Glittering future brightened with help of scientific visualizations at SDSC

May 7, 1991

Media Contacts: Julie Shisler, 534-5137; Warren Froelich, 534-8564

DIAMOND FILM: GLITTERING FUTURE BRIGHTENED WITH HELP OF SCIENTIFIC VISUALIZATIONS AT SDSC

Diamonds, those pure crystals long associated with lasting affection, wedding anniversaries and jubilees, are now considered the glittering hope for some seemingly less-romantic ideas ... like scratch-resistant lenses and advanced semiconductors.

Today, a new generation of diamond hunters has left the mine for the laboratory in a high-tech search for low-cost gems.

For many, the goal is the production of synthetic diamond film, strong enough to withstand adverse conditions on land, in space and at sea.

"You won't be able to put them just in the front of your car, you'll be able to put them in the rocket engine," said Bernard Pailthorpe, an applied physicist from the University of Sydney, in Australia.

Recently, Pailthorpe turned to the CRAY Y-MP8/864 supercomputer at the San Diego Supercomputer Center to help him understand what happens when diamond film is grown in the laboratory.

Combined with the graphics workstations and expertise at the center's Advanced Scientific Visualization Laboratory (VisLab), Pailthorpe was able to create color video images simulating the growth process, atom-by-atom.

The results offer new insights into the process which Pailthorpe says could bring diamond film -- created only in small amounts today -- into large-scale production within a few years.

"We think we have an edge," said Pailthorpe.

An edge in the diamond business could represent an edge in durable industrial profits. Not only are diamonds the hardest known substances, they are extremely good electrical insulators, and are transparent to visible light, as well as infrared and ultraviolet radiation. They also are the best known conductors of heat and melt at 4,500 degrees C.

"One of the uses people talk about now is to coat silicon chips," Pailthorpe said.

"Next, we will have diamond chips," he added, "so this could be the next-generation semiconductor."

Diamonds may be forever, but they're also precious, and therefore expensive. Less than 20 tons of natural diamonds are mined each year throughout the world, mostly in Brazil, India and South Africa.

As a result, many interested in diamonds for industry have turned to artificial gems. Technological breakthroughs during the 1980s for growing diamond film triggered rapid and furious interest in this new industry.

As if to underscore the new-found interest, Science magazine the journal of the American Association for the Advancement of Science -- named the diamond as "Molecule of the Year" in 1990.

The process that has attracted most of the interest is called chemical vapor deposition (CVD). In this process, hydrogen gas is heated to temperatures of 2,200 degrees C. with a simple hydrocarbon compound such as methane.

Carbon atoms produced in this manner are then condensed onto a substrate, (ie., glass, plastic, ceramic, metal) resulting in a film about a tenth of the thickness of human hair. Film grown by this method already is being used on a limited basis to coat lenses, for cooling computer chips and as diaphragms for tweeters in stereo speakers.

However, the film generally isn't pure enough, or durable enough, for some of the more exotic applications envisioned for its future, particularly in the electronics industry.

In his laboratory at the University of Sydney, a team of researchers working with Pailthorpe has been experimenting with a new method for growing thin film called a filtered vacuum arc. Here, a block of graphite is placed in a vacuum tube and exposed to a low-voltage welder's arc. The resulting blast of carbon material is then filtered by a magnetic field producing carbon ions which, in turn, are deposited on a substrate.

"It's like we're electrically sandblasting the graphite," said Pailthorpe.

Film grown by this method is about 300-500 atoms in thickness -- about 300 times thinner than film produced by CVD. It's also purer, with none of the residual hydrogen characterized by the more traditional process.

However, growing thin films still is more art than science. The process can result in failure when the film cracks during production.

"It's cookbook chemistry," said Pailthorpe. "You try a little of this and a little of that, a dash of this and a dash of that."

To find a better way, Pailthorpe turned to the computer to simulate what happens when thin film is grown. The simulations required large-scale and complex calculations, involving the interactions of all the carbon atoms and their motions in thin film. The addition of one atom of carbon to the film required a half-hour of computer time on the CRAY Y-MP.

Once these calculations were completed, Pailthorpe turned to the VisLab to create a videotape representing 10 picoseconds (10- trillionths of a second) in the history of the production of diamond film. The video, created with the help of SDSC computational chemist Jerry Greenberg, shows tiny red and blue spheres -- corresponding to newly introduced and already established carbon ions -- hitting the growing film one atom at a time. After each sphere hits, the film depresses a bit, somewhat like a mattress; the sphere then springs back and forth, until it eventually nestles in place.

The simulation demonstrates that there is an optimum range or "window of energy" needed to grow the film without breaking it.

"So it's like a working sheet of metal in a blacksmith shop," explained Pailthorpe. "You're hammering on it and squashing it. But it doesn't spring back all the way.

"But if you use too much energy, it's like hitting it with a pointy hammer and you break holes in it. The atoms go into the surface and damage it and fire through."

Pailthorpe recently presented his results to meetings in San Diego and Anaheim. Several U.S. industrial representatives have expressed interest in the process and his findings, although one large Japanese firm already is helping to fund his work.

"It takes a while for the message to sink in because the big labs don't think it can be done anyplace else," said Pailthorpe. "But if we're right, if it gets borne out, people will believe us and it will take off.

"We think we're onto something."

Pailthorpe added that the use of computer graphics and simulations could represent a new and rational approach to the design of advanced materials, somewhat akin to the way in which drugs now are being designed by pharmaceutical companies.

"To design drugs, it's now part of the commercial practice to use supercomputer simulations and graphics to see where they fit in," he said. "If they don't look right, you try again.

"I believe this can be important for the design of materials too; it offers a more efficient route to the design process."

SDSC, established in 1985 in cooperation with the National Science Foundation, is administered and operated by General Atomics at the University of California, San Diego. Its primary goal is to support leading-edge computational science and engineering for academia, industry and government. Aside from its advanced supercomputer resources, SDSC offers education, training and consulting services, in addition to fostering collaborative research and development programs.

(May 7, 1991)