LOS ALAMOS NATIONAL LABORATORY
WHERE SCIENCE MAKES A DIFFERENCE

DATELINE
LOS ALAMOS

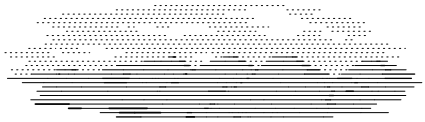
LOS ALAMOS WINS TWO R&D 100 AWARDS

OUTSTANDING TECHNOLOGIES WITH COMMERCIAL POTENTIAL

Two Los Alamos technologies have been honored with 1996 R&D 100 Awards. *R&D Magazine*'s international awards program is now in its 34th year. The program each year recognizes the most significant products, materials, processes, software, and systems with commercial promise.

Technologies are nominated in an open competition, and the Illinois-based magazine uses technical criteria to pick the most unique, important, and useful entries.

The two 1996 awards bring Los Alamos' total to 46 R&D 100 Awards won over the past nine years.



DATELINE: LOS ALAMOS

"Technologies recognized with an R&D 100 Award are some of the top commercial opportunities developed each year," said Pete Lyons, director of the Los Alamos Industrial Partnership Programs office. "We're glad to see continued recognition of the excellence of Los Alamos efforts in these awards."

This issue of *Dateline: Los Alamos* features the Laboratory's two winning technologies. The first is PLASMAX, an innovative method of keeping silicon wafers clean of contamination as they undergo the numerous manufacturing steps that transform them into integrated circuit chips.

The second winner, TRACER, is an analytical instrument with a long fiber-optic probe that can be carried into the field in a station wagon or truck bed to provide remote, on-site analysis of environmental contamination.

Brief descriptions of the Laboratory's other 23 entries are also included in this issue.

DATELINE LOS ALAMOS

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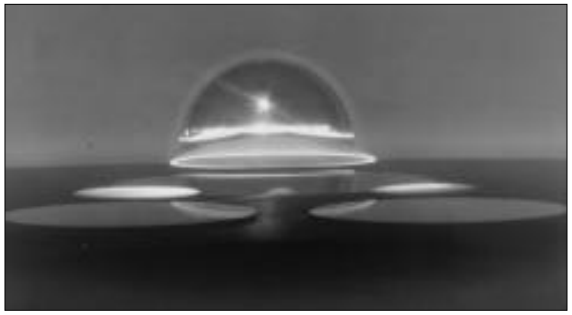
DATELINE: LOS ALAMOS

GOOD VIBRATIONS

PLASMAX CLEANS SILICON WAFERS WITH NO POLLUTING BYPRODUCTS

Every integrated circuit begins life as a silicon wafer. Even though the silicon wafers are processed under the cleanest possible conditions, using special rooms 1,000 times cleaner than hospital operating rooms, particle contamination still plagues the circuit chip industry. In fact, 30 percent of the steps required for production of silicon-based circuits are cleaning steps. This penchant for cleanliness is not a fetish; a particle of contamination less than 0.5 micrometer in diameter can result in a circuit chip that fails to operate.



The suspension and trapping of particle "clouds" over three silicon wafers in a plasma-processing chamber.

Researchers from Los Alamos and Beta-Squared Inc. of Allen, Texas, have developed a new cleaning method for removing particles of contamination from a wafer's surface. The "Plasma Mechanical Cleaner for Silicon Wafers," or PLASMAX, process combines plasma, an ionized gas, with mechanical vibration to clean wafers inside a vacuum chamber. The invention is one of two 1996 R&D 100 Awards received by Los Alamos.

Beta-Squared Inc., a wholly owned subsidiary of Photronics Inc., develops, manufactures, markets, and services plasma etch equipment used in the fabrication of integrated circuits for the semiconductor industry.

The PLASMAX system has several advantages over existing technologies. Current wafer cleaning methods use solvents, including some harsh chemicals. In contrast, PLASMAX uses harmless, inert gases to clean the wafers, thereby enhancing worker safety.

The PLASMAX system also can be incorporated directly into plasma etching tools already required for the silicon fabrication process. Because the PLASMAX process is directly integrated into the tools used for

processing, no extra clean room space is needed and the wafers are cleaned inside the tools immediately prior to the normal plasma etch or deposition steps, reducing process cost and the need for additional clean room space.

Furthermore, PLASMAX is an environmentally sound dry-cleaning process that produces no polluting byproducts and reduces the water usage of semiconductor manufacturers. This savings is especially important for companies located in arid regions.

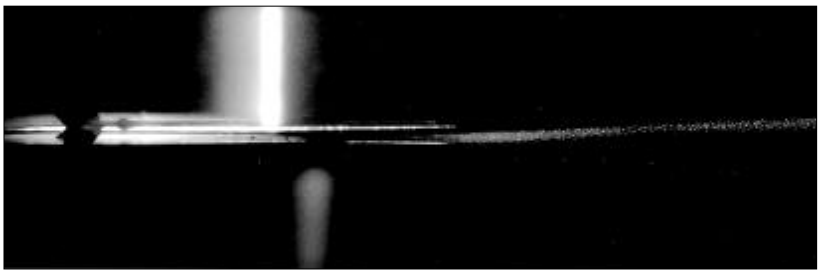
PLASMAX will make it possible to recycle blank silicon wafers used to test the cleanliness of manufacturing equipment. Such wafers are typically discarded; recycling them would save companies tens of millions of dollars yearly.

