PHYSICS NEWS FLASH

Ultrathin Metal Alloys as Potential “Hydrogen Sponge”

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UT physicists, together with ORNL scientists, have won $1.2 million to study hydrogen storage; an endeavor built on metal, magic, and the power of one tiny electron.

The Department of Energy grant actually began with “Tuning the Quantum Stability and Superconductivity of Ultrathin Metal Alloys,” published in the June 15 issue of *Science*. Professors Jim Thompson, Hanno Weitering, and Zhenyu Zhang co-wrote the paper with lead author Murat Özer (Ph.D., 2006) and Yu Jia, a visiting professor from Zhengzhou University (ZZU) in Zhengzhou, China.

The UT/ORNL/ZZU collaborative team reports on an alloy made from lead and bismuth, as well as the discovery that thin films made from these metals can be “tuned” at the atomic level. While they have had previous success using lead alone to grow very flat, smooth films, the addition of bismuth revealed some interesting new ideas about how materials behave at the nanoscale.

Ultrathin films are typically only five to 20 atoms thick. While a metal or an alloy may be well understood in bulk form, in quantum systems like this, Weitering explains, all bets are off.

“Small scale materials can just behave very differently,” he says. “The properties are dictated by quantum mechanics.”

As he explains it, the group drove the bismuth-lead alloy into the “quantum regime” by changing the temperature. Bismuth and lead sit side-by-side on the periodic table, with bismuth having one more electron than its neighbor.

“That extra electron does the trick,” Weitering says. By changing the number of electrons in the film, “we’ve found that you can tune the growth morphology. That means you can do microscopic measurements as a function of thickness, where you know exactly what the thickness and compositions are. To have that perfect control is usually very hard.”

Although scientists have grown thin films for years, in the past it was difficult to control their size and structure because extremely thin films usually self-destruct, forming tiny droplets. Weitering explains that it wasn’t until the late 1990s that researchers discovered how to clear those hurdles. Zhang and his collaborators, in fact, discovered “magic layer thicknesses” in these tiny systems that can stabilize the film, making it possible to grow smooth layers.

The UT group found that by fine-tuning the way a film develops, they can determine its behavior.

"By tuning the growth mode," Weitering says, "we were able to tune superconducting properties."

That discovery inspired them to consider the idea that if you could tune the physical properties of quantum systems, perhaps it's possible to change their chemical properties as well, in effect devising "a knob" of sorts to tune chemical reactions.

Quantum Leap to Hydrogen

When DOE requested proposals for research supporting the President's Hydrogen Fuel Initiative, UT's physicists saw an opportunity to apply their quantum tuning concept to hydrogen chemistry.

"The hydrogen grant proposal was inspired by this quantum growth," Weitering says.

With fellow physicists Zhang and Distinguished Professor Ward Plummer, Weitering submitted a proposal to investigate "Quantum Tuning of Chemical Reactivity for Storage and Generation of Hydrogen Fuels." In May 2007, the Department of Energy announced $11.2 million in funding for hydrogen research, and the trio's proposal won one of only seven grants awarded to study novel materials for hydrogen storage and the only one within the DOE national systems to start this year.

Hydrogen has emerged as an attractive candidate for energy purposes because it has a high energy content and produces no harmful emissions when used in fuel cells. How to store hydrogen, however, has been a challenge, in part because in previous efforts the temperature required to absorb or release it has been either too high or too low.

"What we hope to do first is demonstrate that through these quantum effects one can actually modify the desorption temperature of the hydrogen," Weitering says. "Ideally, you want to bring it down."

Instead of using heavier elements like lead and bismuth, UT's scientists will work with magnesium, aluminum, and sodium to test their chemical tuning principles. For possible fuel cell applications in the auto industry, Weitering says, a lightweight material is the best option.

"Magnesium happens to be a lightweight material that soaks up hydrogen," he says. "But it's not only how strongly does the hydrogen bind to the magnesium, but also how easily it goes in; it's what we call kinetics. Thermodynamics tells you about energetics and kinetics about how easy it is to get in and out. We also think we can control that with quantum size effect."

With bulk magnesium, temperatures of around 300 or 400 degrees centigrade are required to release hydrogen. Zhang and Jia have already worked through preliminary calculations predicting that quantum engineering can lower the desorption temperature by at least 100 degrees.

The project is funded for three years, during which Weitering says he and his colleagues hope to demonstrate that hydrogen chemistry—absorption, desorption, and diffusion—can be controlled. He, Zhang, and Plummer all have joint appointments at Oak Ridge National Laboratory and the research will be conducted both at ORNL and on UT's campus. Weitering says it's a good way for joint faculty to contribute to the national laboratory's mission. It's also a return to a niche he first explored as a Ph.D. student working with lead films on silicon.

"Twenty years later," he says, "you can still have fun with these materials systems."