# Materials Scientists Make Contact in Boston

BOSTON—Looking to bring futuristic materials a step closer to reality, scientists from around the world gathered at the Materials Research Society (MRS) meeting in Boston from 27 November to 1 December, considering a wide array of topics ranging from superconductivity to nuclear waste storage (see p. 1761). Two intriguing presentations focused on efforts to simplify computer chip manufacture patterning and to improve the electrical conductivity of thin films.

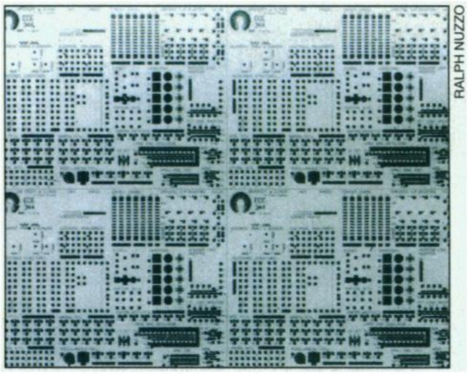
## Stamping Out Microchips

Patterning thin layers of electrical and optical materials may be old hat to chipmakers. But even old hats call for complex craftsmanship, and in this case they require fabrication facilities loaded with clean rooms, vacuum chambers, and lithography equipment, which painstakingly carve out patterns in layer after layer of each chip.

Over the past 2 years researchers have developed an appealing alternative: a benchtop chemistry method, known as microcontact printing, that amounts to little more than pressing an ink stamp on paper. At the Boston meeting a group of researchers from the University of Illinois (UI) reported that a new version of the technique can pattern copper and other materials into features as small as 0.7 millionths of a meter on several substrates widely used in microelectronics, including silicon-oxide. An older version of the technique could print features only on gold surfaces, hardly a cost-efficient substance for chip manufacture.

"It's very nice work," says Ronald Andres, a chemical engineer at Purdue University in West Lafayette, Indiana. "They certainly demonstrated you can make high-resolution patterns this way," adds Edwin Chandross, a chemist at AT&T Bell Laboratories in Murray Hill, New Jersey. The new method could eliminate much of the complexity from chipmaking. Chandross and others do caution, however, that the technique still has to prove it can mass-produce circuits with a low number of defects before it makes it to the factory floor.

The UI researchers—Ralph Nuzzo, David Payne, Nooli Jeon, and Paul Clem—built on the original microcontact printing technique developed by chemist George Whitesides and his colleagues at Harvard University. First, scientists use conventional lithography to etch a pattern in a hard polymer known as a photoresist. This serves as a mold for a liquid polymer called polydimethylsiloxane (PDMS), which is then heated, cured, and peeled off. The PDMS is now a stamp carrying a negative image of the photoresist: Valleys become peaks, for instance, and ridges become grooves.




**Cut! Print!** A new method of stamping copper patterns on a substrate (*above,* circles in top right corners = 300 micrometers) could simplify chipmaking.

The stamp is then dipped in a solution containing organic molecules, which adhere loosely to the PDMS. When the stamp is pressed down on a particular substrate, the organics—which contain functional groups that bind tightly to reactive groups on that substrate—grab this surface and "transfer like ink from a stamp to paper," says Nuzzo.

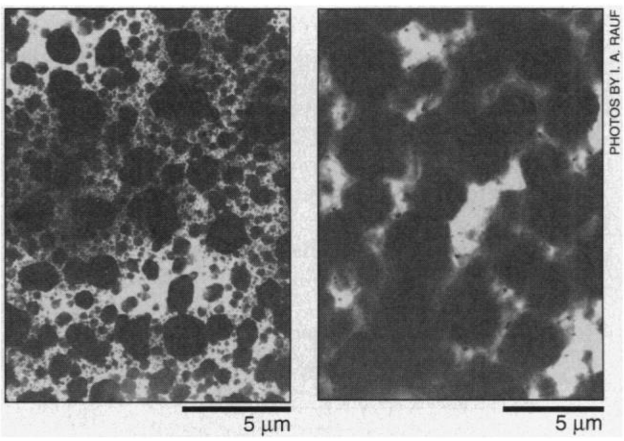
But while Whitesides and his colleagues use organics designed to adhere to gold surfaces, Nuzzo and his co-workers turned to another class of organics, known as alkylsiloxanes, which bind to hydroxyl groups on substances such as silicon- and indium-tin-oxide. When these organics transfer from the stamp to the oxide surfaces, the UI team reported, they take the pattern with them. The scientists then deposit other materials, such as copper, over the pattern, which functions as a mask. Copper binds tightly to the oxides but not at all to the organics, so when the organics are removed with a simple chemical solvent, what's left is an intricate pattern of copper on the oxide surface. The researchers also made features from lithium niobate, a widely used optical material, and lead-lanthanum-titanate, used in chips to filter out electronic signals.