Other applications for PLASMAX include cleaning magnetic storage disks and decontaminating radioactive dust from instruments and weapons. The researchers predict that PLASMAX ultimately will be used for cleaning compact disks, flat panel displays intended to replace today's computer monitors, medical instruments, and optical components.

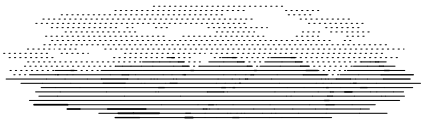
PLASMAX removes contamination from surfaces in the vacuum environment of a plasma processing chamber before, during, or after a processing step.

The basis of the PLASMAX tool is a mechanical activator that resides inside the chamber and supplies the necessary vibrations. Pins extend from the vibrator to the wafer, which is clamped in place. The vibrations, combined with the physical and electrical phenomena that occur in the plasma processing chamber, drive contaminants away from the wafer and keep them from redepositing on its surface.

Particles adhere to surfaces because of electrical attraction, chemical bonds, or surface tension if liquid is present. During fabrication, silicon wafers are flooded with a flux of ions and electrons that reduce the



The PLASMAX cleaner in operation — particles are being lifted off a wafer and ejected from the chamber.



intensity of electrical attractions. However, reducing these electrical forces results in minimal removal of contaminating particles. More cleaning is needed.

To break the chemical bonds, PLASMAX vibrates the wafer's surface at the same time the wafer is exposed to the plasma that acts to reduce electrical attractions. This combined effect greatly enhances the efficiency of the cleaning process. The vacuum also helps because any moisture present on the wafer vaporizes, reducing adhesion of the particles due to surface tension.

Once the process removes particles from the wafer's surface, it lifts them away from the wafer due to the electrical fields present in the plasma. The lifting action also directs the particles to special ports contained in the vacuum chamber. In this way, the particles are electrostatically prevented from returning to the wafer.

The wafer is not removed or exposed to air during the entire plasma process: an important feature because some contaminants become corrosive when exposed to air and moisture.

PLASMAX is an effective, energy efficient, fast, and inexpensive technology that will allow circuit chip engineers to develop new manufacturing steps that are considered too “dirty” in the absence of a suitable cleaning method. PLASMAX also provides benefits to workers, neighboring communities, and consumers by reducing the cost of computer products while permitting the production of ever more advanced circuits.

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DATELINE: LOS ALAMOS

PORTABLE, REMOTE UNIT SCREENS SOLID AND LIQUID MATERIALS FOR METAL CONTAMINATION

REDUCES COST OF ANALYSIS BY A FACTOR OF 200

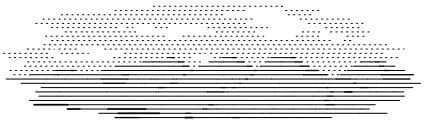
A complete "lab-in-a-box" instrument that analyzes materials under conditions and at locations other analytical techniques do not allow is the second Los Alamos 1996 R&D 100 winner.

Los Alamos researchers, together with ICF Kaiser Inc. engineers, developed the instrument to analyze soils for metal contaminants, but the technology also works on other solids and liquids. The Transportable Remote Analyzer for Characterization and Environmental Remediation, or TRACER, can be carried into the field in a van or station wagon to perform the measurements on site. A probe, which attaches to the main analytical unit, can be located up to 80 feet away from the unit, allowing access to difficult sites such as down a mining borehole.

TRACER's main analysis unit fits in the back of a vehicle and is connected to a probe by fiber-optic cables. A material — in this case soil — is analyzed by holding the probe against the surface.

TRACER's remote analysis capability is possible because of its ability to transmit intense laser pulses through a long fiber-optic cable that connects the end of the probe to the box. By focusing powerful laser pulses on the ground to form a series of laser sparks, a small mass of the sample is vaporized, and the resulting atoms become excited and emit light.

The analytical unit sitting in the van then automatically identifies the composition of elements contained in the soil by their unique spectral fingerprints. The automated procedure eliminates the need for highly skilled operators and virtually eliminates the possibility of an operator error. The lab-in-a-box analytical unit uses the SPECTRA hardware/software system developed at Los Alamos specifically for the TRACER unit.



Although optical fibers have been used for decades to transmit low-power low-energy light pulses, TRACER combines the transmission of intense — megawatt — laser pulses with laser spark spectroscopy.

In addition to remote analysis, TRACER has other advantages, including rapid analysis in less than one minute, no need for sample preparation as samples are analyzed directly in the field, and the ability to detect multiple elements in a single sample.

Los Alamos and ICF Kaiser Inc. developed TRACER primarily to determine the types and extent of elemental contamination at industrial and governmental facilities and waste sites. The instrument has undergone a field test sponsored by the Environmental Protection Agency, the Department of Energy, and the Department of Defense.

