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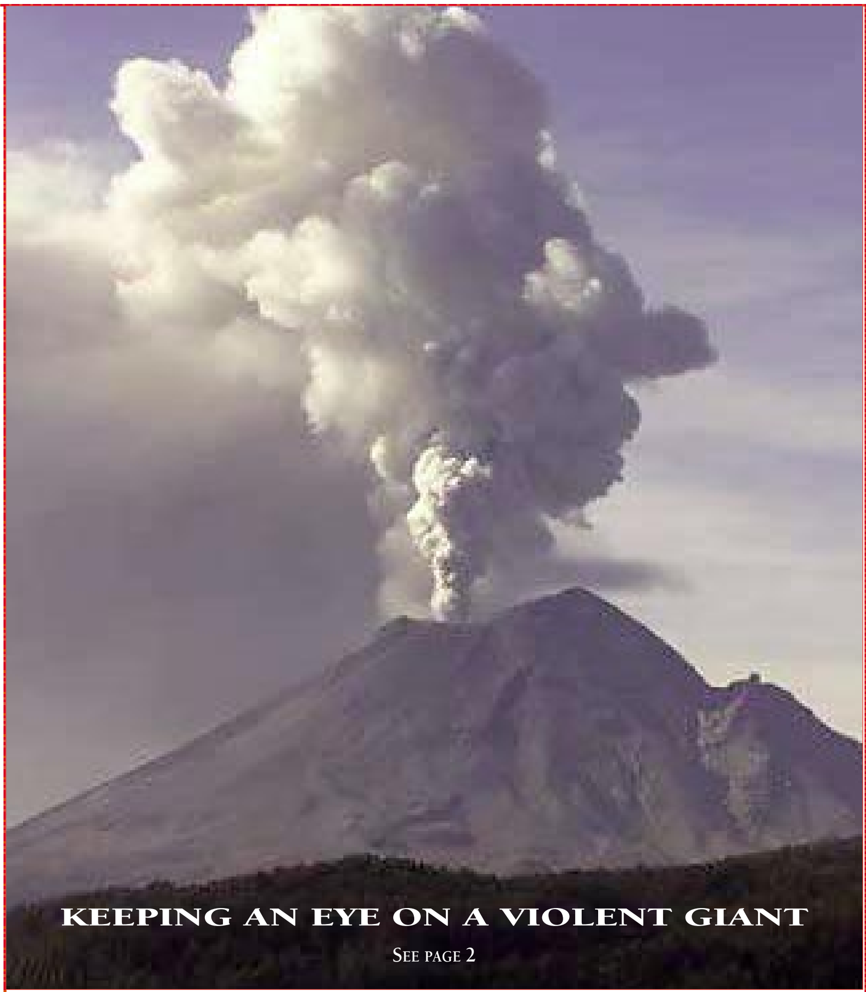

KEEPING AN EYE ON A VIOLENT GIANT

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A MONTHLY PUBLICATION OF LOS ALAMOS NATIONAL LABORATORY

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KEEPING AN EYE ON A VIOLENT GIANT

Researchers at Los Alamos National Laboratory are developing new techniques to remotely monitor volcanic gases at a safe distance.

Volcanic gases provide important insights into deep-Earth processes and gas composition. Changes in variations of the gases may show promise as predictors of eruptive activity.

The methods were recently tested on Mexico's Popocatépetl, a volcano with a history of human impacts. The 17,800-foot volcano is nearly 50 miles southeast of Mexico City. Living directly in the danger zone on the lower flanks of the mountain are more than 300,000 people who farm the rich volcanic soil for their livelihoods.

To the people living around the base of the mountain, the volcano is spiritual. The nearby native population interprets the periodic eruptions as omens portending the future. There is reference in ancient literature about the feathered serpent rising from the mountain. The famed Spanish conquistador Cortez took advantage of a small eruption and the belief systems that

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surrounded it in the 1500s to persuade locals to help him defeat a group of indigenous peoples.

Popocatépetl has not experienced a major eruption in more than 1,200 years when the mountain laid waste to the surrounding area, particularly to the southeast.

Yet the local population is reluctant to leave their farms and animals when the volcano threatens. Emergency planners walk a fine line, careful not to cry "wolf" in deciding when it is necessary to evacuate the area. Planners are trying to build credibility with the locals to save lives.

There is much that scientists don't know about volcanoes and why they erupt when they do. As a result, these eruptive mountains remain a threat to those who live around them.

