

# News Briefs

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## General Developments

*Inquiries about News Briefs, where no contact person is identified, should be referred to the Managing Editor, Journal of Research, National Institute of Standards and Technology, Building 820, Room 126, Gaithersburg, MD 20899-0001; telephone: 301/975-3572.*

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## UPDATED NVLAP DIRECTORY NOW AVAILABLE

Approximately 700 testing and calibration laboratories accredited by the National Voluntary Laboratory Accreditation Program are listed in the 1997 edition of the NVLAP Directory (NIST Special Publication 810). Accreditation by NVLAP under international standards provides assurance to U.S. manufacturers, exporters, government agencies and others that their test reports and services will be accepted in the global marketplace.

A NIST spokesperson stated that the number of NVLAP-enrolled laboratories has grown this past year due to developments such as (1) the Federal Communication Commission's decision to accept certain products tested in NVLAP-accredited EMC testing laboratories; (2) the commencement of the NVLAP fasteners and metals accreditation program; and (3) the expansion of the Calibration Laboratories accreditation program.

The directory's indexes list laboratories in alphabetical order, by field of accreditation, by state or country, and in numerical order by NVLAP Lab Code.

For a copy of NIST SP 810, contact NVLAP, Room 282, Building 820, NIST, Gaithersburg, MD 20899-0001, (301) 975-4016, fax: (301) 926-2884, <nvlap@nist.gov>. Additional information on NVLAP may be found on the World Wide Web at <<http://ts.nist.gov/nvlap>>.

## WORKSHOP PROCEEDINGS HIGHLIGHT MATH MODELING

Recently, NIST sponsored a four-day workshop to discuss the use of mathematical techniques—such as Green's functions and boundary element analysis—for modeling the mechanical behavior of advanced materials. The proceedings from the workshop, NIST Special Publication 910, are now available for purchase.

A total of 29 participants from universities, industries and national laboratories attended the workshop. Discussion groups focused on fracture, quantitative nondestructive evaluation and computer-aided engineering. Each group was charged with identifying key technology issues, establishing the relevance of these issues to Green's functions and boundary element analysis, and identifying specific projects. The key issue was the relevance of the technology discussed at the workshop to specific problems in industry.

For a copy of Green's Functions and Boundary Element Analysis for Modeling of Mechanical Behavior of Advanced Materials (NIST SP 910), contact the Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402. Order publication no. 003-003-03441-0 for \$15 prepaid.

## NEW MONITORING TECHNIQUE GETS REAL WORLD TEST

Automobile manufacturers and others who use strong but lightweight composite materials to make parts say that they critically need better methods to monitor and control their manufacturing processes. Now, a fast optical fiber process monitoring system, developed and laboratory tested by NIST, also has been evaluated in a pilot industrial composites processing environment at one of the major U.S. automobile companies.

The new system uses optical fibers to measure the chemical reactions and fluid flow inside a mold as a composite changes from liquid to solid form. This eliminates the need for the large or intrusive sensors used by other techniques. Faster process monitoring and reduced waste are likely benefits, preliminary laboratory tests indicated.

Molding tests at the automobile company demonstrated that the NIST system can provide useful information for process and quality control. However, the sensor requires further development to maximize its sensitivity to specific commercial systems.

For more information on the process monitoring system, contact Richard Parnas, B108 Polymer Building, NIST, Gaithersburg, MD 20899-0001, (301) 975-5805, <richard.parnas@nist.gov>.

### **REFLECTOMETER ENHANCEMENTS PRODUCE RECORD SENSITIVITY**

A neutron reflectometer recently installed in NIST's Cold Neutron Research Facility is now operating with one of the highest sensitivities of any comparable instrument in the world.

The neutron reflectometer is used to probe the composition and magnetization depth profiles of polymer, ceramic, semiconductor, and metal multilayers. These materials have molecular-level structures that can significantly influence their properties and, in turn, the performance of devices made from them. The higher neutron intensity now provides compositional and structural information at a 1/10 nanometer-level resolution and can detect layers as thin as  $5 \times 10^{-10}$  m to  $10 \times 10^{-10}$  m.

In addition to its high sensitivity, the instrument has been fitted with a molecular beam epitaxy chamber that allows for thin film and multilayer growth under ultrahigh vacuum conditions while making reflectivity measurements.

The new MBE chamber is the only one in the world available in a neutron scattering facility. Scientists will use it to study structural and magnetic properties of materials being developed for advanced electronics and magnetic sensors. For example, it already has been used to study the effect of hydrogen on magnetic properties of iron-vanadium superlattices. More details on the reflectometer and molecular beam epitaxy chamber are available on the World Wide Web at <<http://rrdjazz.nist.gov/ng1refl.html>>.

### **NEW VOLTAGE STANDARD PERFORMS FAST SWITCHING**

Voltage standards that can be switched quickly between levels are needed by industry to characterize digital-to-analog and analog-to-digital converters. NIST has developed such a programmable voltage standard that will enable dc voltage measurements on a microsecond scale.

The new circuit has the equivalent resolution of a 9 bit digital-to-analog converter and an accuracy of 30 bits ( $1 \times 10^{-9}$ ). The heart of the circuit is an array of 32768 Josephson junctions. In order to achieve programmability, the array is divided into a binary sequence of segments in which the least significant bit has 128 junctions and the most significant bit has 16384 junctions. The voltage across the array is programmed by biasing each segment at one of three constant voltage steps. When the array is driven with a 16 GHz microwave signal, it produces 1023 selectable reference voltages in increments of 4.235 mV.

The circuits are based on a novel superconductor-normal-superconductor junction technology developed at NIST. In this technology, a high-resistivity palladium-gold alloy is used as the normal metal barrier sandwiched between two superconducting niobium electrodes. The junctions are about 130 times smaller than those in the present dc voltage standard.

Initial tests have shown the functionality of the full circuit, proving that all 32768 junctions are working properly. A level of junction and microwave distribution uniformity is obtained that is about five times better than previous circuits. For more information, contact Samuel Benz, Div. 814.03, NIST, Boulder, CO 80303-3328, (303) 497-5258, <benz@boulder.nist.gov>.

### **IMPROVED MAGNETIC IMAGING SAMPLE COMING**

Magnetic force microscopy (MFM) is becoming widely used as an analytical tool in the disk drive industry. Presently, MFM images can vary greatly due to variations in tip geometry, magnetic materials used to coat the tip and instrument configuration. A well-characterized, widely distributed reference sample provides vital information about such variations.

NIST is developing an improved magnetic imaging reference sample based on a thin-film magnetic recording disk. It replaces the current NIST prototype sample with a smoother, laser-textured version that minimizes

topographic effects. The magnetic pattern written to the disk also has been changed to enable a quick measure of the polarity of the MFM tip.

