Research Notes

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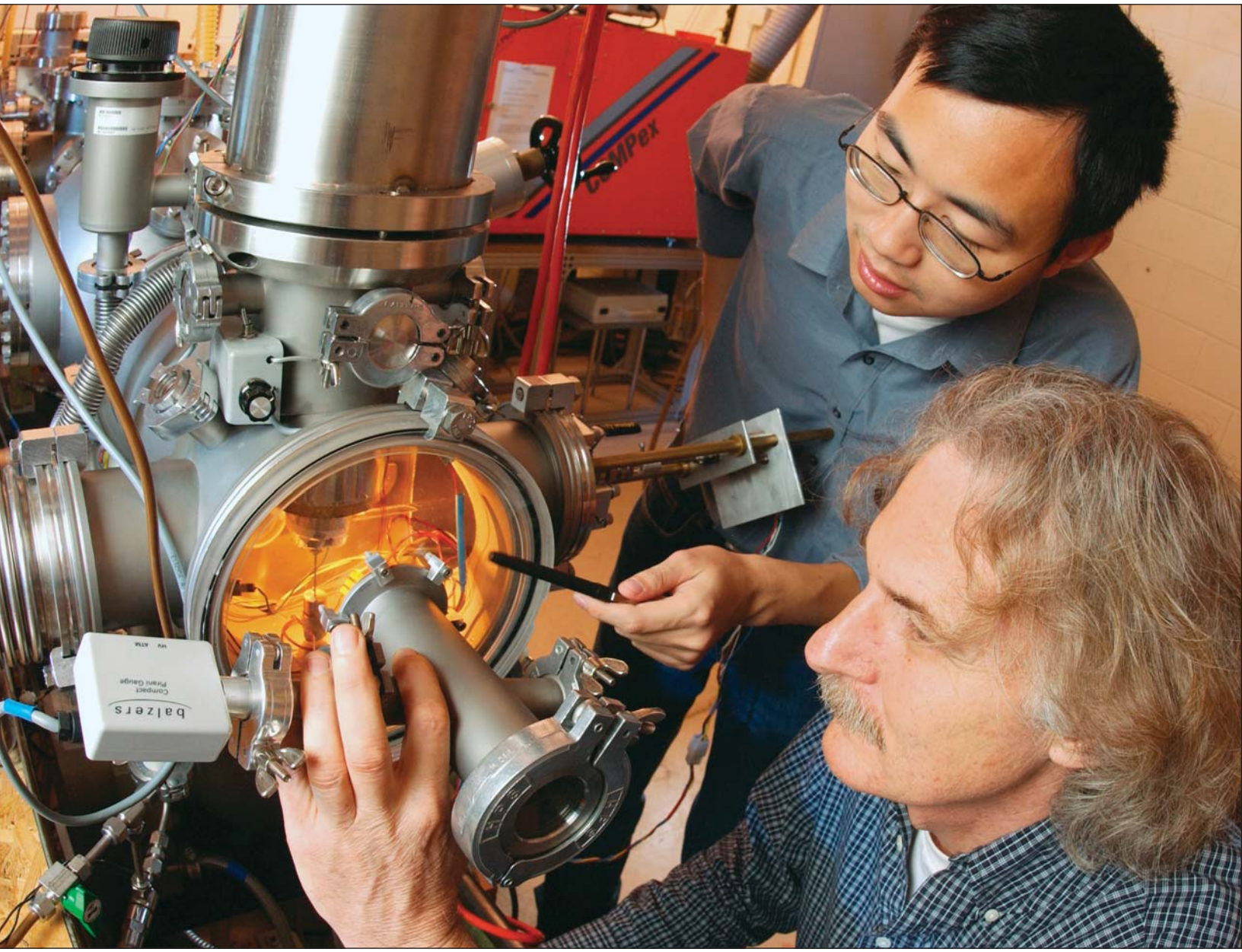


Researchers adjust equipment used to create and study nanometer-scale clusters of the metal niobium. When cooled to temperatures below 20 degrees Kelvin, the clusters exhibit unusual behavior.