If today's emergency planners could rely on an accurate test to know when evacuation is necessary, it could be beneficial in establishing trust among the native people as well as saving lives.

Fraser Goff and Steve Love, safely removed from Popocatépetl, use their newly developed monitoring equipment to analyze volcanic gases.

Los Alamos researchers Steve Love and Fraser Goff may have found such a way. Love and Goff have developed a way to monitor gases, at a safe distance, emitted from the volcano. Volcanic gases provide useful insight into the deep magmatic and chemical processes churning in the heart of the mountain and may aid in predicting eruptive activity, but traditional methods for gathering gases are inherently dangerous.

The most common practice requires a person go to a fumarole or vent, or perhaps into the crater itself to collect the gas manually. Researchers have been killed collecting gas samples. Furthermore, when a large-scale eruption threatens, it becomes too dangerous to sample using these methods.

Goff and Love use infrared (IR) spectroscopy that permits monitoring multiple gases from well outside the crater. Their work is unique in that they are able to obtain IR spectra using the sky as a background, permitting them to work miles from the crater. Other traditional IR monitoring techniques mandate the presence of high-temperature

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rocks or lava, which act as a source of IR radiation, or an artificial IR source placed on the opposite side of the monitored plume, typically requiring close access to the volcano.

Additionally, infrared monitoring is tricky because Earth's atmosphere normally contains gases, mostly water and carbon dioxide, both of which are strong IR absorbers.The team's work takes advantages of recent advances in compact, portable IR spectrometers and laptop computers. The team uses Fourier Transform Spectroscopy, an idea conceived in the 19th century but because of its large computational demands, the technology had to await the development of modern computers to be useful.

One of the strengths of this type of gas monitoring technique is that it allows simultaneous measurement of a variety of gas species and nearly continuous measurements of changes in the gaseous concentrations.

In February 1997, Love and Goff set up their equipment about three miles from the Popocatépetl crater to monitor the volcano. The results, which the team published in the journal Nature, surprised them: From Feb. 21 through Feb. 24, the team monitored the gas venting from the volcano. On Feb. 25 and 26, the volcano erupted in an ash explosion. In the days before the eruption, the monitoring data showed a steady increase in silicon tetrafluoride relative to the amount of sulfur dioxide. Immediately after the eruption, both gas levels were extremely high, followed by a rapid decline.

Previous research indicated that silicon tetrafluoride increases when temperatures fall inside the volcano. The gas is not present at magmatic temperatures. This meant that the gas cooled before the explosion. The team speculates that this cooling indicates an expansion that occurred as the plug in the volcano's plumbing system began to give away before the explosion. As the plug weakened, releasing gas, the pressure and temperature decreased, resulting in an increase in silicon tetrafluoride.

Eventually, the team believes the plug failed catastrophically, producing the observed explosion. A large drop in temperature and pressure followed and the observed spike in silicon tetrafluoride and sulfur dioxide resulted. The team says a new constriction within the volcano formed that caused the gases to return to normal levels.

These data are important because such an explosion is driven by gas as opposed to the movement of magma. Future observations of these trends could warn scientists of similar explosions that occur frequently on Popocatépetl.

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The eruption on Feb. 25 and 26, 1997, could have killed researchers using conventional gas collecting technologies. The eruption would have destroyed any crater-rim monitoring instruments, and even aircraft-based measurements of this eruption would have been risky.

In 1998, the team returned to Popocatépetl and observed large bursts of carbon dioxide not seen the previous year. Normally difficult to observe with IR spectroscopy because it is also present in the atmosphere, the volcanic carbon-dioxide levels were high enough to be seen easily in February 1998. These observations, taken together with geological sampling of new ash and pumice, suggest that Popocatépetl is incorporating the nonvolcanic limestone underlying the volcano into its magma as it rises to the surface. These results, which will appear in the journal Chemical Geology, provide an example of how IR remote sensing can give new clues about processes deep inside the Earth.

Such results make researchers confident that infrared spectroscopy can be uniquely valuable to volcanoes like Popocatépetl. More research is necessary to develop an early warning device. This work was funded under the special research pot of money called Laboratory Directed Research and Development Program, which was drastically cut in 1999. Love and Goff currently seek other sources of funding to continue this exciting work.