NIST researchers have demonstrated the usefulness of this proposed sample by comparing a number of tips and showing their variability. They also have shown how a tip's magnetization direction can affect the image and how signal is increased when scanning an area of interest.

The NIST team, working with a scientist from a private company is currently trying to solve some lithography problems with the reference sample. It also is developing software to present magnetic field profiles at various heights from the sample surface. For a copy of paper 9-97, which describes the improved reference sample, contact Sarabeth Harris, Div. 104, NIST, Boulder, CO 80303-3328, (303) 497-3237, <sarabeth@micf.nist.gov>.

#### **NIST REFINES PROBE MODEL, IMPROVES PERFORMANCE**

Refinements to a NIST-developed computer model that estimates and corrects the "lobing errors" of touch-trigger probes used on most coordinate measurement machines and, increasingly, on machine tools, are expected to increase both the power and practical value of the tool.

NIST manufacturing researchers have extended their "Superfit" model to account for inaccuracies caused by misalignment of the measurement stylus. For example, misalignment can result from a bent stylus or from inexact placement of the stylus in its holder. Adding probe asymmetry to error sources already addressed (such as friction and rotational displacement) substantially improves the NIST model's performance. The upgraded model typically can correct for 80 % to 90 % of the systematic error due to probe-lobing effects.

NIST researchers also made the model easier to use by significantly reducing the amount of data (and therefore, time) required to tailor it to a particular machine.

Preprint copies of an upcoming Precision Engineering article on the improved model can be obtained by contacting Steven Phillips at (301) 975-3565, <steven.phillips@nist.gov> or Tyler Estler at (301) 975-3483, <tyler.estler@nist.gov>. The mailing address for both is NIST, B113 Metrology Building, Gaithersburg, MD 20899-0001.

#### **NEW STANDARD MAKES SENSE OF MICROCIRCUITS**

Work performed by NIST scientists has helped the Navy's ManTech program describe electronic circuit

packages in a computer-sensible form. One such assembly, the hybrid microcircuit, has many characteristics that are typical of both printed-wiring boards and integrated circuits. The NIST/Navy project has led to a new American National Standards Institute standard for the transfer of product data for these circuits.

The standard, expected to be published in May 1997 by the U.S. Product Data Association as "ANS US PRO/UPO-111-1996" should facilitate error-free transfer of electronic product data between computer-aided design programs via the Initial Graphics Exchange Specification. It also will improve electronic product data transfer between CAD and computer-aided manufacturing programs. The standard provides a means of data exchange that permits engineers to concurrently design electronic packages, including hybrid microcircuits, despite different, normally non-communicating CAD tools. In addition, the new standard reduces the chance of error between the design and manufacturing steps. For more information, contact Curt Parks, B343 Metrology Building, NIST, Gaithersburg, MD 20899-0001, (301) 975-3517, <curtis.parks@nist.gov>.

#### **FQA IMPLEMENTATION NOW SET FOR MAY 1998**

NIST has announced that the implementation date of the Fastener Quality Act of 1990 is being extended one year until May 26, 1998.

The FQA establishes a national program to protect public health and safety by ensuring that certain nuts, bolts and other fasteners used in critical situations (such as attaching aircraft engines to fuselages) conform to specifications. Its original implementation date of May 27, 1997, was contingent on having an adequate number of accredited laboratories to carry out fastener testing. To date, four organizations have applied to NIST's Accreditation Body Evaluation Program for approval to accredit laboratories that perform testing of fastener products and materials, and 42 laboratories have applied individually to NIST's National Voluntary Laboratory Accreditation Program for approval as fastener testers.

Since approximately 425 accredited laboratories are needed to carry out the FQA, NIST has determined that more time is needed to complete the accreditation process. Therefore, the date of implementation has been extended.

The Fastener Quality Act of 1990 protects public safety by (1) requiring that fasteners identified by the act conform to the exact specifications represented by the manufacturer; (2) providing for accreditation of laboratories engaged in fastener testing; and

(3) requiring inspections, testing and certification, in accordance with standardized methods for fasteners covered by the act.

For more information on the FQA, contact Subhas G. Malghan, Rm. 311, Building 820, NIST, Gaithersburg, MD 20899-0001, (301) 975-4500, fax: (301) 975-2183, <malghan@nist.gov>. Additional information is available on the FQA page of NIST's World Wide Web site at <<http://www.nist.gov/fqa>>.

### **READING GREEN TEA LEAVES FOR BETTER HEALTH**

Scientists have known for many years that people with diets high in certain foods are less likely than others to get certain types of cancers. Sorting out exactly what compounds in these foods and what amount of the food provide the apparent protective effect is a long-term, difficult undertaking.

Working in cooperation with the National Cancer Institute, NIST chemists have several ongoing projects contributing to this research, including a new effort to improve ways of measuring the concentration of catechins in blood plasma.

Catechins are compounds found in green tea and are thought to prevent certain human cancers. NIST chemists are developing methods to measure accurately concentrations of specific catechins in green teas using a variety of techniques.

The application of this research to the measurement of catechins in blood plasma should be useful to clinical researchers investigating links between tea consumption and cancer prevention.

For technical information, contact Jeanice Brown Thomas, B208 Chemistry Building, Gaithersburg, MD 20899-0001, (301) 975-3120, <[jeanice.brownthomas@nist.gov](mailto:jeanice.brownthomas@nist.gov)>.

### **KEEPING BABIES—AND THEIR PARENTS—BREATHING EASIER**

Researchers at NIST are assisting in the development of a new therapy for newborns with a serious breathing disorder. In collaboration with the National Institute of Child Health and Development, NIST chemists are evaluating measurement methods and developing standards for very low concentrations of nitric oxide and nitrogen dioxide in high oxygen environments.

Pediatric researchers have found that inhaled nitric oxide can be very beneficial to newborns with persistent pulmonary hypertension, a syndrome that can result from several serious cardiovascular conditions. However, a potential problem with the treatment is the formation of nitrogen dioxide when nitric oxide mixes

with oxygen. Nitrogen dioxide can cause additional respiratory problems if present in high enough concentrations.

Working with NICHD, NIST scientists have determined the rate of nitrogen dioxide formation under therapeutic conditions. Information from these collaborative studies helped assure pediatric researchers that clinical trials of the nitric oxide treatment were of safe design. Since clinical studies demonstrated favorable results, nitric oxide therapy is likely to become widely available.

### **NEW METHOD COMBINES QUICK IMAGING, CHEMICAL ANALYSIS**

Scientists have long relied on infrared spectroscopy as an analytical tool to identify the chemical components of an unknown sample. Likewise, they have used a variety of imaging techniques to study spatial relationships between chemical components. Now scientists at NIST have joined with a team at the National Institutes of Health to improve a system that combines infrared spectroscopy, an array detector, and microscopy to rapidly obtain sensitive spectral images of complex samples.