When is a Metal not a Metal?

Nanoclusters of niobium display distinctly non-metallic properties at ultra-cold temperatures.

When is a metal not a metal? Georgia Tech researchers answered that question in the May 23, 2003 issue of the journal *Science*. The article reported the surprising behavior exhibited by nanometer-scale clusters of the metal niobium. When the clusters are cooled to below

20 degrees Kelvin, electrical charges in them suddenly shift, creating structures known as dipoles.

"This is very strange because no metal is supposed to be able to do this," says Walter de Heer, a professor in the School of Physics and co-author of the paper published in *Science*. "These clusters become spontaneously polarized, with electrons moving to one side of the cluster for no apparent reason. One side of each cluster becomes negatively charged, and the other side becomes positively charged. The clusters lock into that behavior and stay that way."

This ferroelectric phenomenon has so far been observed in clusters of niobium, vanadium and tantalum – three transition metals that in bulk form become superconducting at about the same temperature that the researchers observe formation of dipoles in the tiny clusters. De Heer believes this discovery will open a new field of research – and provide clues to the mystery of superconductivity.

In bulk metals — and even in niobium clusters at room temperature — electrical charge is normally distributed equally throughout the sample unless an electric field is applied. But in the clusters of up to 200 niobium atoms created by de Heer and collaborators Ramiro Moro, Xiaoshan Xu and Shuangye Yin, that changes when the particles are cooled to less than 20 degrees Kelvin.

The Georgia Tech researchers discovered this "spontaneous symmetry breaking" while searching for signs of superconductivity in the nanometer-scale clusters. It was completely unexpected, and de Heer admits he has no explanation for it.

"When this happens, these particles that are made out of metal atoms no longer behave as if they were metallic," he says. "Something changes the particles from a metal into something else."

For the smallest clusters, the strength of the dipole effect varies dramatically according to size. Clusters composed of 14 atoms display strong effects, while those made of 15 atoms show little effect. Above 30 atoms, clusters with even numbers of atoms display stronger dipole effects than clusters with odd numbers of atoms.

"Structure matters greatly to this process," de Heer says. "A small change can affect the position of the phase transition rather profoundly, and the exact arrangement of atoms really does matter to these systems."

He attributes the size sensitivity to the quantum size regime, which is related to restrictions on how electrons can move in very small clusters.

De Heer sees strong "circumstantial evidence," but no solid proof, that the phenomenon is connected to superconductivity in these metals.

"Our assumption is that superconductivity in the bulk materials has something to do with the spontaneous production of dipole in the small particles," he says. "At this point, it is circumstantial evidence – the same materials and the same temperature regime, and the odd phase transitions occurring in both. By studying several different metals, we found that those that are superconducting in bulk have this effect, and those that are not superconducting do not have it. That strengthens our belief that this is connected to superconductivity in some way that we don't yet understand."

So far, researchers have studied in detail clusters of up to 200 atoms, though de Heer believes the effect should continue in larger clusters, perhaps up to 500 atoms or as many as 1,000.

"This is just the beginning of what will ultimately be a very exciting story," he says. "We certainly have a lot of work to do."

The research has been sponsored by the U.S. Department of Defense, the National Science Foundation and Georgia Tech.

— John Toon

■ For more information, contact Walter de Heer, School of Physics, Georgia Tech, Atlanta, GA 30332-0430. (Telephone: 404-894-7879) (E-mail: deheer@electra.physics.gatech.edu). The full-text, news release version of this article is on the Web at **gtresearchnews.gatech.edu/newsrelease/niobium.htm.**

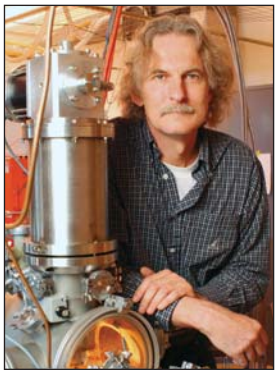


PHOTO BY GARY MEEK

In his Georgia Tech laboratory, Professor Walter de Heer uses specially designed equipment to create and study nanometer-scale clusters of the metal niobium.