In addition to its use in environmental remediation, TRACER can be used in mining to determine the locations of high-yield ores and for prospecting and process control during mining operations.

Decontamination and decommissioning activities require on-site sensors to monitor toxic materials before, during, and after cleanup. TRACER's capability of remote analysis could easily be adapted to robotic systems intended for remote cleanup.

Another application has to do with the nation's infrastructure. Because existing U.S. bridges, railways, roads, and nuclear power plants are aging, authorities need methods that can efficiently determine the condition of such structures and facilities. TRACER can be used to determine conditions such as the state of protective coatings on bridges and buildings, the extent of radiation embrittlement in the cooling pipes of a reactor, and the degree of metal corrosion.

ICF Kaiser Inc. is an international company involved in environmental characterization and mining. As the co-developer of TRACER, Kaiser intends to develop the technology further for its customers. A patent is pending on this product. The inventors estimate the cost of a commercial TRACER unit to be $30,000 to $80,000, depending on its range of analytical capabilities.

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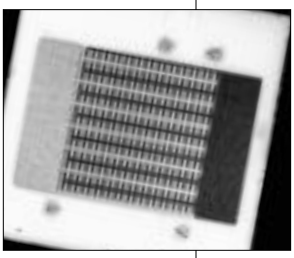
SOLID-STATE ELECTROCHEMICAL CARBON MONOXIDE SENSOR



Interdigitated configuration of the solid-state electrochemical sensor.

Half of all poisoning deaths in the United States are caused by carbon monoxide, a deadly, colorless, odorless gas produced when heating fuels burn incompletely. Sensors currently on the market detect the gas slowly and only at levels of hundreds of parts per million. A new, inexpensive ceramic sensor developed at Los Alamos can detect CO concentrations as low as one part per million in less than a minute. The Solid-State Electrochemical Carbon Monoxide Sensor rapidly returns to its pre-exposure condition once the gas is removed, meaning there will be few false alarms. Because it operates at elevated temperatures (400° C to 700° C), this sensor also is suited to monitoring exhaust streams from furnaces, power plants, or automobile engines for active combustion control. CONTACT: FERNANDO H. GARZON, (505) 667-6643, E-MAIL: garzon@lanl.gov

FOAMING CAPACITY MONITOR

A close-up view of a foam that the Foaming Capacity Monitor generates for a dilute detergent solution.

Foam is a common by-product of surfactants — surface-active agents such as detergents — which are used in many industries to stabilize emulsions, improve surface wetability, and remove contaminants. In many applications, the presence of the foam, and the amount of foam that is formed, is extremely relevant to the efficiency of process operations. Too much or too little foam, depending on the process, can damage the final product. Los Alamos has developed the Foaming Capacity Monitor, also known as the "Solution Monitor," to measure the foaming potential of a solution and control it by adding exactly the right amount of antifoaming agent or surfactant to keep the process operating at peak efficiency. The simple, inexpensive device can measure surfactants and other foaming or bubbling substances on-line, continuously, and in real time. Because the monitor eliminates the use of hazardous chemicals in the test process, such as chloroform, it is more worker- and environment-friendly. The monitor also costs much less to produce than conventional instruments. The Los Alamos device will be useful in many industries, including ceramics, wood pulp and papermaking, waste water treatment, and electroplating.

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QUICK-FLIP LOCATOR FOR MICROMACHINING

A close-up view of a Quick-Flip Locator attached to the spindle of a polishing machine.

Securing millimeter-size parts to a lathe for precise machining ranges from difficult to impossible, especially when the parts are complex and must be machined on two sides. The Los Alamos Quick-Flip Locator snaps onto a magnetic chuck with a positioning error of less than 0.25 micrometer. For multi-step fabrication, the part travels in the locator from one machine to another or is flipped on a single tool to allow machining of both sides. On small parts requiring multiple machining steps, for which setup and inspection time account for a large part of the total cost, the locator offers significant cost savings. Machining accuracy with the locator is 100 times greater than with conventional part holders.

CONTACT: LEANDER J. SALZER, (505) 667-9666

PALLADIUM MEMBRANE REACTOR

The Palladium Membrane Reactor with its heater and insulation is seen in the middle glovebox window. Inset shows the reactor's active components.