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THE DARK AGES MAY HAVE REALLY BEEN DIMMER

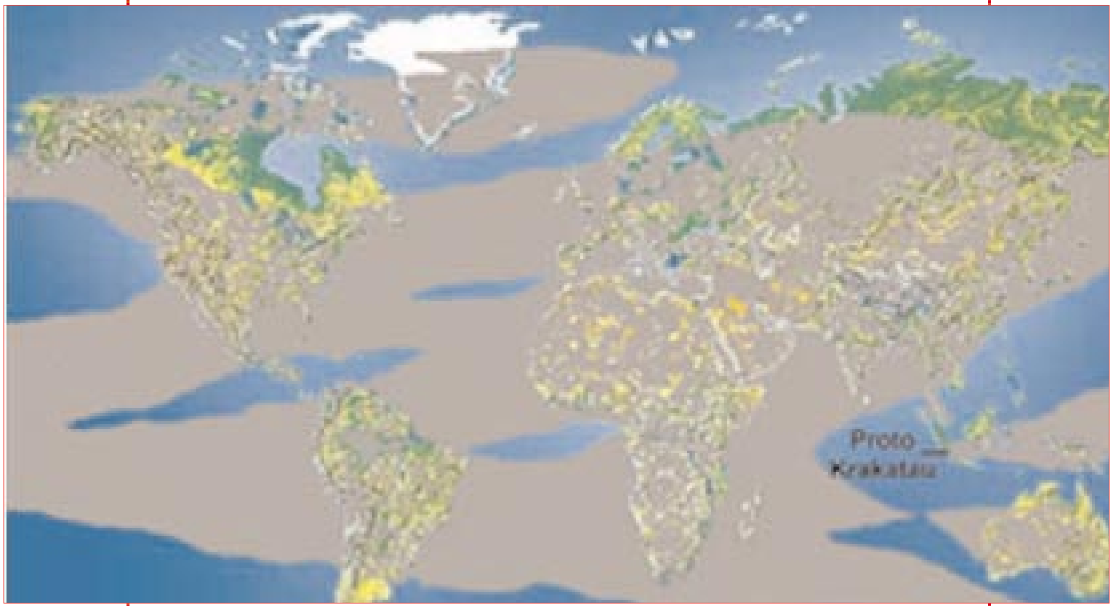
The beginning of the Dark Ages may have been literal, as well as figurative, as the result of a massive volcanic eruption in the 6th century, according to a volcanologist at the Department of Energy's Los Alamos National Laboratory.

Ken Wohletz said an eruption in the Indonesian archipelago could have produced a 150-meter-thick cloud layer over the entire Earth, triggering a chain of climatic, agricultural, political and social changes that ushered in the Dark Ages.

Evidence supporting the catastrophe includes tree-ring and ice-core measurements, indications of a huge underwater caldera, and ash and pumice in the same area, said Wohletz, who discussed his work modeling such an eruption at the December meeting of the American Geophysical Union.

The 6th century was a turbulent, unsettling period in human history. The Roman Empire began to fall; nomads of central

Ash and water vapor blown from a presumed Indonesian volcano called proto-Krakatoa (Krakatau) in a massive 6th-century eruption could have covered Earth for many months, as shown in this artistic rendering. Such a cloud layer would have destabilized the climate around the globe, possibly triggering major political and social changes that ushered in the Dark Ages.



Asia migrated to Europe and the Near East; civilizations in Persia, Indonesia and South America collapsed; major religions experienced considerable change as natural events were viewed as omens.

Many of these social transformations resulted from widespread crop failures and the explosion of plague around the globe, which in turn were caused by major climatic changes, Wohletz said.

Beginning in about the year 535, according to historical and archeological records, the weather was colder and drier, sunlight diminished, snow fell in summer and regions of persistent drought suffered floods.

Wohletz was a resource for a book postulating that the climate changes resulted from a huge volcanic eruption. The book, "Catastrophe: A Quest for the Origins of the Modern World" by David Keys, was published last year.

Wohletz said he worked with Keys to try to identify a volcano that could produce such dramatic climate change. "We came up with an eruption that would certainly be the largest in recorded history, some four or five times bigger than the (1815) eruption of Tambora, which is usually considered the biggest eruption in the past few millennia," he said.

Such an explosion, he said, would eject some 200 cubic kilometers of material, and one-third to one-half of it would be lofted into the stratosphere, where it would remain suspended for months to years while being carried around the globe.

"It would have produced enough dust and water vapor (in the form of ice crystals) to form a cloud layer 150 meters thick over the entire globe, and that's a conservative estimate," he said, adding that a cloud of particles that thick may have diminished the transmission of sunlight by as much as 50 percent.