Georgia Tech researchers discovered this "spontaneous symmetry breaking" while searching for signs of superconductivity in the nanometer-scale clusters.

Less Expensive Displays

New technique allows polymer processing of a key solid-state fluorescent material.

By chemically attaching a difficult-to-process solid-state fluorescent material to a universal polymer backbone, researchers at the Georgia Institute of Technology have built what may be a foundation for a new generation of optoelectronic display devices based on inexpensive organic light-emitting diodes (OLEDs).

Until now, the aluminum tris (8-hydroxyquinoline) (Alq_3) material – which is used as the emission and electron transport layer in organic light-emitting diodes – had to be deposited under high vacuum conditions, which requires costly equipment. Attaching it to a polymer backbone

PHOTO BY GARY MEEK

Researchers Marcus Weck and Amy Meyers examine vials containing dilute solutions of polymers with functionalized Alq_3. By allowing the fluorescent material to be applied as a polymer, the researchers could help lower the cost of manufacturing organic light-emitting diodes.

Vials containing dilute solutions of polymers with functionalized Alq_3 show the ability of the system to be tuned to different wavelengths.

PHOTO BY GARY MEEK

allows the material to be applied using solution processes – simple spin-coating methods already widely used for applying thin films of materials.

Beyond the implications for less costly and more flexible flat panel displays and similar devices, the new technique demonstrates that small molecules with interesting properties can be self-assembled onto standard polymer backbones. Using this "Lego-like" approach could have applications to other materials that are easier to process in polymeric form.

"This could have a significant impact for industry because it would make the manufacture of organic light-emitting diodes much easier," says Marcus Weck, an assistant professor in Georgia Tech's School of Chemistry and Biochemistry. "You can do this on a lab bench without million-dollar equipment. Being able to spin coat these organic systems could allow production of large surfaces suitable for displays."

Details of the work were presented March 27, 2003 at the 225th American Chemical Society National Meeting in New Orleans. Sponsored by the National Science Foundation and the Office of Naval Research, the study has also been published in the journal *Macromolecules*.

Because they are based on polymers, organic light-emitting diodes produced with the new technique could offer another significant advantage – physical flexibility. That would allow production of displays that are less prone to damage and that can operate in shapes and forms not possible with current technology.

Using the polymer poly(norbornene) as a backbone, Weck and graduate student Amy Meyers designed a functional monomer containing Alq_3, also known as aluminum tris (8-hydroxyquinoline). The Alq_3 was covalently bonded to the poly(norbornene) backbone, which was selected because it can be polymerized by ring-opening metathesis, a method that tolerates many functional groups.

Though the prototype material shows great potential, Weck cautions that much work remains to be done before the new material finds its way into laptop computers and other display systems.

"From a scientific standpoint, this is a milestone, but there is a lot of optimization and evaluation that must be done," he says. "We've shown that we can change the polymer backbone and that we can change the connection of our Alq_3 to the polymer."

The Georgia Tech researchers are working with scientists at the University of Arizona to assess how well the new material would work in OLEDs. If long-term testing shows the new polymer has the desired stability and other properties, it could help open up new applications for OLEDs.

The Alq_3 system is the first demonstration of a technique Weck hopes will allow his research group to build many new types of polymers using modular scaffolds programmed to attract building blocks of small molecules. Weak and easily reversed chemical interactions would self-assemble those molecules to form complex structures with predictable physical and chemical properties.

