the material.

Helping develop the material were Argonne scientists Orlando Auciello, Jeffrey Elam and Xingcheng Xiao.

TeraGrid to enhance access for research

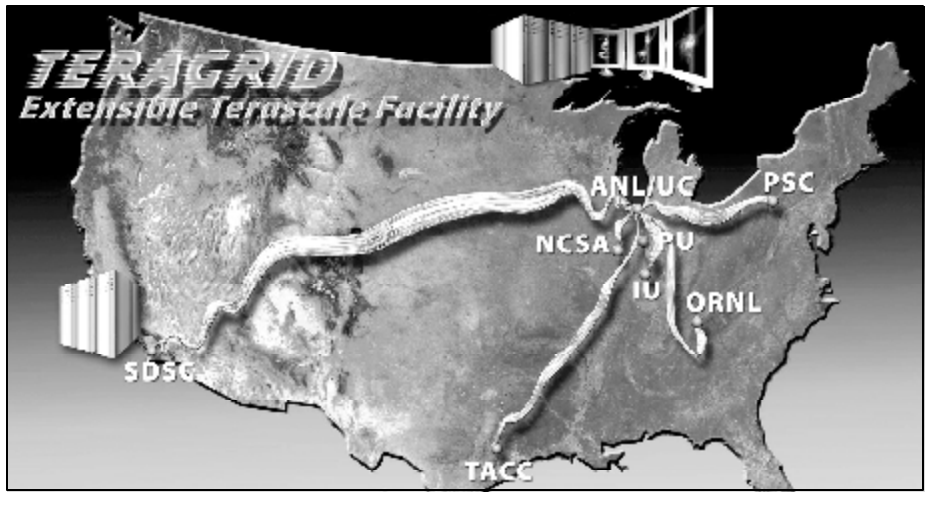
By Steve Koppes

The National Science Foundation has awarded $48 million to the University of Chicago over the next five years to operate and expand TeraGrid, a national-scale system of interconnected computers that scientists and engineers are using to solve some of their most challenging problems.

The NSF has concurrently granted another $100 million to the University of Chicago, Argonne and seven other institutions to provide computational, storage, instrument and visualization resources that make up the TeraGrid, along with user support and related services.

TeraGrid is the world's largest open computer, storage and networking system.

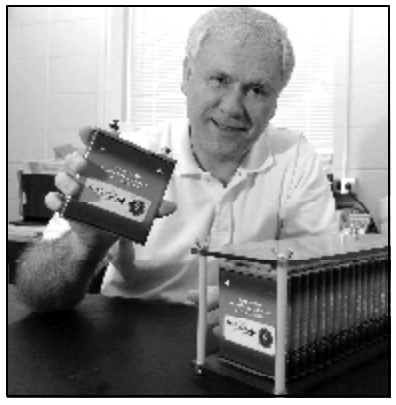
The TeraGrid team expects the system to affect virtually every scientific discipline that requires intensive computing capabilities, from disease diagnosis and weather forecasting to the study of drug interactions with cancer cells and aircraft design simulation.



Overseeing the TeraGrid will be Charlie Catlett, a senior fellow in the Computation Institute, a joint effort between the University of Chicago and Argonne.

One way that TeraGrid is measured is in teraflops: the total number of mathematical operations that can be done in one second, Catlett said. Currently, the TeraGrid's power is just over 60 teraflops. If each of the 300 million people in the United States were to do one calculation per second, it would take them 55 hours to compute as much as the TeraGrid can compute in one second.

For more information about TeraGrid, see *www.teragrid.org/*.



Argonne scientist Gary Henriksen, a Downers Grove resident, works on advanced automotive battery technology that may help reduce the nation's dependence on foreign sources of oil. *Photo by George Joch.*

Meet an Argonne scientist

By Kevin Trim

With the price of gas escalating at record levels, Argonne scientist and Downers Grove resident Gary Henriksen recently felt a sense of pride when he considered the potential significance of the battery research program he directs.

Henriksen, 60, leads a group of researchers in the Battery Technology Department, part of Argonne's Chemical Engineering Division, which focuses on both nuclear fuel cycle and electrochemical (battery and fuel cell) programs.

"We are involved in a large research and development (R&D) program with five other government laboratories, spending between $5.5 and $6 million per year, to develop more optimal batteries for use in hybrid electric vehicles (HEVs)," said Henriksen, an Argonne employee since 1990.

According to Henriksen, the U.S. automotive industry

(See "Henriksen," page 4)

Office of Science U.S. DEPARTMENT OF ENERGY

THE UNIVERSITY OF CHICAGO ARGONNE NATIONAL LABORATORY

Argonne National Laboratory is operated by the University of Chicago for the U.S. Department of Energy.

