Materials Science

A hard mystery solved

Why are silicon and other substances that are known as covalent solids so much harder and more brittle than pure metals? This has long mystified materials scientists. In fact, John J. Gilman has pondered the phenomenon for 40 years.

Scientists know that covalent solids are particularly hard because electrons in them pair up to form tight bonds. And one indication of silicon's hardness is that dislocation lines in the crystal structure move very slowly through it. A dislocation is a line in the crystal where the atoms are not arranged perfectly — like a big wrinkle in the middle of a rug. A dislocation moves when stress is applied. When it moves, the crystal deforms plastically — that is, one part of it slides over another and the crystal gradually deforms without shattering or cracking. But no one had ever explained adequately why dislocation lines move slowly, says Gilman, a materials scientist at the Lawrence Berkeley (Calif.) Laboratory.

A material as important as silicon — to which computer chips, solar cells, and other electronic devices owe their existence — deserves better, Gilman thought.

He found the explanation by analyzing how silicon's electronic structure changes when a dislocation line moves, he reports in the Sept. 10 SCIENCE. Other scientists had looked at electrons' general mechanical properties but not at their arrangement and behavior, he says.

Gilman argues that kinks along a dislocation line determine the rate of the line's movement. For the line to move, the kinks have to separate the paired electrons in front of them. Then the line moves through the electrons, and the electrons close up behind it.

The strength of the electrons' bonds depends on the size of the gap between the energy levels of the electrons that are bonded and those that are not bonded. The wider the gap, the stronger the bonds and, therefore, the harder the material.

"This suggests that the kink mobility is directly related to the electronic structure," Gilman reports.

Showing how the electronic structure affects kink mobility enabled Gilman to calculate the amount of stress needed to form the kinks, break up electron pairs, and move the kinks. This is a measure of how much silicon resists being plastically deformed.

More recently, Gilman has found that the reasons for silicon's hardness apply to other covalent solids, including silicon carbide, which is used in abrasives.

A gem of a mistake

In 1955, General Electric Co. scientists reported two processes for synthesizing diamonds. But the shining example from their first effort, a tiny stone that has held a place of honor for 38 years at GE's research center in Schenectady, N.Y., just fell off its pedestal.

New measurements of the infrared absorption spectrum of that diamond reveal it is a natural gem. Its spectrum has "features in it that are only found in natural diamond — that gave it away," says Peter J. Codella, a physical chemist at General Electric who did the analysis. He and five of the GE researchers who did the original research describe their new findings in a letter in the Sept. 2 NATURE.

Somehow, and they still don't know how, a fragment of a natural diamond seed "got into the experiment inadvertently," they report.

Their mistake proved serendipitous. When they tried to repeat the experiment using the same apparatus, they found they didn't have enough pressure to synthesize a diamond. But their one apparent success "provided the impetus to experiment with the system at higher pressures," which was all they needed to actually make synthetic diamonds.

Science & Society

Feds propose new pesticides policies

Following the recent publication of a report from the National Academy of Sciences (NAS) on the health risks of pesticides used on foods, the Clinton administration pledged to revamp policies for studying, regulating, and policing the use of these chemicals (SN: 7/3/93, p.4). Last week, the Environmental Protection Agency, the Food and Drug Administration, and the Agriculture Department told Congress how they intend to fulfill that promise.

Among their proposed initiatives:

- setting an upper bound on the lifetime cancer risk that any pesticide can pose. They defined this "negligible" risk as one anticipated malignancy for every 1 million exposed persons.
- imposing a blanket prohibition on the export of pesticides banned in the United States.
- speeding up the ongoing federal safety review of all currently marketed pesticides.
- granting a grace period of up to five years for phasing out certain pesticides that do not meet the safety standard but that could result "in significant disruption in the food supply" if pulled from the market immediately. However, EPA said, such temporary waivers would be granted only for chemicals whose risks did not exceed 10 times the "negligible risk" level.
- adopting the NAS' recommendation that EPA consider possible exposures to a chemical from more than one food source when establishing permissible residue limits.

One of the more controversial elements of the revised pesticide policy is the intended amendment of the Delaney clause — a 35-year-old provision of the Food, Drug, and Cosmetic Act that prohibits the sale of processed foods containing greater concentrations of pesticide residues than were present in the raw ingredients (SN: 5/15/93, p.311). EPA and other agencies have argued that the Delaney rule is too rigid, given improved analytical techniques that can detect residues too small to matter. The amendment would allow residues to concentrate as long as they pose only negligible risk. But critics, such as the Washington, D.C.-based Environmental Working Group, say the change "would weaken the strongest public health standard in all environmental law."

Environmental impacts of the computer age

Worldwide, some 148 million computers are plugged in to crunch numbers, process words, analyze data, and organize the business world, notes John E. Young of the Worldwatch Institute in Washington, D.C. While these machines have the capacity to reduce the use of many resources, to date they have actually fostered the exploitation of many materials, he argues in *"Global Network: Computers in a Sustainable Society,"* a report released last week. For instance, far from threatening the extinction of office paper, business computers have so increased the ease of making documents that they have encouraged the generation of more drafts and copies, Young says. He estimates the annual paper consumption by the world's computers at 230 million reams, or 115 billion sheets.

Computers also account for an estimated 5 percent of U.S. electricity use (SN: 3/20/93, p.186). According to Young, meeting that power demand results not only in the generation of millions of tons of carbon dioxide (a greenhouse gas), but also in the emission of thousands of tons of nitrogen oxides and sulfur oxides — the principal precursors of acid rain.

Finally, personal computer owners frequently mothball obsolete computers long before they actually wear out. Such PCs could be recycled. Young points to a German ordinance due to take effect early next year that will require computer makers to take back old machines at the end of their useful lives. This, he says, will "compel manufacturers to design computer components for upgradability or reuse."