In the natural world, self-assembly techniques produce thousands of varied life forms — bacteria to human beings — based on a relatively small set of amino acids and nucleosides combined in different ways. By emulating this natural system, he hopes to simplify the synthesis of new materials for light-emitting diodes, optical storage materials,

biosensors, drug-delivery materials and other applications.

"The goal is to simplify the synthesis of designer polymers via self-assembly using combinatorial chemistry," Weck explains. "Our group is taking design lessons from Nature by incorporating into one system several of these weak interactions to get a degree of complexity that is difficult to achieve otherwise. We believe we now have the basic proof of principle to show that we will be able to address this problem."

— John Toon

■ For more information, contact Marcus Weck, School of Chemistry and Biochemistry, Georgia Tech, Atlanta, GA 30332-0400. (Telephone: 404-385-1796) (E-mail: marcus.weck@chemistry.gatech.edu). The full-text news release version of this article is on the Web at **gtresearchnews.gatech.edu/newsrelease/alq3.htm**.

Shining Light on Cancer

Improved molecular beacons show promise for cancer detection, rapid viral diagnosis.

Diagnosing cancer may one day involve introducing "molecular beacons" into the body and then watching for specific optical or magnetic signals as the nanometer-scale structures latch onto the unique genetic sequences that are markers for the disease.

Believed to be the first technique for imaging RNA in living cells, a new class of beacons under development at the Georgia Institute of Technology and Emory University also has potential applications in the rapid diagnosis of viral infections, as well as drug discovery and pharmacogenomics. Their ability to rapidly detect viruses makes the beacons potentially valuable in the battle against bio-terrorism.

Georgia Tech and Emory researchers are developing improved signaling, targeting and delivery systems for the beacons, which consist of a fluorescent dye molecule and a quencher molecule on opposite ends of an oligonucleotide engineered to match specific genetic sequences associated with disease.

Initially, the dye and quencher molecules are held close together in a hairpin shape, the quencher preventing fluorescent emission from the dye. When delivered into cells, the beacons seek out matching sequences in genetic material known as messenger RNA (mRNA). If the beacons encounter and bind with their specific mRNA targets, Watson-Crick base-pairs holding the dye and quencher together break, allowing emission of a specific fluorescent signal when excited by light.

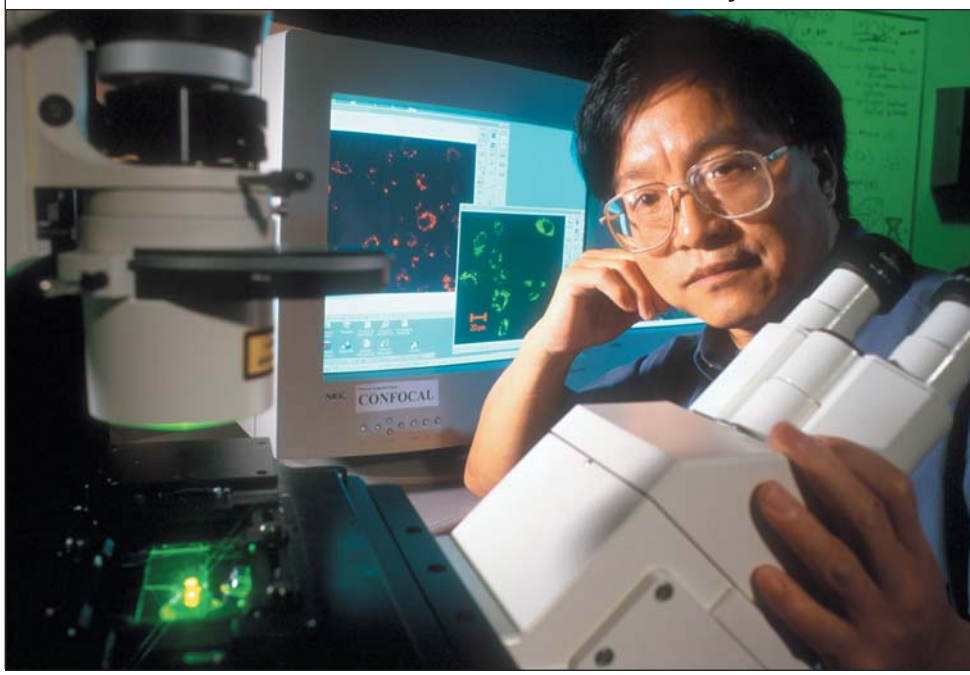
Details of the research, sponsored by the Wallace H. Coulter Foundation and the National Science Foundation, were presented March 26, 2003 at the 225th national meeting of the American Chemical Society in New Orleans.