Generating hydrogen from water and methane is both economically and environmentally advantageous. For example, hydrogen is needed to synthesize ammonia, which is needed for the multi-billion dollar fertilizer industry. While traditional hydrogen production methods require seven processing steps, the Palladium Membrane Reactor developed by Los Alamos researchers generates hydrogen from water and methane in a single, nonpolluting step. This device can also be used to recover tritium from water and methane with extremely high efficiencies. Recovering tritium from the tons of radioactive water that have accumulated at U.S. nuclear facilities is important not only to decontaminating this waste but also to recycling tritium, which is valued at $100,000 per gram. CONTACT: R. SCOTT WILLMS, (505) 667-5802, E-MAIL: rsw@lanl.gov

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PREDICTIVE CODE FOR SUPERPLASTIC FORMING

Superplasticity is a property of certain materials that allows them to undergo extensive tensile plastic deformation. Given the right temperature, pressure, and time, some metals can be elongated up to 1,000 percent. This scientific phenomenon has been translated into a manufacturing technique called superplastic forming, or SPF, a process in which the metal does not get pressed instantaneously into a mold, but is heated and gently pressed while it "creeps" into place over a period of hours. The Predictive Code for Superplastic Forming takes the guesswork out of the industrial SPF process by predicting optimal pressure schedules, overall forming time, and final thickness distribution before a part's forming process begins. Applications for the predictive code include manufacturing complex aircraft parts, aluminum chassis for next-generation cars, jet turbine blades from super alloys, and nuclear weapons parts. The code was developed by Los Alamos under a cooperative research and development agreement with Flameco Plant, Barnes Group Inc. CONTACT: MARTIN PILTCH, (505) 665-6835, E-MAIL: piltch_martin_s@lanl.gov

↑ An aircraft engine's nacelle waffle can be manufactured without costly trial and error, thanks to the Predictive Code for Superplastic Forming.

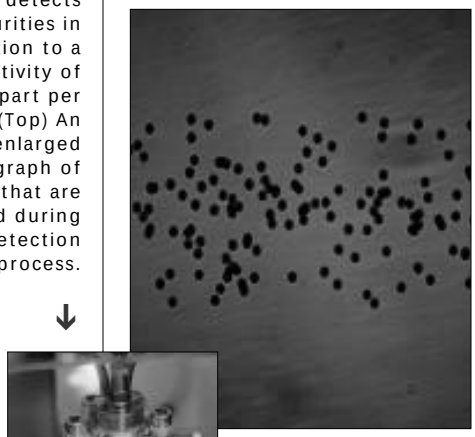
ELECTROLYTIC DECONTAMINATION OF ORALLOY

The end of the Cold War has brought with it accelerated schedules for dismantling nuclear weapons stockpiled around the world. The Electrolytic Decontamination of Oralloy removes plutonium and americium contamination from oralloy (highly enriched uranium) hemishells from dismantled nuclear weapons to levels that will permit its recasting for international inspection and eventual disposal. The previous standard cleaning technology — acid-leaching — is now banned in the United States because of the mixed waste it produces. The new electrolytic decontamination process removes contamination without producing a primary waste stream. The Los Alamos technique also can be used to decontaminate radioactive containers inside gloveboxes and the gloveboxes themselves, saving millions of dollars in future disposal costs for retired gloveboxes. CONTACT: TIMOTHY O. NELSON, (505) 667-2326, E-MAIL: ton@lanl.gov

← Drawing of the fixture used to electrolytically decontaminate oralloy hemishells from nuclear weapons.

DATELINE: LOS ALAMOS

BUBBLE CHAMBER SPECTROSCOPY FOR TRACE CHEMICAL DETECTION



The Bubble Chamber (bottom) detects impurities in solution to a sensitivity of one part per trillion. (Top) An enlarged photograph of bubbles that are created during the detection process.

Chemical analysis using optical absorption is used to analyze many different products for thousands of different chemicals. Los Alamos Bubble Chamber Spectroscopy enhances the usefulness of optical absorption by making it 10 times more sensitive to small quantities than ever before: It can detect impurities in solution to a one-part-per-trillion sensitivity. The technique uses a bubble chamber of superheated liquid to "amplify" the effects of light absorption from a tuneable laser beam by trace impurities in the solution. The new technology can provide increased sensitivity in measurements made for performing environmental monitoring, improving forensic analysis, and providing quality assurance in the production of pharmaceuticals and ultrapure solvents for the semiconductor industry. CONTACT: ROBERT K. SANDER, (505) 667-3001, E-MAIL: bsander@lanl.gov, OR XIN LUO, E-MAIL: luox@lanl.gov

FLOW-THROUGH ION GUN

The Flow-Through Ion Gun can clean surfaces or deposit thin films onto nearly any surface. The glow is from the plasma produced by the gun during operation.

The Flow-Through Ion Gun developed at Los Alamos is a new type of tool that can clean surfaces or deposit thin films onto both conducting and insulating surfaces. By cleaning surfaces just before deposition, the gun can produce thin films with superior adhesion. It also can deposit thin films two to 10 times faster than normal ion beam deposition methods. The thin films produced with this gun are up to 10 times smoother than those produced with other guns. The technology has uses in the automotive, aerospace, and aircraft industries, where coating machine tools and jet-engine parts with the superior thin films will improve their longevity and performance. The gun also has applications for various cleaning and coating processes in the semiconductor industry. CONTACT: R.W. SPRINGER, (505) 667-4258, E-MAIL: rwspringer@lanl.gov

