MATERIALS SCIENCE

Another Step Toward a Diamond-Beater

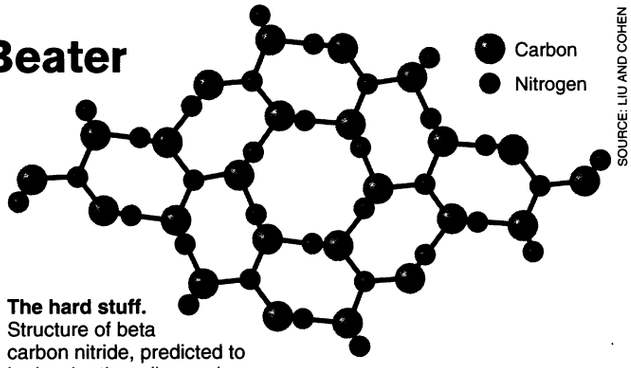
Five years ago, two researchers used a supercomputer to conjure up a crystalline material that could be harder than diamond—if it ever gets made. Since then, materials scientists have struggled without success to take that theoretical material—a form of carbon nitride—out of the computer and into the real world. But last week, at the annual meeting of the Minerals, Metals, and Materials Society in Las Vegas, Yip-Wah Chung reported that he and his colleagues at Northwestern University had created a new composite material that may include the predicted diamond-beater.

The composite, made up of atoms-thick layers of titanium nitride and carbon nitride, is already about as hard as diamond's nearest rival, cubic boron nitride. And it should be far easier than either diamond or boron nitride to apply as a wear-resistant coating to mechanical components such as computer disk drives and jet engines. But aside from any practical value, the composite demonstrates a strategy that could be the key to creating pure carbon nitride with the superhard crystal structure that was first predicted at the University of California, Berkeley, by physicist Marvin Cohen and materials scientist Amy Liu (*Science*, 25 August 1989, p. 841). "It's an exciting result," says Harvard University chemist Charles Lieber, although to really evaluate it, he says, "I'd like to see some data, or a manuscript."

Cohen and Liu had calculated that the short, strong covalent bonds of a hypothetical crystal form of carbon nitride could make it harder than diamond. Their computer model also predicted that this "beta" phase should be relatively stable. But researchers who have tried to create films of carbon nitride with the predicted structure have generally ended up with an amorphous form of the compound—one that has no predictable structure at all.

In fact, the only actual sightings of the desired structure, outside of the computer, have been contested reports from Lieber (*Science*, 16 July 1993, p. 334) and others of finding tiny areas of the beta phase in amorphous carbon nitride films. Lately, Lieber says, he has made progress toward creating films with a crystalline structure—albeit a different one from the structure predicted by Cohen and Liu.

The problem, Chung says, is that carbon and nitrogen atoms don't readily array themselves in the beta structure: "If you leave it to Mother Nature it just won't form." So 2 years ago, he and Northwestern materials scientists Ming-Show Wong and William Sproul decided to give beta carbon nitride "some incentive" to form by providing a template—titanium nitride—whose lattice nicely matched the predicted structure. The titanium nitride, they hoped, would coax the carbon nitride to adopt the sought-after crystal form. Using a deposition process called magnetron sputtering, they coated steel with alternating layers of the two materials.



SOURCE: LIU AND COHEN

The hard stuff. Structure of beta carbon nitride, predicted to be harder than diamond.

The resulting composite is remarkably hard. At 45 to 55 gigapascals (a measure of the pressure needed to dent the material), it's nearly twice as hard as amorphous carbon nitride and approaches the hardness of diamond, which ranges from 60 to 100 gigapascals. What's more—"and this is the exciting part," says Sproul—electron micrographs suggest the carbon nitride layers are nearly 100% crystalline. Because the layers are so thin, measuring just 4 or 5 nanometers, their crystal structure is very hard to discern, says Chung, so he and his colleagues don't know yet whether they really have created the predicted beta phase. They are now at work on electron diffraction studies that may yield a verdict.

Even if the diamond-beater has eluded them, they believe they have created an industrially valuable coating. Because the sputtering technique is widely used in industry, scaling up the process should be easy, and expressions of interest have already come in from the Air Force and several of the commercial partners of Northwestern's Basic Industry Research Lab, where much of the work was done. "To see something that is widely used, that would make me happy," says Chung.