The new spectral imaging technique is being used to study biological samples, such as brain tissue, as well as advanced polymer composites. The imaging technique has many potential applications in industry and biomedical studies.

The advantages of infrared spectral imaging are its high data acquisition speed and spatial resolution—on the scale of 10  $\mu\text{m}$ . The new system produces images in about an hour that otherwise would be impractical. NIST holds a patent on the use of the detector for time-resolved chemical analysis. NIH holds the patent on the imaging approach.

### **KID-SIZED DATA GOES ONLINE**

Say you are starting a small business designing bicycle helmets for children, and you want to know the range of sizes to make for young cyclists. You have spent hours searching the Internet for some electronic data to plug into your computer-aided design software, to no avail. Now, your search is over.

Body measurement data gathered for a 1975 Consumer Product Safety Commission (CPSC) study entitled "Physical Characteristics of Children" now are available on a World Wide Web site called AnthroKids, located at <<http://www.nist.gov/itl/div894/ovrt/projects/anthrokids/>>. This information, the only public domain electronic database of child anthropometric data, should prove to be a valuable resource

for product designers of all types who are concerned with the safety of their products when used by children. This resource is due to a cooperative effort between NIST and the CPSC. NIST also is working with the University of Pennsylvania to incorporate the data into a software system for three-dimensional modeling of human form and movement. For more information, contact Sandy Ressler, A216 Technology Building, NIST, Gaithersburg, MD 20899-0001, (301) 975-3549, <sressler@nist.gov>.

### **NEW DEVICE DEBUTS FOR MEASURING THERMAL CONDUCTIVITY**

Composite ceramic materials and layer-coated ceramics have grown in use in the last decade. These materials are extremely valuable to industry because of excellent chemical and wear resistance, a wide range of electrical and thermal properties, and high service temperatures. Therefore, it has become essential to have reliable methods to measure their thermal conductivity and diffusivity.

A researcher at NIST has produced an absolute, steady-state device to measure thermal conductivity over the temperature range 400 K to 1400 K. Measurements are made in an atmosphere of low-pressure helium. Specimens are 70 mm in diameter with thicknesses between 1 mm and 8 mm. Internal heated components are composed entirely of high-purity aluminum oxide, boron nitride, beryllium oxide, and fibrous alumina insulation board. Pure nickel and thermocouple-grade platinum-based alloys are the only metals used in the system. The instrument has a combined measurement uncertainty of plus or minus 5 %.

Because of its complexity, the new NIST measurement device probably will not be used outside a research facility. However, it can provide primary data measurements needed to calibrate commercial instruments used in industry. It also will be useful for analyzing high-performance thermal-barrier coatings and complex high-temperature composites where direct comparison with known materials is not possible or potentially misleading. For a copy of paper no. 14-97 describing the NIST apparatus, contact Sarabeth Harris, Div. 104, NIST, Boulder, CO 80303-3328, (303) 497-3237, <sarabeth@boulder.nist.gov>.

### **EMMA AND THE ROBOCRANE CLEAN UP TOGETHER**

A Menlo Park, CA, robotics company, has teamed with NIST to prototype an innovative, remotely operated system for cleaning out underground nuclear waste storage tanks.

The system integrates the NIST-developed RoboCrane—a mobile, spider-like crane that agilely wields cargo or tooling platforms while positioning them with millimeter-level accuracy—with EMMA (for Easily Manipulated Mechanical Armature). EMMA is a long-reach manipulator, or robotic arm, that resembles an elephant's trunk in both appearance and dexterity. Its sinuous movements are controlled by a set of steel cables that activate individual stages in the arm. A 12 m version is now being evaluated at a NIST testbed. Measuring 0.6 m in diameter, it supports a 45 kg payload at full reach and carries a waste retrieval hose. To dislodge stubborn waste, an ultra-high-pressure waterjet is attached at the end of the arm.

Smaller EMMA prototypes have been successfully demonstrated with NIST's 6 m-tall RoboCrane. The unique crane can hold its work platform rigidly in place, even at an angle. It provides a stable base that permits EMMA to move around inside a tank and to perform cleanup tasks. For reaching into congested waste storage tanks, a 12 m EMMA would be mounted to a larger version of the RoboCrane—big enough to straddle underground tanks, which measure about 23 m across, and, therefore, avoid exerting forces on tanks of unknown structural integrity.

Besides addressing a national problem, the collaboration provides NIST with an opportunity to refine advanced intelligent control concepts. It also furthers NIST's efforts to advance standards and measurement techniques for intelligent machine systems. For more information, contact Roger Bostelman, B124 Metrology Building, NIST, Gaithersburg, MD 20899-0001, (301) 975-3426, <rbostelman@nist.gov>; or Robert Kent, GreyPilgrim, at (800) 365-3352, <pilgrim@greypilgrim.com>.

### **NIST AND AIST/JAPAN HOLD INFORMATION EXCHANGE**

The United States and Japan held the Second Joint Information Exchange Forum on standards and conformity assessment issues on Jan. 9-10, 1997, at NIST. These dialogues are aimed at building lasting relationships in mutual activities in the Asia-Pacific region.

A NIST spokesperson reviewed the NIST plan for implementing the Technology Transfer and Advancement Act of 1996, which requires NIST to play a leadership role in coordinating standards and conformity assessment activities with Federal, state, and local government agencies, and with the private sector to meet the needs of U.S. industry in the global marketplace. She also gave an overview on the proposed National Council for Laboratory Accreditation, a cooperative partnership between the public and private

sectors to provide a comprehensive U.S. laboratory accreditation infrastructure.

The Japanese delegation described recent developments in their standardization activities and the current status of their “Eighth Long-term Standardization Plan.” They presented background information on Japanese Industrial Standards (JIS), including the administration of the JIS mark approval system for mining and industrial products. JIS standards are voluntary national standards, similar to ANSI standards. They are developed in recognition of the increased importance of international standards in accordance with the Technical Barriers to Trade (TBT) Agreement of the World Trade Organization. A Japan spokesperson expressed their intention to develop the JIS mark for use in mutual recognition agreements between Japan and its trading partners.

Both the U.S. and Japan participants described their involvement in the Asia Pacific Economic Cooperation and their national laboratory accreditation programs, NVLAP and the Japan Calibration Service System. They also exchanged information on management systems applications, registration, and the accreditation of registrars as related to ISO 9000 and ISO 14000. An ANSI official gave an update related to the International Organization for Standardization and the International Electrotechnical Commission in Geneva. There were updates on the NIST fastener program and the criteria for accrediting foreign entities under the Fastener Quality Act of 1990.

#### **ENERGY-RELATED INVENTIONS PROGRAM MAKES RECOMMENDATIONS**

During January 1997, the NIST Office of Technology Innovation recommended two innovative technologies for commercialization to its Department of Energy partner under the Energy-Related Inventions Program.