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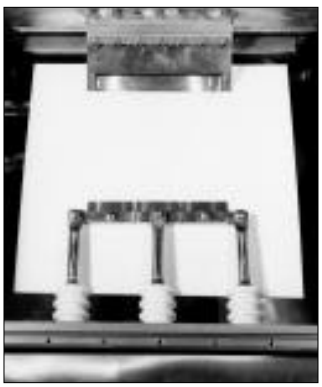
MICRO-ATMOSPHERIC MEASUREMENT SYSTEM

Airborne emissions are released from industrial processes, hazardous-waste incinerators and storage containers, and during the cleanup of contaminated soil. Accidental releases of hazardous aerosols may require emergency response teams to track and characterize emission plumes. The Micro-Atmospheric Measurement System is the only system of its kind that can be deployed aboard small, mobile platforms to monitor and collect atmospheric aerosol emissions. By providing real-time monitoring of these emissions, the Los Alamos technology makes possible more thorough monitoring of industrial emissions and real-time tracking of inadvertent releases of hazardous aerosols. CONTACT: JOHN R. STEPHENS, (505) 667-7363, E-MAIL: jrs@lanl.gov

The Micro-Atmospheric Measurement System is a portable sensor package and control station for monitoring emissions from stacks and from open areas such as landfills or hazardous waste sites undergoing remediation.

SLIDING-ARC UV FLASHLAMP

The Sliding-Arc UV Flashlamp produces ultraviolet and visible light that is intense enough and covers a large enough area to process an entire liquid-crystal display for a laptop computer screen in a single flash. The intense light can potentially melt and crystallize the silicon in the transistor driver circuits of the display to increase its brightness. In addition, the flashlamp processes the surfaces without contaminating them. The flashlamp is expected to have its greatest impact in fabricating liquid-crystal displays, a multibillion-dollar industry projected to see large growth in the next few years. The same Los Alamos technology can also be used to treat liquid-waste streams by breaking down hazardous materials with intense UV radiation. CONTACT: ROBERT C. SZE, (505) 667-4300, E-MAIL: sze@lanl.gov



The Flashlamp produces ultraviolet light that is intense enough and covers a large enough area to process an entire liquid-crystal display for a laptop computer screen in a single flash.

DATELINE: LOS ALAMOS

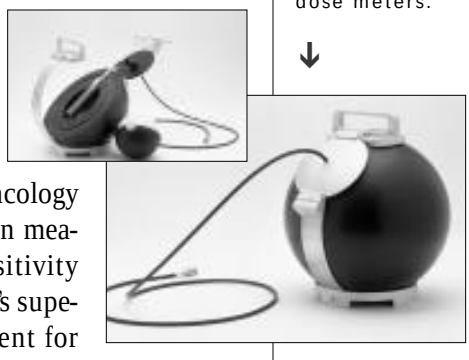
LIGHT APPLIQUÉ SYSTEM TECHNIQUE (LAST) ARMOR

The cockpit of a US Air Force C-141 (top) wears LAST Armor designed to protect the crew and critical components from small-arms fire.The armor is composed of several mats of 4-inch-square cermet tiles (bottom).

Although armor has been used since medieval times, modern protection methods only date from 1962 and the introduction of Kevlar, an incredibly strong fiber patented by DuPont, and the application of very hard ceramic materials to stop hard-point bullets. Researchers from Los Alamos, Foster-Miller Inc., and Lanxide Armor Products Corp. have extended the use of these materials to new bullet protection applications with the development of LAST armor. Panels of the armor are constructed of 4-inch-square silicon carbide tiles. These tiles are backed with Kevlar to make modular, lightweight, easy to install, and easy to repair panels. The attachment to the vehicle is with a Velcro-like hook and loop material. The LAST armor was initially designed to protect the USMC LAV-25 armored personnel carrier during Desert Storm. The Los Alamos-industrial team adapted this design to the cockpit crew of the U.S. Air Force C-141 aircraft for protection from all .30-caliber armor-piercing bullets. The armor is now being adapted to the C-17 and C-130 aircraft. Other potential applications for the armor include counter panels in banks and convenience stores, door and floor panels in police cruisers, and body armor for anyone living or working in dangerous situations.

CONTACT: S. ROBERT SKAGGS, (505) 667-1134; E-MAIL: bobskaggs@aol.com

WIDE-ENERGY NEUTRON DETECTION INSTRUMENT (WENDI)

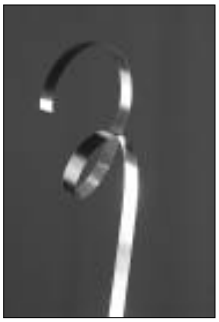


WENDI measures the amount of neutron radiation received by human beings with an accuracy and sensitivity unequaled by other neutron dose meters.

Workers at nuclear power plants and other facilities where neutron radiation is present are monitored closely to determine the amount of radiation, or dose, their bodies have received. The Wide-Energy Neutron Detection Instrument developed by Los Alamos, Varian Oncology Systems, and San Jose State University Foundation measures neutron dose with an accuracy and sensitivity unequaled by other neutron dose meters. WENDI's superior accuracy will help create a safer environment for people working in nuclear power plants, medical centers where accelerators are used to treat cancer, oil-well-logging sites, research centers that

use particle accelerators, and nuclear-materials laboratories. CONTACT: RICHARD OLSHER, (505) 667-3364, E-MAIL: dick@lanl.gov

FLEXIBLE SUPERCONDUCTING TAPE



A piece of superconducting tape that carries high current with no resistance even in magnetic fields.