Wohletz said tree-ring data collected around the world and ice-core measurements in Greenland and Antarctica support the possibility of a huge eruption in the 6th century. Ocean depth measurements between Sumatra and Java — where Krakatoa exploded in a well-known 1883 eruption — indicate the presence of a caldera up to 50 kilometers in diameter, and a recent survey uncovered evidence of ash and pumice layers formed in the area during the appropriate time frame.

Under a likely scenario, a large volcano, which Wohletz calls proto-Krakatoa, connected the islands of Sumatra and Java. When it erupted and then subsided, it created the Sundra Strait and left a ring of smaller

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volcanoes, including the present-day Krakatoa. The ash, dust and water vapor blown into the stratosphere would disperse across both the Northern and Southern Hemispheres.

"This volcano would have had the potential to be a major player in destabilizing the climate around the world," he said. "An eruption that could produce a caldera 50 kilometers across would have been big enough."

Although definitive evidence for such a catastrophic eruption has not been discovered, the possibility deserves a full-scale field study, Wohletz said, in part because of the potential impact on the world if another such catastrophe happens.

"(Key's book) is the first detailed account of how closely humanity is linked to the natural world," he said. "If the natural world goes through some large upheaval, we'll all be affected."

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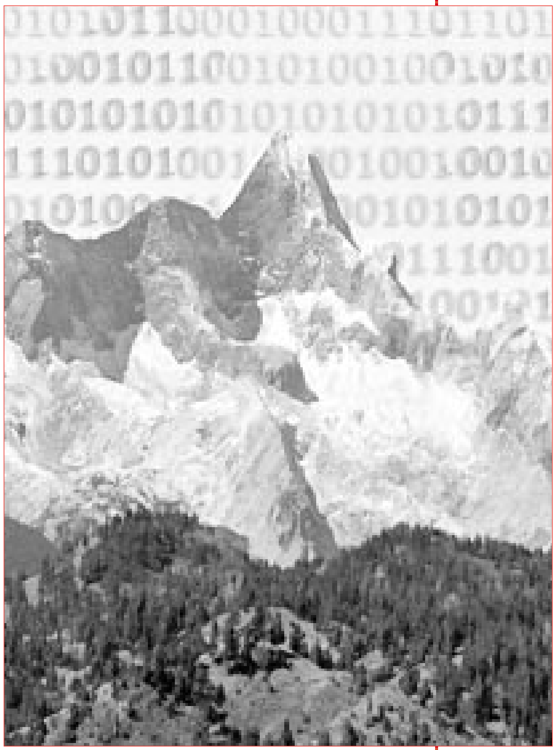
BLANCA PEAKS

The Los Alamos Blanca Project achieved a major milestone for the Accelerated Strategic Computing Initiative Program, completing its computer simulation of a nuclear detonation safety test ahead of deadline.

Blanca ran two calculations on the ASCI Blue Mountain computer system. It simulated a hydrodynamics experiment previously conducted at PHERMEX (High-Energy Radiographic Machine Emitting X-rays facility) and a one-point safety test that was actually done in 1990 at the Nevada Test Site.

Blanca calculations were nearly 10 times larger than previous safety calculations run on older computer systems.

"The Blanca Project Team deserves tremendous credit for dedicated efforts under extreme circumstances," Project Leader Forrest Brown said. "They completed the milestone on schedule despite uncertainty and stress caused by the Cerro Grande fire in which two members of the team lost their homes. Challenges for the team continued during the missing hard drive incident and subsequent security stand-down."



The two calculations used a detailed, 3-D model with 115 million cells. The first calculation, a simulation of the hydrodynamics experiment, required 47 CPU-years of computation and was completed in 206 hours using 2,016 processors on Blue Mountain. The calculated data compared very well with the previously measured experimental results.

The second calculation, simulation of an NTS event,

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required 32 CPU-years of computation and was completed in 180 hours. The results compared well to measured experimental results.

The second simulation used a windowing technique, where the number of processors was varied according to the extent of the active portion of the computational mesh, growing from an initial 126 processors up to 2,016 processors at the end of the problem. This technique reduced the overall calculation by a factor of two to three and contributed to Blanca's early completion of the milestone.

The Blanca Project is one of the major ASCI code projects that are developing full-physics-simulation capabilities for Los Alamos National Laboratory's contribution to the Department of Energy's national science-based stockpile stewardship program. Blanca is responsible for developing multidimensional production codes for modeling the safety and performance of nuclear devices and predicting other weapons phenomena.

By adapting emerging computational approaches to large-scale scientific software systems that scale well for parallel architectures, the Blanca Project is facilitating the addition of more complex physics and promoting rapid implementation of new computational models for code verification/validation testing.