The Hydrostatic Mooring—a mooring system for anchoring vessels in open seas having wave heights of up to 8 m.

An Efficient Compressor Valve—a patented compressor valve for use in positive-displacement gas compressors.

#### **NIST HELPS INDUSTRY TO EVALUATE A KEY GEOMETRICAL PARAMETER DESCRIBING OPTICAL FIBER CONNECTOR ENDS**

A recently completed study of geometrical parameters of optical fiber connectors provides dramatic evidence of the importance of appropriate definitions in determining a manufacturer’s ability to specify its product. As more optical fiber moves into the local loop, the

number of connections will greatly increase; the annual North American market for connectors is projected to be \$362 million by 1999.

A very important parameter specified for the connector is the amount of protrusion or undercut of the fiber end from the spherically polished ceramic connector ferrule. This parameter is typically less than 50 nm. A gap between fiber ends can lead to a reflection from the connector; for some demanding applications, the reflections must be less than –50 dB.

NIST scientists, working with members of the Telecommunications Industry Association (TIA), recently completed a round-robin study to evaluate potential candidates for a protrusion/undercut definition. At present, there is no recommended TIA definition. Two definitions were studied based on protrusion/undercut: (1) measured from the edge of the ferrule bore and (2) measured from a sphere fitted to the ferrule surface. The study involved 18 ferrules being circulated in series among 15 laboratories. Measurement specimens had protrusion (positive) and undercut (negative) values ranging from +65 nm to –330 nm. In total, 19 sets of data were analyzed to reveal a remarkable difference in performance between the two definitions. The spherical fit exhibited significantly improved precision over the edge definition. Of more concern were large systematic offsets of up to 100 nm observed among some of the participants for the edge definition. Further analysis suggests differences in edge-fitting algorithms may have accounted for the offsets. Systematic differences were not apparent for the spherical definition. Nearly all of the measurement methods used in the study involved some form of optical interferometry. The study is being expanded to include mechanical stylus measurements. The final result will be a recommended industry test procedure from the TIA.

#### **NIST REFERENCE SAMPLE RESPONDS TO MAGNETIC RECORDING INDUSTRY NEEDS TO COMPARE IMAGING METHOD CAPABILITIES**

In response to magnetic recording industry needs, NIST has developed and demonstrated a magnetic imaging reference sample that provides a method for comparing the capabilities of different magnetic imaging instruments and techniques. Nanoscale magnetic imaging is crucial in the development of advanced magnetic media, recording heads, and magnetic solid state memory. In particular, information on magnetization of structures is needed. Simple in concept, the reference sample consists of a 8 mm-sized piece of hard disk, which has a special magnetic bit pattern recorded on it. A series of fiduciary marks, in the form of 100 numbered frames, provide identification of the location of a given set of

magnetically written bits, so the user may compare images of the same set of bits produced by different means such as NIST's SEMPA (scanning electron microscope with polarization analysis), various forms of magnetic force microscopy, magneto-optical Kerr imaging, and Lorentz microscopy.

In one specific use, the reference sample provides a link between magnetic force microscopy measurements on media and the magnetization of that media. As its name suggests, the magnetic force microscope measures the force of attraction of a tip to media; these measurements can be calibrated in terms of measurements of the same media sample by SEMPA, which images the magnetization directly. Reference samples have been sent to a number of potential users for evaluation. These include manufacturers of scanned-probe microscopes, magnetic force microscopes, and magnetic disk drives, together with university laboratories. NIST will determine the next step depending on the results of these evaluations. Industry has indicated an interest in having NIST make the reference sample available for sale.

#### **IMPROVEMENTS REALIZED IN THE AWAMS SIGNAL PROCESSING ALGORITHMS**

The Automatic Waveform Analysis and Measurement Systems (AWAMS) are commercial 20 GHz bandwidth, high-speed, equivalent-time sampling oscilloscopes interfaced to desk-top computer systems and used for providing the NIST pulse waveform measurement services (Test Numbers 65 100S – 65 400S). Special NIST-developed software programs provide the processing needed to acquire the measurement data, to make corrections based on both time and amplitude calibrations, and to perform signal processing operations on the data to reduce the hardware limitations of analog bandwidth, noise, time-base jitter, etc. Recent research on the algorithms used in the AWAMS has resulted in improved software that eliminates the prior requirement for operator judgment, for example, in coping with the effects of local minima that may interfere with computational convergence, and thus reduces the uncertainty attributed to the NIST signal processing software.

In one phase of this work, a NIST scientist examined the histogram method used for obtaining pulse parameters; the results showed that pulse parameters (transition duration, amplitude, overshoot, undershoot, etc.) can be sensitive to the number of histogram bins and that using a fixed number of bins is not desirable. An optimizing histogram algorithm was developed and written that searches for stable regions in the pulse parameters. This algorithm was tested on four step-like waveforms that are representative of the pulse trains

typically recorded using the AWAMS. In each case, the optimizing algorithm selected histograms for which the pulse parameters were least affected by the number of histogram bins.

In a second phase of this work, a visiting guest scientist from the Technical University of Budapest, researched optimal waveform deconvolution approaches for implementation in the AWAMS. The guest scientist and the NIST scientist compared the performance of four different deconvolution algorithms, and implemented them as LabVIEW™ software virtual instruments (VIs), which can be called by the LabVIEW™ main control program. Work also was carried out on estimating the uncertainties of the guest scientist's model-based deconvolution process. It was found that bounds on the reconstructed spectrum can be determined with reasonable confidence and an estimate provided of the signal-to-noise ratio. Bounds on pulse parameter estimates can be obtained from the pulse parameters derived from the inverse Fourier transforms of the spectral bounds. A grant was established for the Technical University of Budapest so that the guest scientist can pursue this deconvolution work further in Hungary.

#### **NIST HOSTS ION IMPLANT USERS GROUP MEETING PRESENTING INFORMATION ON ALTERNATIVE SOURCES, THIN-FILM METROLOGY**

NIST recently hosted a meeting at Gaithersburg of the NIST-sponsored Ion Implant Users Group that provided information on commercially available ion-implantation services and on NIST's perspective on challenges to thin-film metrology. Ion implantation is now the principal means for introducing dopants in semiconductor processing.

The meeting first considered ion-implantation services that ion implant users could call on as alternatives to using their in-house systems. Selection of this topic was motivated by the interest on the part of members of the group in identifying facilities capable of (1) carrying out custom ion implants, for example, when their own ion-implantation systems were unavailable as a result of high workload, and (2) providing ion-implantation services in the development of a process sequence for a new device. Members of the group also wanted to identify facilities that have implant capability for elements that fall outside the realm of the usual dopants for semiconductor manufacture. Representatives from four facilities that offer ion implantation services gave technical presentations on issues concerning implantation into semiconductor materials, other ion/substrate targets, specialized equipment and procedures, and interesting and novel applications, as well as on characterization and modeling capabilities.