Software speeds emergency planning, response

By Catherine Foster

All Hazards Management, LLC, of Denver, Colorado has obtained worldwide exclusive rights to the Sync Matrix technology portfolio, a unique toolset of emergency preparedness software and systematic, structured services developed at Argonne.

This toolset enables the development of completely integrated, coordinated and synchronized emergency plans. Sync Matrix visually displays information to enable first responders to deliver an impeccably executed, multi-jurisdictional response to a terrorist attack or natural emergency of any source.

> The program supports the development of any number of emergency plans to any type of homeland defense emergency scenario.

It is the first and only systems-based application developed to address the complexities of planning and testing emergency responses by multiple agencies, disciplines and jurisdictions.

The program supports the development of emergency plans, from hurricanes, tornados, forest fires, chemical spills, etc., to any type of homeland defense emergency scenario. Sync Matrix is the first systems-based application to address the complex problem of planning and integrating responses to emergencies, particularly those involving different teams or agencies.

Argonne assists those affected by hurricane

"We at Argonne are deeply saddened by the suffering from Hurricane Katrina," said Argonne Director Robert Rosner. "Our thoughts are with those who have lost their loved ones, their communities, and those that have been hurt and injured. We are supporting organizational and individual efforts from the lab to help in whatever way we can."

Argonne's Infrastructure Assurance Center is supporting the Department of Homeland Security's Protective Security Division in identifying vulnerabilities, recommending potential protective measures, and evaluating damages at critical infrastructure and key resources directly affected by the storm. Two Argonne employees, Becca Haffenden and Greg Handke, were deployed to the Gulf Coast to support these efforts.

Argonne's Infrastructure Assurance Center, a member of the Department of Energy (DOE) virtual team, which provides data, analysis, and visualization tools to the Office of Infrastructure Security and Energy Restoration in response to energy emergencies and exercises, has been working long hours.

The virtual team was activated more than 48 hours prior to Hurricane Katrina's landfall to identify critical infrastructure assets that may be affected by the storm, as well as to estimate potential impacts and response challenges. During and after landfall, the team has focused on collecting and analyzing facility and system impact and restoration information.

Argonne's role centers on analyzing oil and natural gas infrastructures, along with interdependencies among the infrastructures. The team also includes experts from Los Alamos, Oak Ridge and Sandia national laboratories and the National Energy Technology Laboratory.

Brett Hansard, an emergency risk communication specialist in Argonne's Decision and Information Sciences Division, has been deployed to Baton Rouge to work with the Federal Emergency Management Agency. Other Argonne emergency communications specialists working in Louisiana are Jerry DeFelice and Jim Chesnutt. Argonne firefighter/paramedic Jimmy L. Ross was dispatched to the New Orleans area with a group from the Mutual Aid Box Alarm System, an Illinois state-wide mutual aid system.

Also in Louisiana is Moses Lee, M.D., an emergency medicine specialist at Stroger Hospital in Chicago, currently on special appointment at Argonne. Lee also serves as director of the Illinois Emergency Medical Response Team and was deployed for the relief efforts as part of that organization.

On the educational front, Argonne has offered extended appointments to its summer students from New Orleans who are unable to continue their work at Southern University. This past summer three Southern University researchers have been working at Argonne in the Environmental Assessment Division, and they will be able to remain in those positions.

Argonne is also hosting two students to continue their research on a project called "Development of Toxicological Matrices for Contaminants Released in Water and Air." Argonne, through the Division of Educational Programs, has also found resources to support their faculty mentor, Shirley Scott Williams.

At Argonne's request, DOE will make resources available in order to provide opportunities to other students and faculty members to host them at Argonne in research projects. Potentially, Argonne's program to host students displaced by Katrina could reach the size of its summer program.

Argonne's computer expertise is also assisting in connecting those separated from family members because of the destruction. Argonne information technology specialist Jay Johnson is providing computer networking capabilities at a shelter for Katrina refugees in Tinley Park. Using the computer network allows individuals to communicate with family members and others.

Associate Laboratory Director Murray Gibson, an accomplished pianist, explains "The Physics of the Blues" in a series of videos available on the Argonne Web site.

'Explorer' online has text, videos

The online version of *Explorer*, Argonne's new semi-annual magazine, includes video and other interactive features in addition to the full text of the magazine's articles about Argonne research and other activities.

The online version contains additional material on the articles featured in the magazine, including video of Associate Laboratory Director Murray Gibson demonstrating the relationship between physics and music; Robert Janssens and a "team" from the Physics Division explaining the Gammasphere with a baseball analogy; and footage from the Argonne-sponsored Rube Goldberg Contest. Also included is a photo slide show showing how actor Bill Landry, who performed the one-person play "Einstein the Man" at Argonne, transforms himself into the great scientist.