Los Alamos researchers achieved a breakthrough in superconductor technology with a piece of thin metal tape coated with a high-temperature superconducting material. The tape carries high current with no resistance at liquid nitrogen temperatures — even in high magnetic fields — and is flexible enough to be wrapped into a tight coil. The tape's flexibility and high current-carrying capacity give it a wide range of potential applications, including electromagnets, motors, generators, transformers, and magnetic separators that use high magnetic fields to separate materials in suspension. In addition, the tape may find major applications in microwave cavities used for digital communications and in particle accelerators, current leads, and fault current limiters, which are used in the electric power industry to protect sensitive current-carrying operations when electrical shorts occur. CONTACT: DEAN PETERSON, (505) 665-3030, E-MAIL: dpeterson@lanl.gov

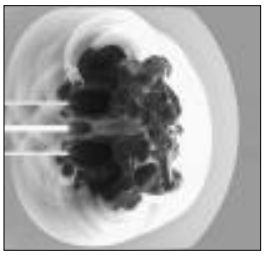
ADVANCED LASER-DRIVEN FUEL IGNITOR

The Advanced Laser-Driven Fuel Ignitor produces a laser spark that ignites jet fuel.

Los Alamos researchers have developed several novel, laser-driven ignition methods that reliably and efficiently initiate jet-fuel combustion over a broad range of temperatures and fuel-air compositions. One of these advanced ignition methods has the potential to replace currently used capacitive discharge ignitors. The Advanced Laser-Driven Fuel Ignitor yields enhanced turbojet engine reliability and safety, increased fuel economy, and reduced pollution. Specialized laser-light pulses are focused within a cloud of fuel to produce a laser-induced plasma, known as a "laser-spark," that ignites the fuel. The ability to reliably ignite fuel within the optimal zone of the engine's combustion chamber, in a manner unobtrusive to engine flow dynamics, will enhance the performance of existing turbojet engines as

well as expand the design possibilities for the next-generation high-efficiency, clean-burning turbine engines. CONTACT: JIM EARLY, (505) 667-5678

DISTRIBUTED-DATA IMAGING SYSTEM



One frame of an animated visualization of two gases mixing in a tank displayed by the Distributed-Data Imaging System.

Visualization — displaying computational data in a pictorial form — teams the strength of the computer with the pattern-recognition ability of the human brain. Because supercomputers can handle the most complex simulation problems, they are ideal for creating representative models of scientific data. Unfortunately, their multi-million-dollar pricetag is more than most organizations can afford. The Distributed-Data Imaging System developed by Los Alamos and Digital Equipment Corp. links eight desktop computer workstations into a computing cluster capable of producing seamless, colorful, animated images that equal the quality and complexity of those generated by supercomputers. Some applications include scientific studies such as weather and ocean current modeling, chemical and biological process modeling, and fluid-flow simulations. In private industry the technology could be used in creating movie and video special effects, developing new drugs through pharmacological modeling, or improving airline scheduling and freeway design through traffic-flow modeling. CONTACT: DONALD TOLMIE, (505) 667-5502, E-MAIL: det@lanl.gov

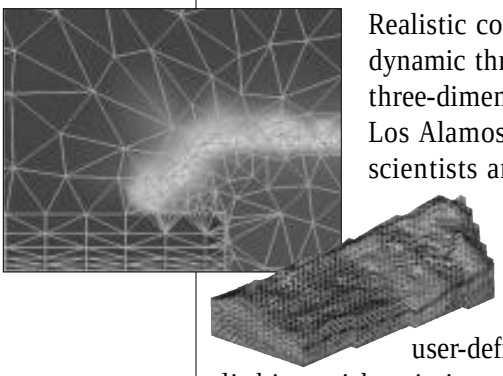
TRANSPORTABLE ACTINIDE MASS SPECTROMETER (TAMS)

TAMS provides fast, accurate isotopic analysis of uranium and plutonium compounds.

Nuclear materials such as uranium and plutonium are used in research, energy production, and nuclear weapons. The isotopic composition of a nuclear material is like a fingerprint that reveals the material's physical characteristics, often its source, and its potential applications. Los Alamos researchers have developed a portable system for rapid on-site isotopic analysis. Easy to use, with low power requirements,

the Transportable Actinide Mass Spectrometer, or TAMS, eliminates the need for laboratory analysis, which requires time-consuming sample delivery and receipt of results. TAMS combines proven, reliable actinide chemistry and mass spectrometry techniques. The system's transportability and simple operation allow researchers, field inspectors, customs agents, military personnel, and law enforcement officers to quickly identify and analyze actinide samples. Analysis requires no sample preparation and takes less than 30 minutes, which allows fast decisions to be made for remediation of nuclear materials. CONTACT: JOSE OLIVARES, (505) 665-5190, E-MAIL: olivares@lanl.gov