Researchers led by Gang Bao, an associate professor in the Wallace H. Coulter Department of Biomedical Engineering operated jointly by Georgia Tech and Emory, are improving earlier beacon systems to overcome problems specific to their use in living cells. They have also made progress developing magnetic beacons suitable for use in body tissues too deep for optical imaging to work.

"We want to cover the whole spectrum," Bao explains. "The idea is to use the optical molecular beacons for cellular studies outside the body. You can combine that with a delivery system and additional technologies to do shallow tissue imaging. With the magnetic beacons, we could do deep-tissue imaging."

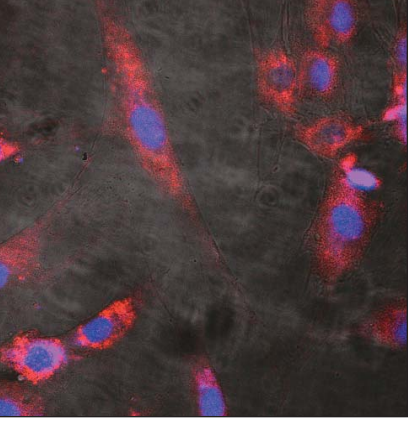
Developed in the mid-1990s, molecular beacons are used today by researchers to detect sequences of nucleic acids in homogeneous solu-

Their ability to rapidly detect viruses makes the beacons potentially valuable in the battle against bio-terrorism.



Researcher Gang Bao uses a confocal microscope to image molecular beacons in cellular samples. The instrument is in the Coulter Department of Biomedical Engineering, which is operated by Georgia Tech and Emory University.

PHOTO BY GARY MEEK



Shown is a fluorescent image of dual FRET molecular beacons targeting K-ras mRNA in human dermal fibroblasts. K-ras is a member of the G-protein family and is involved in transducing growth-promoting signals from the cell surface.

tions. Bao and collaborators Andrew Tsourkas and Phil Santangelo have improved the basic system to enhance accuracy and efficacy in living cells.

Bao and colleagues are pursuing other improvements, including an ability to target specific organ systems, more rapidly disperse the beacons into cells, and recognize genetic sequences that signify the presence of viruses. The latter work, in which the researchers have shown their ability to detect viral mRNA, could be the basis for tests able to identify viruses within a few hours – instead of days.

With Dr. Karim Godamunne, who holds both a medical degree and an MBA, Bao has formed a start-up company – Vivonetics – to commercialize the patent-pending technology. The company recently received a $50,000 commercialization grant from the Georgia Research Alliance.

Many challenges lie ahead.

In early and more curable stages of cancer, the amount of marker RNA in bodily fluids such as blood or pancreatic fluid is low. That means the researchers must develop a detection system sensitive enough to pick up very faint signals.

A definitive cancer diagnosis requires recognizing several markers, so they will also have to use several beacons systems together, each targeting different markers and producing different signals. For in-vivo use, researchers will have to show that the beacons don't harm healthy cells.

For cancer, Bao envisions a comprehensive system in which molecular beacons detect cancerous cells in lab-tested bodily fluids. When appropriate fluids cannot be obtained, other beacons could be introduced into the body to detect the cancerous cells. Beacons could then be used to monitor the success of cancer therapy. And because they specifically attach to mRNA, beacons could perhaps also be used to slow down or halt the growth of cancer cells.