To see the online version of Explorer, visit the Argonne home page at *www.anl.gov,* click on "Media Center," and "Publications."

ARGONNE NATIONAL LABORATORY

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Research to enable the hydrogen economy

George Crabtree is senior scientist and director of the Materials Science Division at Argonne National Laboratory. This article is based on testimony he gave before the subcommittee on energy and research of the House Science Committee.

Crucial energy challenges motivate the need for a hydrogen economy. First, our dependence on fossil fuel requires that much of our energy come from foreign sources; securing our energy supply for the future demands that we develop domestic energy sources. Continued use of fossil fuels produces local and regional pollution that threatens the quality of our environment and the health of our citizens. Finally, fossil fuels produce greenhouse gases like carbon dioxide that threaten our climate with global warming.

Hydrogen as a fuel addresses all of these issues: it is found abundantly in compounds like water that are widely accessible without geopolitical constraints, it produces no pollutants or greenhouse gases as byproducts of its use, and it converts readily to heat through combustion and to electricity through fuel cells that couple seamlessly to our existing energy networks.

Critical Challenges: Production

The enormous appeal of hydrogen as a fuel is matched by an equally enormous set of critical scientific and engineering challenges. Unlike fossil fuels, hydrogen does not occur naturally in the environment. Instead, hydrogen must be produced from natural resources like fossil fuels, biomass or water. Currently nearly all the hydrogen we use is produced by reforming natural gas. To power cars and light trucks in the coming decades we will need 10 to 15 times the amount of hydrogen we now produce. This hydrogen cannot continue to come from natural gas, as that production route simply exchanges a dependence on foreign oil for a dependence on foreign gas, and it does not reduce the production of environmental pollutants or greenhouse gases. We must find carbon-neutral production routes for hydrogen.

Critical Challenges: Storage

The on-board storage of hydrogen for transportation is a second critical basic science challenge. To allow a 300-mile driving range without compromising cargo and passenger space, we must store hydrogen at densities higher than that of liquid hydrogen. This may seem a daunting task, but in fact there are a host of materials where hydrogen combines with other elements at densities 50 percent to 100 percent higher than that of liquid hydrogen. Since the 1970s over 2,000 hydrogen compounds have been examined for their storage capability; none has been found that meet the storage demands. The challenge is to satisfy two conflicting requirements: high storage capacity and fast release times. High hydrogen capacity requires close packing and strong chemical bonding of hydrogen, while fast release requires loose packing and weak bonding for high hydrogen mobility. This critical storage challenge cannot be met without significant basic research: we must better understand the interaction of hydrogen with materials and exploit this knowledge to design effective storage media.

Critical Challenges: Fuel Cells

The use of hydrogen in fuel cells presents a third critical scientific challenge. Fuel cells are by far the most appealing energy conversion devices we know of. They convert the chemical energy of hydrogen or other fuels directly to electricity without intermediate steps of combustion or mechanical rotation of a turbine. Their high efficiency, up to 60 percent or more, is a major advantage compared to traditional conversion routes like gasoline engines with about 25 percent efficiency. The combination of hydrogen, fuel cells and electric motors has the potential to replace many of our much less efficient energy conversion systems that are based on combustion of fossil fuels driving heat engines for producing electricity or mechanical motion.

Argonne Materials Science Division Director George Crabtree testified before the House Subcommittees on Energy and Research, sharing thoughts on the role of basic research in ushering in the "hydrogen economy" to reduce the nation's dependence on foreign energy sources. "Revolutionary breakthroughs are needed, of the kind that come only from high-risk, high-payoff basic research," Crabtree said. Here, Crabtree meets with 13th District U.S. Rep. Judy Biggert, who chairs the Science Subcommittee on Energy.

Conclusion

The vision of the hydrogen economy as a solution to foreign energy dependence, environmental pollution and greenhouse gas emission is compelling. The enormous challenges on the road to achieving this vision can be addressed with innovative high-risk/high-payoff basic research. The great contribution of basic research to society is the discovery of entirely new approaches to solving our most pressing needs. The phenomenal advances in personal computing enabled by semiconductor materials science and their impact in every sphere of human activity illustrates the power of basic science to drive technology and enhance our daily lives. The challenges for the hydrogen economy in production, storage and use are known. Recent developments in nanoscience, in high-intensity sources for scattering of electrons, neutrons and x-rays from materials at DOE's user facilities, and in numerical simulation using density functional theory open promising new directions for basic research to address the hydrogen challenges. The breakthroughs that basic research produces in hydrogen materials science will enable the realization of a mature, sustainable, and competitive hydrogen economy.