X3D: THREE-DIMENSIONAL UNSTRUCTURED GRID TOOLBOX



Realistic computer modeling and simulation of static or dynamic three-dimensional processes require high-quality three-dimensional grids. The X3D software developed by Los Alamos and Semiconductor Research Corp. enables scientists and engineers to realistically model complex, multiple-material, three-dimensional structures that change over time. It also minimizes the need for computer resources. Easily modified through user-extensible data objects, user-defined commands, and easy-to-use interfaces for linking with existing user-specified application software, X3D is well-suited for a wide range of practical applications. Two examples are semiconductor manufacturing process simulations such as material deposition and etching, and geologic models of fluid flow and material transport. CONTACT: DENISE GEORGE, (505) 667-6248, E-MAIL: dgeorge@lanl.gov

← The background image is a two-dimensional grid extracted from a three-dimensional semiconductor process simulation. The three-dimensional grid in the foreground is a stratigraphic geologic model of mountainous terrain used to model fluid flow and track migration of environmental contaminants.

PC-GSAS: CRYSTAL STRUCTURE ANALYSIS SOFTWARE FOR THE PERSONAL COMPUTER

In today's computer-based laboratory environment for basic and industrial research, the trend is away from high-end workstations and mainframe computers and toward personal computers, or PCs. Due to their user friendliness and cost effectiveness, PCs are becoming the computers of choice for handling data and operating sophisticated

data-collection instruments. New software developed at Los Alamos allows laboratory users of IBM-compatible PCs to determine crystal structures and crystalline properties from multiple sets of X-ray and neutron diffraction data. PC-GSAS is beneficial to researchers in any field in which properties of molecular and crystal structure are of interest. By combining the data-analysis tools with word processing, spreadsheet, and graphical presentation software on a single computer, PC-GSAS greatly increases productivity. As a full-featured analysis software for determining crystal structure on IBM-compatible PCs, it is the right tool for the time. CONTACT: ROBERT VON DREELE, (505) 667-3630, E-MAIL: vondreele@lanl.gov

↑

PC-GSAS provides an easy-to-use, menu-driven interface for handling a wide range of crystallographic analyses on IBM-compatible personal computers.

PLUME-IN-A-BOX: AN EMERGENCY RESPONSE TRAINER

Chemical processing plants, nuclear reactors, and facilities that produce hazardous materials — all are potential sources of radioactive or hazardous releases into the environment. Personnel working in such areas are trained periodically so that they can protect themselves and the general public in the event of accidents. Although extremely valuable, theoretical classes do not fully prepare workers for what happens in real emergencies. Plume-in-a-Box is an interactive training system that simulates environmental emergencies outdoors, under conditions as close to real ones as the users choose to create. The system integrates off-the-shelf Global Positioning System, or GPS, electronics with a portable computer that includes notebook, pen, laptop, or palmtop and a software package developed by the inventors. Plume-in-a-Box was successfully tested during a nuclear weapons accident exercise at the Yorktown Naval Weapons Station in Virginia. CONTACT: LARRY HOFFMAN, (505) 665-8890, E-MAIL: hoff@lanl.gov

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Plume-in-a-Box is the first emergency response trainer to simulate instrument response to any hazardous release into the environment.

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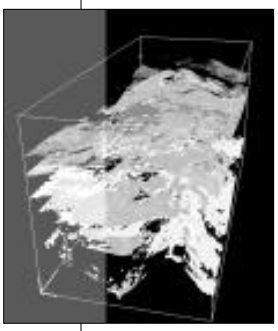
FALCON: ADVANCED RESERVOIR SIMULATION SOFTWARE

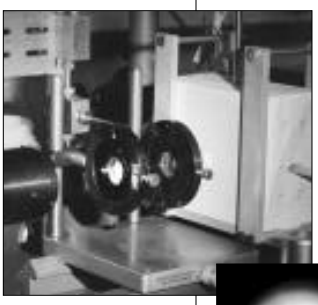


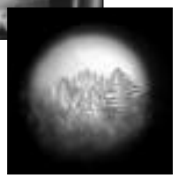
Falcon provides the first ever computer simulation of multibillion-barrel oil and gas reservoirs.

Simulations that predict the flow of oil and gas in underground reservoirs are used by all major oil and gas companies to determine the best recovery strategies. However, current production simulations are limited because they run on small, slow, single-processor computer systems. Worldwide, reservoirs produce 70 million barrels of crude oil per day. Of this production, 40 million barrels are from huge fields that cannot be modeled with present-day computer simulation software. Falcon software developed by Los Alamos, Cray Research, and Amoco makes it possible to model large, economically important oil fields in their entirety. Run on massively parallel computers, Falcon is 100 times faster than currently available simulators. Falcon allows oil and gas companies to perform best- and worst-case analyses of drilling scenarios and to calculate "what if" operational scenarios for reservoirs, both of which are crucial to developing economical recovery strategies. CONTACT: OLAF LUBECK, (505) 667-6017, E-MAIL: oml@lanl.gov

DIAMOND-WINDOW OPTICAL CELL FOR FLUID MONITORING

The Diamond-Window Optical Cell (top) allows direct observation of phase behavior in fluids under high-temperature, high-pressure conditions. The magnified image (inset) appears on a monitor.