Whitesides calls the new results "leading work." But Chandross notes that patterned electronic and optical devices can easily be degraded if large numbers of impurity atoms are incorporated during their manufacture, and the UI team hasn't yet demonstrated that the stamping method can keep these numbers low. That's "clearly true," agrees Nuzzo. "But if it's this good at this level, how good could it be if you put the level of engineering into it that has gone into the Pentium chip?" He says the team has begun discussions with one major microelectronics company to transfer the stamp of the new technology to industry.

## Return of the Thin Film

The desire for superior films reaches beyond Hollywood. Materials scientists too long for better crystalline thin films, which among their other roles act like wires to pass electrical current in everything from computer chips to flat panel displays for laptop computers. Most of these films consist of an ultrathin layer of tiny crystalline grains. But these so-called polycrystalline films typically are poorer electrical performers than films grown as a single crystal—which is an expensive and difficult process.

At the MRS meeting, however, physicists Ijaz Rauf and Michael Sayer from Queens University in Kingston, Ontario, Canada, described what may be a low-budget way to make an award-winning film: Grow it on a substrate that's heated in strips to alter the microstructure of the material. In a film of polycrystalline indium-tin-oxide (ITO), the result was an electrical performance to equal that of a single-crystal ITO film. The feat intrigued a critical audience. "It looks interesting," says Michael Parker, a thin film expert with IBM's Storage Systems Division in San




**Winning performance.** Grains in a copper thin film can have poor alignment *(left),* but a temperature gradient during film-making improves the match *(right)*—and electrical conductivity.

Jose, California. Parker notes that the technique could reduce electrical losses in ITO films used in flat panel displays, and polycrystalline silicon films used in photovoltaic devices, which convert sunlight to electricity.

The strategy works by sweeping away some of the obstacles that slow the passage of electrons through a conducting film. Defects such as impurity atoms or vacancies in the lattice structure slow the passage of electrons through many crystalline materials, but in a polycrystalline film, electrons are also slowed as they pass from one grain to the next, because the grains usually don't line up in nice neat rows—and if they do, their crystalline lattices don't usually align well at the boundary.

The Queens University researchers found that all three of these problems were reduced if they made their films on a substrate that's warmer and colder in alternating strips. But they are still trying to figure out why this occurs. Rauf does have some ideas. The material in films such as ITO, he explains, is typically deposited as a high-temperature vapor of atoms. As hot atoms in a vapor land on a substrate, they initially liquefy and congregate, forming tiny droplets. As the droplets cool, they crystallize, forming the neighboring grains in a polycrystalline film.

Rauf believes that the temperature gradients in the substrate sweep defects to the warmest side of each grain. Within each grain, he explains, the warmer side can dissolve more defects, just as warmer water can dissolve more salt than colder water. As a result, as the drops in the film crystallize, the defects are pushed to one side, creating a defect-free channel for current within each grain. And as the defects migrate within each grain, they force the lattice into a particular alignment, like a comb. Because defects are migrating the same way in neighboring grains, all the lattices end up similarly aligned. Finally, Rauf believes the alternating warm and cool regions also change the energetics between neighboring grains, making it favorable for grains to line up in rows atop regions of equal temperature.

While others found data for improved performance compelling, the explanations are "plausible," says Parker, but need to be proven. Rauf says that he and his colleagues are now working to test their theories by studying the nucleation and growth of their crystals.

Whatever the explanation, Rauf notes that his group has found that the process improves polycrystalline films of copper in addition to ITO. The researchers also used the technique recently to grow a film of the superconducting material yttrium-barium-copper-oxide. It improved grain alignment, and they are now testing the film's electrical properties to see if they can produce a new "Best Performance" nominee.