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P&G AND LAB RELEASE OWN PRODUCT OF COLLABORATION

The modern assembly line involves thousands of high-speed precision parts that work together to produce quality products at a rapid pace. However, any small component has the potential to shut down an entire production system for minutes, several hours and possibly days, creating waste and scrap materials while not generating profitable products.

Keeping assembly lines moving, like the generic one below, is the object of the collaboration between Los Alamos National Laboratory and Procter and Gamble.

Such a scenario prompted the billion-dollar consumer products company, Procter and Gamble Co., to develop improved approaches to manufacturing reliability. During the P&G internal program, the company realized that the available reliability statistics and models used for manufacturing system analysis were inadequate.

P&G worried about how long its assembly lines were up and how often they were down, said Donna Smith of Los Alamos National Laboratory's Industrial Business Development Office. The internationally recognized company was working to make its production system more reliable and to predict better what parts should be replaced during down times and how new assembly lines would perform before they were built.

This is why P&G approached the Laboratory 10 years ago to collaborate on the development and implementation of new statistical approaches and models for a continuous assembly line that fails for a myriad of reasons and can undergo maintenance and repairs.

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Laboratory statisticians Harry Martz and colleagues in the Decision and Application Division went to work in an effort to identify parts on P&G's assembly lines that were most prone to breakage. Thus, there are fewer times that the lines go down after being brought up to full speed.

"If any machine breaks down, you're not making a profit," said Smith.

To predict performance, the system accounts for a multitude of competing reasons for why assembly lines stop.

The work done in collaboration with P&G has been performed under a cooperative research and development agreement. A CRADA is a legal document that researchers and industrial partners enter into when collaborative research is performed; it details who has rights to use such material created under joint collaborative efforts.

According to P&G's Tom Lange, the new manufacturing system benefits the consumer because the cost to produce a product decreases because the assembly line has more time in operation between repair and maintenance.

P&G is the manufacturer of such brands as Pringles, Folgers, Jiff, Pampers, Crest, Cascade and Tide.

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CLEANER CHIP MAKING METHOD USES CARBON DIOXIDE FLUID

Scientists at Los Alamos National Laboratory have developed a new technology application that could all but eliminate the use of hazardous corrosives and the production of wastewater in the fabrication of integrated circuits, or chips, for computers.

Chip making is sometimes called a “clean industry” because of the images of technicians in white lab suits working in ultra-clean rooms with shiny pristine silicon wafers. But it is estimated that on an average day of operations at a chip-making plant, four million gallons of wastewater are produced and thousands of gallons of corrosive hazardous materials, like hydrochloric and sulfuric acid, are used.

The new technology, called SCORR, or supercritical CO_2 resist removal, focuses on photoresist removal, one of the steps in a process called photolithography, in which high-intensity light along with aggressive acids and corrosives are used to create a chip’s tiny integrated circuits by altering the topography of a

Each image shows a photoresist-coated silicon wafer on which different metallizations have been deposited: (a) aluminum, (b) platinum over titanium, (c) indium oxide/tin oxide mixture, and (d) titanium over tungsten). The photos, each at a different magnification, were taken after the wafers had been treated with SCORR. They prove that the photoresist has been removed even from the deepest recesses formed by the individual structures and that SCORR has not caused any discernible effect on the metal structures.

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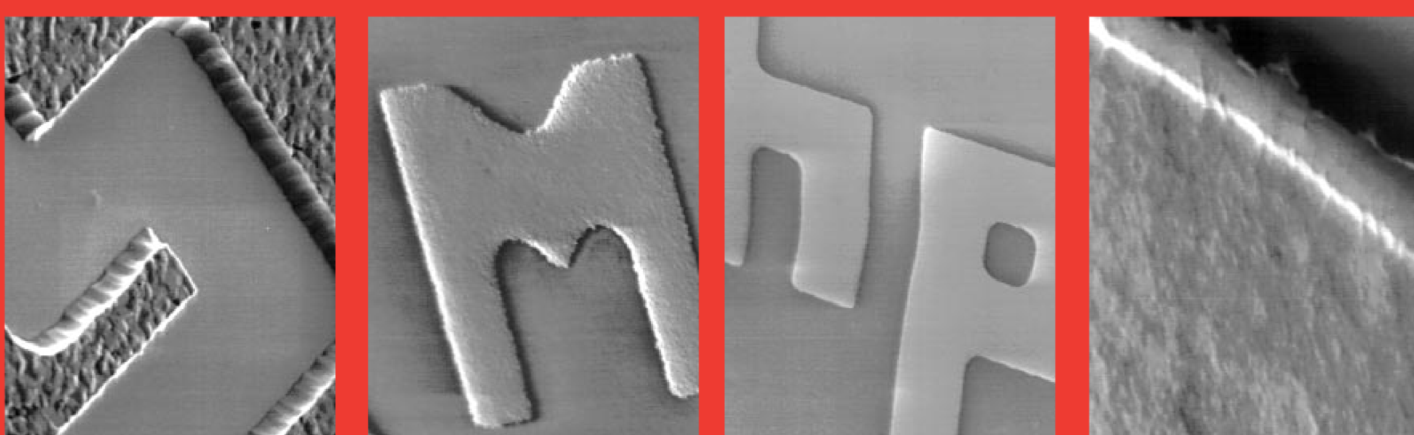