Density is a property of matter that directly affects its flow, heat transfer, and mixing ability. Other properties are dependent on how fast density changes with temperature and pressure. If a fluid chemical processing system is to perform reliably, its designer must take into account how the fluid's density and density-dependent properties relate to the temperatures and pressures involved. This information is known as "characterizing" the fluid. The Diamond-Window Optical Cell makes it possible for essential information to be obtained visually and cost-effectively. Because it quickly and accurately measures fluid density in hydrothermal conditions, the cell is uniquely suited for enabling the development of hydrothermal waste-treatment systems and for providing real-time monitoring of treatment processes. Some of the complex aqueous wastes the optical cell can characterize include military wastes such as streams containing propellants, explosives, and dyes; aqueous mixed wastes left over from weapons buildup during the Cold War and the subsequent initial steps at dismantling those weapons;

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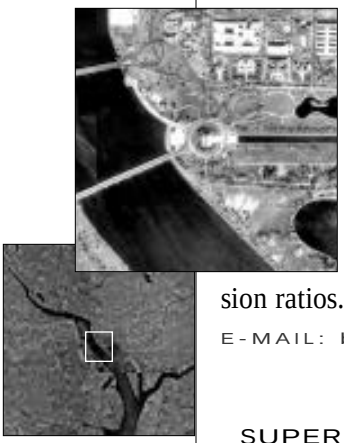
industrial wastes containing metal salts, which include waste streams from paper production, and electroplating; and municipal wastes. CONTACT: GRAYDON ANDERSON, (505) 667-7213, E-MAIL: graydon@lanl.gov

MULTIRESOLUTION SEAMLESS IMAGE DATABASE (MrSID)

MrSID is a set of cross-platform software applications that compress large images and image databases.

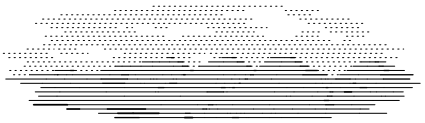


In the face of the Internet's recent explosive growth, the storage, retrieval, communication, and manipulation of information have become everyday problems that must be solved fast. Users often need to retrieve and then store large images or even entire image databases, a task they cannot accomplish on desktop computers without efficient image compressors. MrSID fills that need. Developed by researchers at Los Alamos and LizardTech, MrSID allows efficient retrieval and storage of very large digital images, such as the geographical images provided by the United States Geological Survey. MrSID also allows seamless multiresolution browsing and viewing and provides superior image quality even at high compression ratios. CONTACT: JONATHAN BRADLEY, (505) 665-2722, E-MAIL: bradley@lanl.gov

SUPERSCAN COUNTERFEIT CURRENCY DETECTOR

Because of its relative stability, U.S. currency is one of the preferred currencies for use worldwide. It is also one of the easiest of the world's stable currencies to counterfeit. Unfortunately, new reprographic technologies are making counterfeiting U.S. currency even easier. The SuperScan Counterfeit Currency Detector developed at Los Alamos quickly discriminates between genuine and counterfeit U.S. $20 and $100 bills regardless of their age or condition. Through the use of near-infrared spectroscopy and chemometric analyses, SuperScan detects minute differences in the paper and inks used to create genuine and counterfeit currency. CONTACT: DONALD BURNS, (505) 665-4186, E-MAIL: dburns@lanl.gov

SuperScan quickly discriminates between genuine and counterfeit $20 and $100 bills regardless of their age or condition.



BRIEFLY ...

LOS ALAMOS PARTNERS WITH INDUSTRY. Since 1991, Los Alamos has entered into 215 Cooperative Research and Development Agreements, or CRADAs, with private industry valued at $478 million. Los Alamos, which is operated by the University of California for the Department of Energy, has two partnership "firsts" to its credit. Los Alamos is the lead laboratory in the largest-dollar-value CRADA with a small business partner ever put together. The Contaminant Analysis Automation CRADA involves five DOE-funded laboratories and SciBus Analytical Inc. of Palo Alto, Calif. Los Alamos' share of this $65.8 million CRADA is $25.4 million. Los Alamos is also the sole national laboratory in a CRADA with 24 oil and gas companies — the largest number of partners for any DOE CRADA. The partners include major companies and small independent operators. For information about the CRADA as a means of working with industry, contact Varda Main at (505) 665-6697 or Donna Smith (505) 667-9473 in the Los Alamos Industrial Partnership Office.

IN THIS ISSUE:

R&D 100 AWARD-WINNING TECHNOLOGIES

GOOD VIBRATIONS: PLASMAX CLEANS SILICON WAFERS WITHOUT POLLUTING
PAGE 3

PORTABLE UNIT SCREENS MATERIALS FOR METAL CONTAMINATION
PAGE 6

23 OUTSTANDING TECHNOLOGIES
PAGE 8

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