–Robert F. Service

MATERIALS SCIENCE

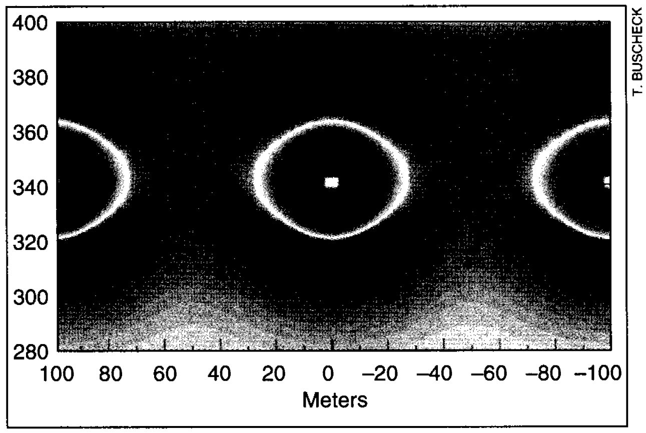
# Can Nuclear Waste Keep Yucca Mountain Dry—and Safe?

Disposing of spent nuclear fuel by placing it deep in the earth is a race against time and corrosion—a race the designers of the proposed long-term nuclear waste repository at Yucca Mountain in Nye County, Nevada, know they will eventually lose. The central scientific question in this controversial project isn't whether the waste will leach out of the large metal casks that contain it, but when. In that race, repository designers are looking for every advantage they can get—including the heat generated by the waste's own radioactive decay.

Two weeks ago, at the fall meeting of the Materials Research Society in Boston, geophysicists Thomas Buscheck and John Nitao from Lawrence Livermore National Laboratory, with geologist Lawrence Ramspott of TRW Environmental Safety Systems Inc., proposed some new twists on an old idea: using that heat to boil corrosive moisture out of the surrounding rock. The researchers suggest that blanketing the waste canisters in gravel, then stowing them more densely and in storage tunnels placed farther apart than has been suggested previously, will keep the fuel warm and dry long enough for much of the danger to decay away. The plan, they say, will help keep the canisters intact for at least 10,000 years—the goal set by Environmental Protection Agency regulations, but still long before many of the most dangerous isotopes have decayed away—and perhaps as long as the 1 million years that a National Academy of Sciences (NAS) panel has recommended.

Like nearly every other aspect of this project, such as the viability of such a repository in the first place (*Science*, 30 June, p. 1836), the plan has divided scientific opinion. Some researchers see a great deal of promise. "State of the art," William Murphy, a geochemist at the Southwest Research Institute in San Antonio, Texas, calls it. And officials at the Department of Energy (DOE), which runs the Yucca Mountain project, call the plan "an important input." But critics say that, as with previous plans, prolonged heating could alter the rock's stability and porosity, perhaps allowing corrosive liquid to seep back into the tunnels.

Some 29,000 metric tons of nuclear waste from U.S. civilian reactors—an amount that grows by 1900 tons each year—are waiting for a permanent home, along with high-grade radionuclides, such as cesium, from the nation's nuclear arsenal. That home needs to be as moisture-free as possible, to minimize the chances for canister corrosion (see box on next page). In the major previous plan for storing the waste in the mountain, called "extended dryout," designers left as little as 20 to 40 meters between waste tunnels. The idea was to use the heat coming from the canisters to keep a thick slab of rock above and below the tunnels boiling hot—and thus dry—for thousands of years. But researchers also feared that, as the waste cooled, condensing water might seep through the rock and back down onto the containers, eating through their double skin of steel and alloy and leaching out wastes.




**Nuclear space heater.** In one plan, widely spaced waste storage tunnels will have a hot, dry zone around them *(red)*, driving moisture into the wetter rock *(purple)*, where it can drain away.

So Buscheck and colleagues used customized computer models, based on known properties of water and heat flow in porous, fractured media such as the Yucca Mountain rock, to test a new approach, dubbed "localized dryout." The scheme would essentially put drains into the rock by spacing the tunnels farther apart. Separating the tunnels by up to 100 meters would keep the zones of boiling-hot rock created by each tunnel from overlapping, allowing the condensate from each zone to drain through the cooler rock in between. With tunnels spaced further apart, waste containers within them could be placed closer to one another, generating a more intense, uniform boiling zone around each tunnel that adds assurance