For the second topic, a NIST scientist gave a presentation on "Challenges to Thin Film Metrology." She discussed selected issues in the measurement, analysis, and use of standards in the characterization of thin dielectric films, such films being a crucial element in the fabrication of semiconductor devices. Advances in metrology are especially critical to achieving the thinner dielectric films called for by the Semiconductor Industry Association's National Technology Roadmap for Semiconductors in future generations of devices such as dynamic random-access memories. A workshop on this topic, is scheduled for Oct. 30–31, 1997, at NIST Gaithersburg.

### **SWITZERLAND JOINS INTELLIGENT MANUFACTURING SYSTEMS; EUROPEAN COUNCIL APPROVES MEMBERSHIP**

The European Council approved Intelligent Manufacturing Systems (IMS) membership for the European Union (EU) at its Jan. 27, 1997, meeting and authorized the necessary exchange of letters. This represents the penultimate step in the EU's joining IMS as a full participating region. The council's approval of IMS membership comes two years after the conclusion of the IMS feasibility study. Several months earlier, Switzerland joined as an official participating region. While not a member of the EU at the present time, Switzerland may convert its IMS membership into the full EU membership in the future. The Swiss already have submitted two project abstracts, which is a good indicator of their enthusiasm for the IMS program. The news of these additional members makes this an exciting time for all IMS participating regions. The office of the U.S. IMS Secretariat is located at NIST.

### **MEASURING PROTEIN ELECTRON TRANSFER RATES USING ELECTROREFLECTANCE SPECTROSCOPY**

Electron transfer in and between proteins is one of the hot topics in theoretical biochemistry and in biocatalysis. New measurement techniques are needed to establish parameters for such theoretical analyses as Marcus theory, and to improve the efficiency of reducing power utilization in industrial biocatalysis. In recent work NIST scientists have developed a new technique called electromodulated reflectance (electroreflectance) spectroscopy for measuring the heterogeneous electron transfer rate constant between the iron-sulfur protein putidaredoxin and silver electrodes. This protein is representative of the kinds of electron transfer proteins found in enzyme systems that mammals use to metabolize fats and detoxify xenobiotics, and in industrial bio-

catalytic processes such as the synthesis of indigo dye. These new measurements indicate that electron transfer may be up to two orders of magnitude faster than previously measured by the classical technique of cyclic voltammetry. This work will appear soon in the Journal of Colloid and Interface Science; meanwhile the investigators have begun to use electroreflectance spectroscopy to study other redox proteins and to incorporate the synchrotron uv light source at SURF II. They hope to learn if multiple routes of electron transfer exist between the protein and the electrode or if some new previously unrecognized mechanism is involved in transferring electrons into protein redox centers.

### **ELECTRICAL OPTIMIZATION OF FLUORINATED GAS PLASMAS**

A private company and NIST have developed new methods for optimizing processes and equipment used to generate plasmas in fluorinated gases. Fluorinated gas plasmas are used widely in the semiconductor industry to etch silicon, silicon dioxide, and silicon nitride films. They also are used to clean the plasma-enhanced chemical vapor deposition reactors that are used to deposit these films. Deposits on the reactor surfaces must be removed periodically; if the deposits become too thick they will generate particles that can contaminate the substrates. Fluorinated gas plasmas offer a means of removing the deposits in situ, without disassembling or venting the reactor.

To be commercially successful, any chamber cleaning process must be extremely rapid, which would appear to require high pressures of the reactive fluorine species. Previous studies, however, have shown that the etch rate of deposited materials is often increased by lowering the total pressure and diluting the fluorine-containing species. By optimizing these operating conditions, maximum etch rates can be obtained with the additional benefits of significant savings of reactant materials and reduced effluents. Unfortunately, optimum process conditions vary unpredictably from reactor to reactor.

In recent experiments, conducted at the private company, the optimization of  $\text{NF}_3/\text{Ar}$ ,  $\text{CF}_4/\text{O}_2/\text{Ar}$ , and  $\text{C}_2\text{F}_6/\text{O}_2/\text{Ar}$  plasmas was studied with optical emission spectroscopy and radio-frequency electrical measurement techniques developed at NIST. The experiments showed that previously observed local optima in etch rate are explained by electrical effects. It was found that the impedance of the discharge was strongly dependent both on the overall gas pressure and the concentration of the fluorine containing species. Local optima occurred at gas pressures and concentrations at which the power losses in the plasma were minimized, and the power most efficiently coupled into energetic plasma electrons,



electrons, which, in turn, create the reactive species necessary for chamber cleaning. This behavior is quite general; it was observed for all gas mixtures studied, and it can be represented by a simple equivalent circuit model.

The generality of these results suggests that measurements of the plasma electrical impedance can simplify greatly the task of finding and maintaining optimal reactor cleaning processes, even in reactors or gases different from those studied here. The results also suggest methods to improve the design of the reactors and the circuitry that powers them, to minimize power losses in the external circuitry, and thus to obtain further improvements in etch rate and efficiency. By allowing electrical effects to be distinguished more easily from purely chemical effects, this work also provides a firmer foundation and a better defined basis of comparison for studies of other plasma chemistry issues, such as the need to reduce the global warming effects of plasma effluents.

#### **AEROSOL MINERALIZATION OF CHLOROFLUOROCARBONS BY SODIUM VAPOR REDUCTION**

Scientists at NIST have developed a new method for the destruction of chloro-fluorocarbons (CFCs). The process consists of mixing vapor-phase CFCs with a vapor of elemental sodium at atmospheric pressure and 800 °C in an exothermic single-pass process. The thermochemically preferred Na-halide mineral and elemental carbon are efficiently produced from this process. The process has demonstrated high destruction efficiencies (greater than 99 %) for a surrogate CFC (CF<sub>4</sub>) as well as high efficiency (mass balances within 99 %) for the formation of the equilibrium predicted products of reaction: benign salt coated carbon aerosols, large enough to be filtered with existing filtering technologies, with no volatile products. The rapidity of the chemistry and condensation process and the low cost of sodium should enable the construction of industrial-scale reactors that are fairly small and economical to build and operate. Potential applications of this chemistry would be toward destruction of CFC stockpiles and as a treatment of the effluent of plasma reactors used in semiconductor processing.

#### **THERMODYNAMICS OF CYCLODEXTRIN SYNTHESIS**

Cyclodextrins are of increasing importance to the technology of drug delivery systems, separations, and foods. At present, approximately  $6 \times 10^6$  kg of these substances (commercial value approximately \$60

million) are manufactured from starch using enzyme cyclomaltodextrin glucanotransferase. There are three principal cyclodextrins in use, namely, alpha-, beta-, and gamma-cyclodextrin. These are cyclic substances that contain, respectively, 6, 7, and 8 D-glucopyranose molecules joined by alpha-1,4 linkages.