— John Toon

■ For more information, contact Gang Bao, Department of Biomedical Engineering, Georgia Tech, Atlanta, GA 30332-0535. (Telephone: 404-385-0373) (E-mail: gang.bao@bme.gatech.edu) or Dr. Karim Godamunne, Vivonetics, Inc., 430 Tenth St. N.W., Suite S-203, Atlanta, GA 30318. (E-mail: karim@vivonetics.com). The full-text news release version of this article is on the Web at **gtresearchnews.gatech.edu/newsrelease/beacons.htm**.

Role Reversal Repercussions

Male pregnancy in seahorses may affect formation of new species in this fish family.

Male pregnancy in seahorses may do more than reverse traditional gender roles. It could also influence the way new species form from single populations of these ancient creatures.

Studies have shown that most new species arise from geographically, and therefore genetically, isolated populations. But some seahorses likely diversify in a process called sympatric speciation, in which new species arise from a single population that has no geographic barriers to inhibit gene flow, according to a paper published in May 2003 in the *Proceedings of the National Academy of Sciences (PNAS)*.

"We think there's a fairly strong case that sympatric speciation may have occurred in seahorses," says Georgia Institute of Technology Assistant Professor of Biology Adam Jones, the lead author on the PNAS paper. "We're not arguing that all speciation in seahorses is sympatric. The majority of speciation is probably due to some geographic barrier to genetic migration. But in some instances it looks like sympatric speciation occurred."

Driving the sympatric speciation process in seahorses is the fish's size-similar mating practice imposed by male pregnancy, extended male parental care and monogamy, Jones says. Seahorses choose similar-size mates to have the best chances for successful reproduction. The

IMAGE COURTESY OF ADAM JONES

Pictured at right is a seahorse species found in western Australia and studied by the authors of the journal article.

female inserts ripe eggs into the male's brood pouch, where the eggs are fertilized, embed and incubate for 10 days to six weeks, depending on the species.

"Male reproductive rates, the size of the brood pouch and the number of eggs that a female produces all increase with the size of the seahorse," Jones explains. "So if you're a large seahorse, you want to mate with another large seahorse so you're not wasting your eggs or your brood pouch space. So this kind of mating is the real mechanism for sympatric speciation. A lot of forms of parental care might not cause that size-specific restraint in mating, but this one does."

In addition to size-specific mating, a process called disruptive selection is also necessary for sympatric speciation to occur, Jones says. Disruptive selection occurs when large-sized and small-sized individuals survive better than mid-sized animals.

To test their hypothesis, Jones and his co-authors developed a computer-based genetic model to determine if the rate of size-similar mating in their field study population was sufficient to produce disruptive selection and, in turn, sympatric speciation. The model allows simulated populations to evolve at the rate of size-similar mating that Jones and his colleagues observed in a seahorse species off the coast of Perth, Australia. Under these conditions, the model indicated sympatric speciation does occur with fairly modest levels of disruptive selection.

"So the remaining question is whether disruptive selection occurs at a sufficient strength in natural populations of seahorses," Jones notes. "The model shows it's plausible, but as in most cases of sympatric speciation, we have no definitive proof."

To determine that size-similar mating was occurring in the field study population, researchers conducted genetic analyses of parentage, much like the DNA "fingerprinting" technique used in humans. Researchers tagged males and females in the field, sampled the DNA of the males' progeny and then determined the mother of those offspring. Then, researchers compared the sizes of male and female partners to chart a statistical trend that indicated size-similar mating.

A third line of evidence for sympatric speciation came from the phylogeny, or family tree, of seahorses, which are found in coastal and ocean habitats throughout the world, except in extreme latitudes. Researchers gathered documentation of species pairs that are close relatives and live in the same place.