Argonne's Human Resources Director Carol Quinn (left) accepts the Diversity and Multiculturalism Award from Robin Robinson of FOX News, Chicago. The award recognizes leadership as an organization that is "open and inclusive to people of differing human qualities, promotes a tolerant work environment, and considers diversity and multiculturalism to be a competitive advantage."

Argonne honored for diversity

Argonne won the Diversity and Multiculturalism Best Practices award — one of the top 10 "Elite" awards of Chicago's Best and Brightest Companies to Work For — presented by the National Association for Business Resources. The awards recognize companies that use innovative practices and tools in human resources activities.

The Diversity and Multiculturalism Best Practices award focuses on the "extent to which the organization is open and inclusive to people of differing human qualities, promotes a tolerant work environment, and considers diversity and multiculturalism to be a competitive advantage."

"This is good news for Argonne and recognition of the laboratory's efforts to leverage the talents of all our employees by supporting diversity," said Carol Quinn, Argonne's director of Human Resources. "It is one more acknowledgement that Argonne is truly an 'Employer of Choice.'"

The livin' is easy

A fallow deer at Argonne National Laboratory enjoys the summer sunshine. Commonly referred to as "white deer," the species is native to parts of Asia. They are remnants of a herd kept by a previous owner of the Argonne site.

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ARGONNE UPDATE

The community newsletter for neighbors of Argonne National Laboratory

Inside this issue

Henriksen

(Continued from page 1)

has been somewhat cautious about entering the HEV market, even though most U.S. automakers have now introduced HEVs or have announced a schedule for doing so.

A major reason for this hesitancy, as well as the slow growth of the HEV market, has been because of the lack of an optimal energy storage device. Today's commercial HEVs use nickel/metal hydride batteries, which are expensive and last about eight years. Argonne's goal is to produce a battery capable of operating for 15 years.

"Better energy storage systems are needed and high-power lithium-ion (Li-Ion) batteries offer the most promise for replacing traditional batteries," noted Henriksen. "Argonne's programs are addressing these needs. With continued R&D, they could become less expensive and have a longer calendar life, and also provide the same amount of power and energy, and be smaller and lighter weight. This could dramatically expand the market for conventional HEVs and help reduce U.S. dependence on foreign oil."

Married with several grown children, this hobbyist who in his spare time enjoys photography and performing home improvements, believes significant progress is being made to understand the factors that limit battery calendar life and inherent safety, as well as in developing new cell materials and chemistries that provide greater stability.

He pointed out that in a related program, Argonne is also developing new electrode materials and electrolyte systems that could facilitate the commercialization of a new generation of HEVs, denoted "plug-in" HEVs. These vehicles can be "plugged" into home electrical outlets at night to charge batteries.

"These batteries could allow 'all-electric' round-trip work commutes of up to 50 miles per day by these types of HEVs, which could help dramatically reduce U.S. dependence on foreign oil," he said.

LAB NOTES

Visit Argonne's Web site at www.anl.gov for more information on these and many other stories.

■ **Faster, easier-to-use X-ray beamlines** at Argonne's Advanced Photon Source are allowing researchers to increase the pace of determining atomic structures of biomolecules important to life. This structural information will help reveal the roles that proteins play in health and disease and lead to structure-based medicines and therapies to treat genetic and infectious diseases.

■ Argonne will soon be home to a new **Sub-Angstrom Microscopy and Microanalysis** (SAMM) facility, which will house four cutting-edge electron microscopes. Construction is expected to be complete next summer.

SAMM will be a user facility, open to researchers at Argonne and from industry and academia. Its powerful electron microscopes will give researchers atom-scale views of the structure of materials, with a focus on nanoscience.

■ Each year as many as 200 students in Ph.D. programs compete to attend Argonne's **National School on Neutron and X-ray Scattering**. Sixty are selected to attend the school here each August, now in its seventh year. Argonne is the only national laboratory with both types of facilities: the Intense Pulsed Neutron Source (IPNS) for neutron scattering and the Advanced Photon Source (APS) for X-ray scattering.

The National School on Neutron and X-Ray Scattering brings the field's top senior scientists from academia, industry and national laboratories together with the brightest young scientists attending U.S. universities.

■ Argonne researcher Michael Wang, a world-leading expert in energy and **environmental benefits of ethanol** as a substitute for gasoline in transportation fuels, presented the results of his research at the Ethanol Energy Open Forum, sponsored by the National Corn Growers Association at the National Press Club, Washington, D.C.

Compared to gasoline, any type of fuel ethanol substantially helps reduce fossil energy and petroleum use, Wang said.