Two scientists at NIST have completed a chromatographic and calorimetric investigation of the hydrolysis and cyclization reactions of these cyclodextrins. They used these techniques to measure equilibrium constants for the cyclization reactions and enthalpy changes for the hydrolysis reactions. These results were combined with results from the literature to obtain a relatively complete picture of the thermodynamics of these reactions. The thermodynamic quantities obtained allow one to predict the position of equilibrium and the enthalpy changes (energy balance) for both the hydrolysis and cyclization reactions. This is essential engineering data that can be used to examine the efficiency of current and proposed processes for the manufacture of these and other closely related substances. The results of this study will be published in *Carbohydrate Research*.

#### **BIOMIMETIC SURFACES FORMED FROM CELL MEMBRANES**

The biological cell membrane is the site of a myriad of important functions in living organisms, and reconstituting these functional materials has led to the development of a number of examples of model cell membranes. Rugged planar model bilayer membranes fabricated from alkanethiol monolayers and phospholipids are being studied at NIST as research tools for protein/lipid structural studies and for use in applications such as sensing and bioremediation. Recent work indicates that using this approach, very complex bilayers can be fabricated from cell membrane preparations. The resulting asymmetric cell membrane hybrid layer was characterized by ellipsometry, surface plasmon resonance (SPR), contact angle, capacitance, voltammetry, and electron and atomic force microscopies. The erythrocyte membrane layer was measured to be about 3 nm to 4 nm in thickness, suggesting that a single lamella of cell membrane adds to the hydrophobic alkanethiol surface. Using SPR, the NIST researchers demonstrated the presence of erythrocyte components on the surface by their selective removal by enzymatic action. They also demonstrated the presence of a contiguous layer of membranous material on the substrate by electron and atomic force microscopy. Demonstration of acetylcholinesterase activity, a membrane anchored enzyme, suggests that the outer leaflet of that enhanced electron transport from a solution redox species accompanies formation of the

erythrocyte layer at the surface. This enhanced electron transport indicates that a transmembrane erythrocyte anion transporter protein, Band 3 protein, is incorporated into the surface layer in an active conformation. This work was performed in collaboration with Roswell Park Cancer Institute, Center for Cellular and Molecular Biology, Hyderabad, India, and NIST.

#### **INFRARED DETECTOR ARRAYS FOR TIME-RESOLVED SPECTROSCOPY**

Time-resolved infrared (IR) spectroscopy is the principal method used for identifying the chemical species present and for measuring their concentrations while chemical reactions are under way. It is possible to measure the transformations of reactants from their initial form through transient intermediate species to final products, because each of these has its own characteristic spectra (determined from the characteristic vibrations of each species) at mid-infrared wavelengths (2  $\mu\text{m}$  to 11  $\mu\text{m}$ ). By obtaining a sequence of instantaneous “snapshots” of spectra with appropriate spectral and temporal resolution, one can understand, and ultimately hope to engineer, the reaction mechanisms in complex, condensed-phase chemical systems.

This approach has been limited until now by use of narrowband light sources (which address only one possible molecular vibration at a time) and single element detectors (which can be used for only one wavelength slice of the spectrum at a time). However, researchers at NIST have demonstrated a new measurement method, exploiting broadband femtosecond infrared pulses and IR focal-plane detector arrays, which results in vastly superior data and much faster data acquisition rates. The researchers employed two  $256 \times 256$  pixel mid-infrared detector arrays that were originally designed for DoD projects, but which are now available for civilian applications.

In femtosecond time-domain vibrational spectroscopy, two broadband infrared probing pulses are transmitted through a sample as probe and reference pulses. The bandwidth of these pulses is sufficient to interact with several different molecular vibrations. At a variable time prior to IR probing, a chemical reaction is triggered in the sample by a tunable ultraviolet, visible, or infrared pump pulse. The probe and reference pulses emerging from the sample impinge on an indium antimonide (InSb) or mercury cadmium telluride (MCT) detector array behind an infrared spectrograph, yielding broadband vibrational spectra of the sample as a function of the time delay between the pump and infrared pulses.

This new apparatus achieves high signal-to-noise and spectral acquisition rates and was used to analyze ultrafast solution-phase hydrogen-bond dynamics, vibrational energy transfer, and photochemical reaction

kinetics. These examples illustrate a wide range of industrial and biochemical applications for this improved research and analytical technique.

#### **NEW HALF-LIFE VALUE FOR THE PET RADIONUCLIDE $^{62}\text{Cu}$ DETERMINED**

Positron emission tomography (PET) is an advanced medical imaging technique that can measure cardiac and brain function. The radiopharmaceuticals administered to the patient have short half-lives, which must be known precisely to compute the proper dose and to assure meaningful results.

One of the new radiopharmaceuticals under investigation is  $^{62}\text{Cu}$  pyruvaldehyde bis( $\text{N}^4$ -methyl) thiosemicarbazone ( $^{62}\text{CuPTSM}$ ). The currently recommended evaluated nuclear structure data file (ENSDF) value for the half-life of  $^{62}\text{Cu}$  is  $9.74 \text{ min} \pm 0.02 \text{ min}$ . However, during a recent calibration of solutions of  $^{62}\text{CuPTSM}$  performed by scientists at NIST, it became apparent that the true half-life is shorter than this value. For this reason, a set of experiments was devised to determine a more accurate value of the half-life.

Using the NIST  $4\pi\gamma$  Ionization Chamber and  $4\pi\beta$  liquid scintillation counting, new half-life values were determined with excellent agreement (0.07 %) between these two techniques. A weighted average of these determinations gives an overall value of  $9.67 \text{ min} \pm 0.03 \text{ min}$ —a difference of  $-0.7 \%$  from the ENSDF value.

The results of this investigation are being prepared for publication in the Journal of Physics G: Nuclear and Particle Physics. This new information will help assure patient safety and provide better quantitative results when using  $^{62}\text{CuPTSM}$  as a PET agent.

#### **INNOVATIVE NEUTRON INTERFEROMETER DESIGN ACHIEVES RECORD PERFORMANCE**

At the NIST Neutron Interferometer and Optics Facility, test samples are placed in one arm of a neutron interferometer. Measured changes in the interference pattern are used to determine characteristics of the samples. Unprecedented performance of single-crystal silicon, neutron interferometers was first demonstrated at NIST in April 1994.