"If there had been sympatric speciation and it was based on assortative mating by size, then when speciation occurs, the result should be a large species and a small species that live in the same place," Jones explains. Indeed, researchers noted two examples of species that are close relatives that are sympatric over part or all of their range.

— Jane M. Sanders

■ For more information, contact Adam Jones, School of Biology, Georgia Tech, Atlanta, GA 30332-0230. (Telephone: 404-385-4435) (E-mail: adam.jones@biology.gatech.edu). The full-text news release version of this article is on the Web at **gtresearchnews.gatech.edu/newsrelease/seahorse.htm**.

Studies have shown that most new species arise from geographically, and therefore genetically, isolated populations.

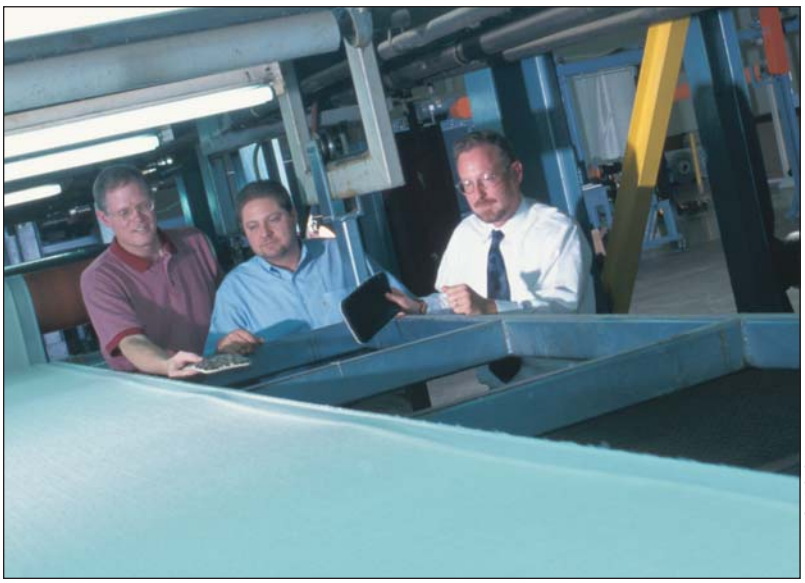


PHOTO BY GARY MEEK

Universal Textile Technologies of Dalton developed a new bio-based carpet backing process, the kind of product innovation that helps boost revenues for Georgia companies. Shown inspecting the product are (l-r) Bill Harrison, the company's environmental coordinator, Eddie Patterson, the firm's production manager, and Jerry Zolkowski, northwest Georgia region manager for Georgia Tech's Economic Development Institute, which provided assistance

Innovation Rules

Georgia manufacturing survey points to profit and wage benefits for innovation.

Georgia manufacturers that compete based on innovation in products and processes rather than on low cost earn higher profits and benefit from higher wages, according to the 2002 Georgia Manufacturing Survey conducted by the Georgia Institute of Technology's Economic Development Institute (EDI) and School of Public Policy. Researchers found that on average, annual wages were $10,000 higher at innovative manufacturing firms, and returns on sales were almost a full percentage point higher.