But he and his colleagues haven't forgotten their original quest. They plan to vary the recipe for the nanocomposite by using different template materials, such as zirconium nitride, that might yield a thicker layer of carbon nitride. In the end, they hope not only to make the superhard beta phase—but to produce enough of it to be sure.

–Antonio Regalado

RISK ASSESSMENT

Agencies Decry Fuzzy Science in Bill

EPA has fought a 20-year war against lead by setting regulations aimed at reducing exposures among those most at risk from its toxic effects—children and, more recently, low-income African Americans. But some scientists fear that pending legislation, part of the House Republicans' Contract with America, could force agencies to base regulations on average risks to the entire exposed population rather than vulnerable subgroups.

"Right now, agencies have had the latitude to focus on whatever part of the population they want to," says Adam Finkel, a senior fellow at the Cecil and Ida Green Center for the Study of Science and Society at the University of Texas, Dallas. "But from the tone of the bill, it's clear the authors think the estimates we're getting are not the best ones," he says.

"I feel like a chemist waking up one morning to find an alchemy bill going through the House."
—Adam Finkel

The changes are part of a broad bill, H.R. 9, called the "Job Creation and Wage Enhancement Act of 1995" that is expected to be approved this week by the House of Representatives. The bill's supporters argue that it would remove what they see as unnecessary regulations that hamper industry. But the Clinton Administration contends it would raise the cost and delay the issuance of regulations. For their part, scientists worry that the bill would sanction environmental policies based on fuzzy scientific concepts. "I feel like a chemist waking up one morning to find an alchemy bill going through the House," says Finkel.

At first glance, the bill's tenets are hard to disagree with: "Too often," it says, "regulatory priorities have not been based upon a realistic consideration of risk. ... Resources need to be allocated to address the greatest needs in the most cost-effective manner."

But "the devil is in the details," says John Gibbons, assistant to the president for science and technology. The details for assessing and weighing risks, Gibbons believes, "may result in less protection for more sensitive or exposed segments of the public," such as children, pregnant women, the elderly, the chronically ill, and certain workers.

The bill would require agencies to use risk assessment and cost-benefit analyses to rank hazards and to decide how much to spend on reducing or removing them. For any proposed action that is expected to cost industry more than $25 million, agencies would need to do the following: assess all relevant scientific data; spell out uncertainties, particularly when extrapolating from animal data; compare the magnitude of the threat to other potential risks; and weigh estimated savings—such as increased productivity from a reduction of injuries in the workplace—against the costs to industry of compliance. Agencies already use some of these analyses in preparing rules estimated to cost more than $100 million, and they apply scaled-down versions of these analyses for lesser rules.

Many industry scientists are eager to see these analyses applied more systematically. The bill would "require agencies to lay out the assumptions they're making," says Colin Park, who handles risk assessment issues for Dow Chemical. But scientists familiar with the bill are also bothered by provisions that would require agencies to "provide the best estimate or estimates" of a risk to people or natural resources. The problem is that there is no way to define a best estimate of risk when different scientific models give widely varying estimates. "That's the alchemy in the bill," says Finkel.

"There's been a lot of controversy about what a 'best estimate' means," says Elaine Faustman, a University of Washington reproductive toxicologist who teaches a course on risk assessment. "Is it a best estimate for the 'average' person? Or should it reflect the variability in the human population?"

Lead regulations are an example of EPA's view of risk as seen through the eyes of the most susceptible populations. Several studies have linked a subtle learning deficit in children to blood lead levels. These findings, although controversial, have caused the Centers for Disease Control and Prevention to lower its "level of concern" for concentrations of lead in the blood to 10 micrograms per deciliter (μg/dl). A relatively successful campaign has reduced blood lead levels to the point where that concentration is exceeded in only 9% of all 10-year-old U.S. children, compared with 88% in 1980. Now, EPA wants to tighten regulations even further to reduce exposures in populations where blood levels are still high, including black children in low-income, urban families, where 20% exceed the 10 μg/dl threshold.