Now, even more remarkable performance has been achieved by innovations in interferometer design and fabrication. In the past, neutron interferometers were machined from single-crystal silicon ingots so neutrons would reflect from lattice planes with the Miller indices (2,2,0). However, NIST scientists designed and built two new large interferometers that use lattice planes with (1,1,1) indices. This choice of crystal orientation makes the interferometers more suitable for use with the

long-wavelength neutrons available from the NIST Cold Neutron Research Facility, and this choice also eliminates first-order contamination from neutrons with a wavelength of half the nominal value.

The results were nothing short of spectacular: fringe visibility near 90 % was achieved at the best points, and a large area with fringe visibility exceeding 70 % was mapped. This large area with stable high performance ensures the possibility of making neutron phase-contrast images of objects as large as 25 mm in diameter.

To date, the most important accomplishments with this facility have been high-accuracy neutron-nuclear scattering-length measurements, and high-resolution neutron radiographs of an operating hydrogen fuel cell. The scattering-length measurements provide a new standard of accuracy for nuclear data and will contribute to fundamental understanding of the interaction of neutrons with electromagnetic and nuclear forces. The fuel-cell radiographs are helping engineers in industry perfect a new generation of fuel cells for low-pollution automobiles. These improvements will reduce the measurement uncertainties in such projects and open up new avenues of research not previously possible.

#### **NIM/VME INSTRUMENT STANDARD PUBLISHED**

The U.S. Department of Energy National Instrumentation Methods (NIM) Committee, chaired and managed by a NIST scientist, has issued a draft standard, NIM/VME-P 9612, VMEbus for Physics Applications: Implementation Rules, Recommendations, and Guidelines (<http://www-vipa.fnal.gov/vme-p/web/draft04/htframe.htm>).

The Versabus Module Eurocard (VME) standard is a computer and electronics standard widely used in science and industry. It has the support of many companies that provide large volume production and a wide variety of devices, but it has many shortcomings that have been troublesome in precise measurement applications. For example, noise from a shortage of ground pins was a problem for sensitive analog circuits. In this new effort, physicists from North America, Europe, and Japan united to extend the VME standard for the benefit of the physics community in such areas as data acquisition, front-end instrumentation, and accelerator controls.

NIM/VME-P 9612 is both a specification and a guide and is oriented to both manufacturers and users. While this release serves the immediate need to begin implementation of the standard, the committee is proceeding to reorganize its contents for high readability. It will submit the reorganized document as VITA 23-199x for processing as a U.S. standard of the American National

Standards Institute and as an international standard of the International Electrotechnical Commission.

The Department of Energy NIM Committee was organized more than 30 years ago to produce the first NIM instrumentation standard. That committee was proposed, chaired, and managed by NBS. Though the NIM standard was produced for the nuclear field (thus the original acronym, nuclear instrument module), its rapid acceptance and spread into other areas of science and technology has made the name misleading. It is now simply known as NIM. NIM instruments continue to be produced and utilized in great number.

The new standard builds on previous ones and enables a new generation of compatible instruments to be designed and marketed by many vendors. An independent economics survey conducted several years ago for the Department of Energy concluded that the popularity and reach of the NIM system has resulted in savings of several billion dollars by U.S. Government laboratories, which were saved the expense of custom-designing the electronics for a myriad of different projects. It is hoped that the new standard will have a similar impact in science and for industrial electronic instrumentation.

#### **IMPROVEMENTS TO THE ELECTRODEPOSITION OF ALUMINUM FROM ROOM TEMPERATURE MOLTEN SALTS**

Aluminum is an excellent protective coating for other metals and alloys due to its low density and high corrosion resistance. Today, there are various methods available for coating workpieces with aluminum. These include thermal spray, hot dipping, roll bonding, mechanical plating, physical/chemical vapor deposition, and electrodeposition. Of these techniques, only electrodeposition offers the potential of coating complex shapes at high deposition rates. The electrodeposition of aluminum must be carried out from nonaqueous solvents because in aqueous solutions hydrogen is evolved before aluminum can be deposited. A number of nonaqueous solvent/electrolyte systems have been examined for the low temperature electrodeposition of aluminum. Among these is the room-temperature melt obtained by combining  $\text{AlCl}_3$  with 1-methyl-3-ethylimidazolium chloride (MeEtimCl). Although aluminum can be electrodeposited from this and similar room temperature electrolytes, deposit quality is often poor and  $\text{Cl}^-$  impurity levels are generally high. In collaboration with a University of Mississippi professor, NIST researchers have determined that the addition of benzene (at levels ranging from 5 % to 50 % volume fraction) to a 60:40 mole ratio  $\text{AlCl}_3$ :MeEtimCl electrolyte tends to decrease the kinematic viscosity of the melt while significantly increasing the specific

conductance. These modifications to the melt dramatically improve the morphology of the aluminum electrodeposit and virtually eliminate  $\text{Cl}^-$  impurities. Electrodeposits produced from such melts exhibit a grain size on the order of 5  $\mu\text{m}$  to 15  $\mu\text{m}$  and have preferred (110) crystallographic orientation. Future efforts will focus on the potential benefits of alternative, environmentally friendly cosolvent systems.

### **IMPROVED ANALYSIS OF HEAT PROPAGATION IN STRATIFIED MEDIA**

Materials systems consisting of two or more layers of different materials, often called stratified media or multilayers, are technologically important for devices such as integrated circuits, optical interference filters, and compact disks. The fabrication and performance of such systems frequently depend on the propagation of heat through the system. Modeling heat propagation through multilayers requires both analytical models of heat propagation and knowledge of the thermal conductivity or thermal diffusivity of the component materials. Thermal waves, which are temperature fluctuations induced by heating with time varying sources such as laser beams, are used frequently both to probe non-destructively for subsurface defects, such as delaminations, and to measure the thermal conductivity or thermal diffusivity of the material components. For proper interpretation of experimental results, calculations that model the experimental conditions are needed and a one-dimensional solution to the thermal diffusion equation forms the basis of many of these models. NIST scientists have developed a modification of a commonly used matrix algorithm that significantly simplifies the solution to the thermal diffusion equation needed for interpreting thermal wave experiments in stratified media. The method is described in a report, NISTIR 5928, Algorithm for Solutions of the Thermal Diffusion Equation in a Stratified Medium with a Modulated Heating Source.

### **NONLINEAR ULTRASONIC TECHNIQUES FOR MICROSTRUCTURAL CHARACTERIZATION DEVELOPED**

Knowledge of a material's microstructure and its relation to performance-related properties is crucial in many industrial applications. NIST is developing nonlinear ultrasonic tools to characterize these microstructural properties. In principle, nonlinear ultrasonics can probe many fine microstructural details more sensitively than conventional ultrasonics. In an essential part of this program, specialized electronics have been obtained through a collaboration with a private

company. Prototype instrumentation has been evaluated by NIST in a series of preliminary experiments over the last year. A beta version incorporating the findings was delivered to NIST; beta testing then will proceed prior to the company commercializing it. Other test participants are researchers at the Johns Hopkins University and NASA-Langley Research Center.