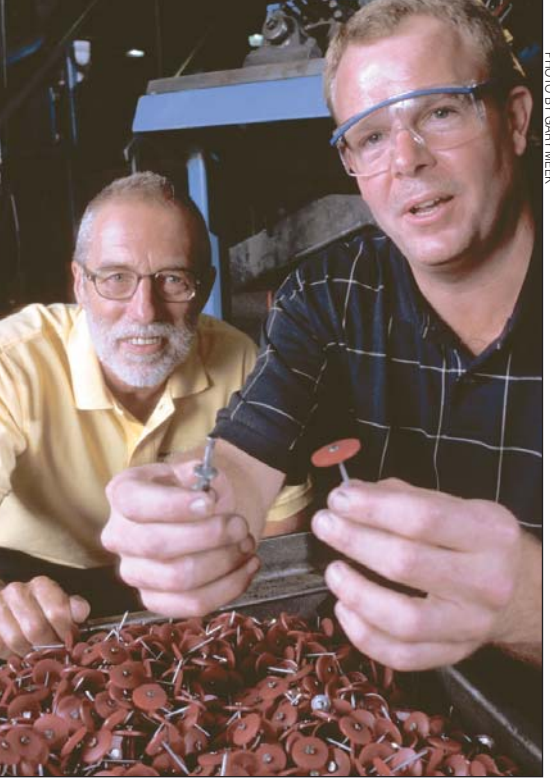


PHOTO BY GARY MEEK

Georgia Tech helped Americus-based Simplex Nails streamline its operations, and the company credits the assistance for helping it return to profitability. The 2002 Georgia Manufacturing Survey found that nearly a quarter of Georgia companies had used Georgia Tech business assistance. Shown, left to right, are John Stephens, a Georgia Tech specialist in lean enterprise techniques, and Jeff Kurtz, plant manager for Simplex.

Researchers defined innovative companies as those that were developing new products or processes, improving products or processes, or changing organizationally.

But the majority of Georgia manufacturers are competing based on cost rather than innovation. That's a bad sign, according to EDI researcher Jan Youtie, because companies competing on low cost are vulnerable to competition from international producers with even lower costs.

The study also showed that more than half of Georgia's manufacturers underwent major changes in strategy or structure in the last two years, and that company concerns have shifted from information technology to marketing and new product development – with nearly two-thirds of manufacturers now improving or developing new products.

"What was disturbing in this survey is that even more of our manufacturers competed on low price than had taken this approach in the last survey when we were in a growth economy," Youtie says. "So when faced with a stressful economic situation, rather than innovating their way out, they are trying to get out of it by dropping their prices. That's not a good long-term strategy for global competition."

Researchers defined innovative companies as those that were developing new products or processes, improving products or processes, or changing organizationally. Researcher Philip Shapira, a professor in the Georgia Tech School of Public Policy, notes that innovation isn't restricted to "high technology" companies.

"There can be innovative companies in traditional sectors such as textiles, food and apparel," he says. "It may be that they use these process and organizational methods to give themselves leverage in the marketplace in order to distinguish themselves from other companies."

In the survey, manufacturers' reasons for not innovating included cost, lack of available financing, uncertainty regarding benefits, organizational rigidity, lack of market information, lack of in-house systems and disinterest from current customers.

"My sense from the survey is that Georgia's manufacturers are weathering the downturn in the economy," Shapira says. "They are changing their priorities and becoming more interested in marketing and product development. I think that is a good sign."

Other results from the study included:

- Manufacturers' priorities shifted from information technology hardware and software to marketing and product development. More than 60 percent of Georgia manufacturers reported doing some type of product development, whether it was developing new-to-the-industry products, offering value-added support services or linking with innovative, out-of-state companies.
- Concerns about information technology hardware and software declined from peak 1999 levels. The survey showed that virtually all manufacturers use e-mail and the majority use company Web sites, shared databases and high-speed Internet connections. More than one-third of manufacturers reported that customer requirements drive information technology adoption, and information technology use rose with facility employment size.
- About half of Georgia manufacturers underwent major changes in strategy or structure in the last two years. About a quarter reported changes in organizational structure; other top changes included marketing concepts and methods, corporate strategies, internal or external training, ownership and management techniques.
- Nearly half of responding manufacturers had at least 20 percent of employees using computers or other programmable machine controllers at least once a week as part of their jobs. One out of five respondents reported that a majority of its employees used computers or programmable controllers weekly. Firms with more than 20 percent of employees using computers had higher than average sales revenues, returns on pre-tax sales and productivity than those with a lower percentage of (or no) computer users.
- Twenty-four percent of manufacturers surveyed used Georgia Tech for business assistance. The top benefits reported were improved management and employee skills, improved existing processes and increased productivity.

— Nancy Fullbright

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