"It would be very difficult to do this" if the current bill were enacted, says Joseph Carra, acting director of EPA's office of pollution prevention and toxics. Such a law, he says, might even preclude the issuance of a regulation if the agency's best estimate was the risk posed to the entire U.S. population. And EPA could be sued if it tried to enforce stricter standards. "It could well be that we would end up constraining our scientists to using certain population estimates to make sure we're not creating a huge cost for the agency in litigation," says Lynn Goldman, EPA's top risk assessment official.

Next month the Senate will hold hearings on a similar bill, sponsored by Majority Leader Robert Dole (R–KS), and opponents hope it will be more deliberative than the House. "Risk assessment is a young science, with a lot of uncertainty," says Faustman. "It makes me nervous that concepts such as 'best estimate' may get codified at this point."

–Richard Stone

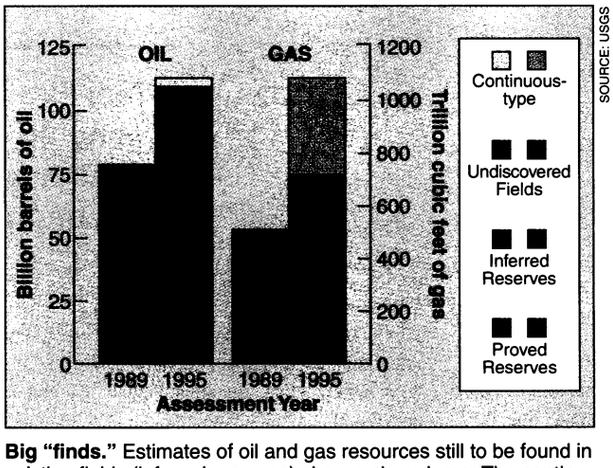
RESOURCES

U.S. Oil and Gas Fields Double in Size

Like a prudent pensioner gauging what remains to support her in her later years, the United States periodically takes stock of how much oil and gas it has in the "bank." The government can't simply consult a ledger, however. It has to rely on innumerable geologic clues to guess at how much oil and gas is left to be found and extracted. But this guesswork, unlike a pensioner's bank account, can produce some happy surprises.

That was the case at last week's annual McKelvey Forum, a conference on energy and the environment in Washington, D.C., sponsored by the U.S. Geological Survey (USGS). The last assessment, in 1989, had been discouraging, but this time around the USGS announced that known oil and gas fields now look far larger than had been thought.* U.S. oil fields were already credited with 20 billion barrels in "proved" reserves, but if intense, sophisticated drilling probes the fields' geologic nooks and crannies, the USGS estimates that they could yield another 60 billion barrels. That's triple the amount of so-called inferred reserves estimated by the USGS in 1989, and equal to an additional 24 years' production at present rates. Inferred reserves of gas enjoyed a similar boost in the new assessment, to 322 trillion cubic feet.

The abundance remaining in known fields isn't exactly like money in the bank; it's more like a long-term bond. At today's prices, much of it would be prohibitively expensive to extract, but it could be extremely valuable early in the 21st century when, USGS researcher Charles Masters told the meeting, "there will be some serious problems" with world oil and gas supply. And the new estimates of inferred reserves are especially welcome because another part of the picture hasn't brightened since the last assessment: the amount of oil and gas in fields yet to be discovered. Those estimates, based on an inventory of likely-looking geologic structures, had declined drastically in the 1980s, and they remain little changed in the new assessment at 30 billion barrels of oil and 259 trillion cubic feet of gas (excluding federal offshore areas).



Big "finds." Estimates of oil and gas resources still to be found in existing fields (inferred reserves) show a sharp jump. The continuous-type category includes widely dispersed, dilute resources.

A combination of geologic peculiarity and oil-industry economics accounts for the dramatic growth of the inferred reserves, explains Donald Gautier of the USGS in Denver, the assessment's project chief. In large, complex oil fields like those in West Texas, he says, the more you drill, the more the known field grows. Previously untapped pools may turn up above or below a known pool, the field may expand laterally as wells are drilled farther away, and a well sunk between two existing wells may tap into oil

*1995 National Assessment of United States Oil and Gas Resources, U.S. Geological Survey Circular 1118, free on application to U.S. Geological Survey, Information Services, Box 25286, Federal Center, Denver, CO 80225.