silicon wafer. Using carbon dioxide at high temperature and pressure, known as supercritical carbon dioxide ($SCCO_2$), in place of the hazardous materials, Laboratory researchers have demonstrated a technology that inexpensively replaces the solvents as well as the tremendous quantities of ultra-pure water that are used wash away those solvents.

"Carbon dioxide, at pressures above 1,050 pounds per square inch and temperatures above 31 degrees centigrade, becomes supercritical," said Craig Taylor, who leads the SCORR team in the Laboratory's Applied Chemistry Technologies Group. "In its supercritical phase the gas becomes liquid, but behaves a little like both — giving it the ability to act as a solvent. But $SCCO_2$ alone is somewhat ineffective, so it is combined with minor amounts of a more effective cosolvent, and we've seen that this mixture is quite effective at photoresist removal.

"On top of that, when the pressure and temperature are lowered the $SCCO_2$ returns to its gas phase, leaving the silicon wafer bone-dry and virtually free of any dirt, eliminating the need to rinse with ultra-pure water and dry with isopropyl alcohol. And the best news, carbon dioxide is cheap, nonflammable, nontoxic, biodegradable, recyclable and plentiful."

The Los Alamos photoresist removal technology produces virtually zero hazardous waste. It is designed as a closed-loop system that reuses the carbon dioxide in the process, adding no greenhouse gas to the atmosphere. Because of their low vapor pressure, the additive cosolvents are easy to separate from the mixture, and so they, too, are collected and reused.

A key element in the process is a tiny high-pressure sprayer that pulses the $SCCO_2$/cosolvent onto the silicon wafer to assist in dislodging the photoresist. Developed by technician Jerry Barton, the sprayer creates enough surface drag to dislodge the microscopic bits of photoresist already softened up by a minutes-long soaking in the $SCCO_2$/cosolvent mixture. This combined process of soaking and spraying, along with an $SCCO_2$-only wash, has produced results that equal the chip fabrication standards currently accepted in industry.

The early work on this technology was accomplished through a cooperative research and development agreement with computer manufacturer Hewlett-Packard. Research and development continues with IBM and GT Equipment Technologies, Inc.

"We want to bring this technology to the attention of the computer industry, as well as the public in general, just to emphasize the environmental advantages of $SCCO_2$," said Taylor. "Even if you were to set aside the hazards and pollution associated with the corrosive materials used in chip making, you still have the issue of water use — and that's especially critical in the Southwest where several large chip fabrication facilities are located. We believe that the $SCCO_2$ process has the potential to save hundreds of millions of gallons of water every year even if it were installed in just one factory, making it not only a very important technological advance, but an environmental advance as well."

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BRIEFLY

The Los Alamos Neutron Science Center (LANSCE) has a new leader, long-time Los Alamos National Laboratory researcher and manager Paul Lisowski.

LANSCE comprises a high-power, 800-million-electron-volt proton linear accelerator; a Proton Storage Ring; production targets at the Manuel Lujan Jr. Neutron Scattering Center and the Weapons Neutron Research facility; and a variety of associated experimental areas and spectrometers. LANSCE produces intense beams of pulsed neutrons at both the Lujan Center and the Weapons Neutron Research Facility, which provide the Laboratory and U.S. scientific community with the capability to perform experiments that support both defense and civilian research.

Lisowski has responsibility for ensuring that LANSCE continues to fulfill its important obligations to the Laboratory's science-based stockpile stewardship efforts and contributes to basic science through the continued, successful operation of the Lujan Jr. Center. Taken together, LANSCE's many features allow for important synergies between different disciplines and encourage the flow of ideas between academic, industrial and defense communities.

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