At NIST, the private company's instrumentation is used in conjunction with a Michelson interferometer to measure absolute ultrasonic displacements. Interferometric detection is inherently noncontacting, possesses micrometer-scale resolution, and has the potential to scan large, curved areas quickly. Finite-amplitude ultrasonic waves are launched in a specimen, and the amplitudes of the transmitted fundamental and second harmonic components are measured for comparison with model predictions. Work is under way at NIST to relate nonlinear ultrasonic behavior to bulk microstructural features such as precipitates in steel. Future plans include examination of nonlinear effects in coatings and other engineered surfaces to characterize properties such as adhesion or wear resistance.

### **PATENT ISSUED FOR SENSING SOLIDIFICATION OF CASTING X-RAY DIFFRACTION**

A U.S. patent has been issued for a transmission x-ray diffraction (XRD) technique, which may be used, in real time, to locate and follow the solidification front in single-crystal investment castings. The concept is to use high-energy x rays (100 keV to 320 keV) to penetrate the mold and casting. Since the x-ray diffraction patterns from the molten metal and crystalline solid differ markedly, it is easy to identify the solidifying region of the casting. The XRD sensing technology is also capable of profiling the fraction solid within the dendritic region of solidification of alloy castings. Feasibility of the sensor was proven on samples of aluminum and copper in a gradient furnace, where it was found that the liquid-solid boundary could be identified easily, even though the samples were surrounded by a mold wall and encased in a furnace.

Recently, the XRD sensor has been tested successfully on a small industrial turbine blade casting furnace. The sensor detected, in real time, the position of the liquid-dendrite-solid region of a nickel-alloy casting during directional solidification and provided data on the proportion of the solid and liquid phases. The high energy x rays (up to 320 keV) produced abundant in-furnace transmission diffraction from a nickel alloy casting, even though the x-ray path through the furnace included furnace ports, the ceramic hot zone of the furnace, and mold material encasing the specimen.

### **NANOCOMPOSITES: A NEW FLAME RETARDANT APPROACH**

A significant reduction in heat release rate without any increase in carbon monoxide and soot production of nylon-6 clay-nanocomposite was found recently by NIST scientists. A clay mass fraction of only 5 % reduced heat release rate by about 65 % even at the high external heat flux of 50 kW/m<sup>2</sup>. Not only is this a very efficient flame retardant system, it does not have the usual drawbacks associated with other flame retardant additives. The physical properties are not degraded by the additive (clay); instead they are greatly improved. Investigation of the mechanism of flame retardancy in clay and other nanocomposite materials is in progress.

### **EXPERIENCE ABOARD THE NASA DC-9 REDUCED GRAVITY AIRCRAFT**

A project to study the combustion of a polymer sphere at reduced gravity is being conducted by NIST scientists. The project is funded by NASA. The objective of the study is to understand the fire hazard associated with combustion in a low gravity environment. In particular, average burning rates will be measured under different oxygen concentrations and total pressures. Reduced gravity (approximately 0.01 g with a duration of about 20 s) is achieved during a parabolic maneuver of the NASA DC-9 Reduced Gravity Aircraft, followed by an approximately 1.8 g pull-up. So far, several flight experiments have been performed successfully. Preliminary results indicate the hazard associated with the spluttering of burning molten polymer in reduced gravity is more severe than at normal gravity. The experimental package was designed by NIST scientists. The experiment is highly automated to facilitate success in a challenging environment, where experimental operators are often nauseated and disoriented.

### **NIST FIRE MODEL USED IN DESIGN OF SWISS TUNNELS**

The Ecole Polytechnique Federale de Lausanne has selected CFAST for use in safety design calculations for automobile and train tunnels in Switzerland. CFAST was chosen in part because they feel it is less prone to user error than other models they have tried. The CFAST (Consolidated Model of Fire Growth and Smoke Transport), developed by NIST, is a zone type fire model that predicts the environment in a structure subjected to a fire. International acceptance of CFAST and other NIST models is evidence of the usefulness of the safety technologies provided by NIST worldwide.

### **A PROTOTYPE COMPUTER-INTEGRATED KNOWLEDGE SYSTEM FOR PREDICTING THE SERVICE LIFE OF REINFORCED CONCRETE EXPOSED TO CHLORIDES**

A prototype computer-integrated knowledge system (CIKS) developed by NIST scientists was described in the December 1996 issue of Concrete International. The CIKS demonstrates a pioneering use of the World Wide Web to disseminate knowledge on complex topics in the material science of concrete to the construction industry. The CIKS integrates a number of NIST's computational material science models into a coherent system for solving a complex problem, viz., predicting the life of a reinforced concrete structure in which diffusion of chloride ions to the reinforcing steel is the main life-determining factor. Starting from a knowledge of the required strength, slump (a measure of the flow properties), and the volume of entrained air to provide adequate frost resistance, the system determines the proportions of the ingredients in the concrete mixture, predicts the chloride ion diffusivity coefficients for the hardened concrete, and goes on to predict the ingress profiles or time-to-corrosion-initiation for a reinforced concrete exposed to a specific chloride-containing environment. The prototype illustrates the high potential of employing a CIKS to aid a designer in the selection of the concrete to be used in a given reinforced concrete application. A variety of mixture proportions can be evaluated quickly for their expected service life when chloride-ion-induced corrosion is likely to be the dominant degradative mechanism; the CIKS also can be used to assess the susceptibility of a massive concrete structure to thermal cracking as a result of the essentially adiabatic temperature rise due to evolution of the heat of hydration of the cement.

Two major extensions of the prototype system are planned. In the first, an online system for assisting in optimization of the mixture proportioning process will be developed. In the second, the service life predictions will be extended to other degradation mechanisms, including sulfate attack and leaching of soluble species.

### **NIST DEVELOPS MEASUREMENT METHOD FOR LEAN FLAMMABILITY LIMITS OF REFRIGERANTS**

The refrigeration industry is examining new refrigerants as chlorofluorocarbons are being phased out due to their harmful effect on stratospheric ozone. Some of the new candidates are flammable. While some of these are being used in the pure state, the more flammable chemicals are often blended with nonflammable partners to

reduce fire hazard. The current standard test method for measuring the flammability of either pure chemicals or blends is time consuming to operate and has a high degree of uncertainty, especially for weakly flammable refrigerants. Under sponsorship of the Air Conditioning and Refrigeration Technology Institute, NIST scientists have developed a new, robust, and rapid method for measuring the lean flammability limit of the refrigerant in air, aimed at each other. A planar flame forms where they meet. As the fraction of refrigerant is reduced, the flame weakens and then extinguishes. The lean limit is determined as the minimum fraction of refrigerant in the mixtures before the flame goes out. The measurements are performed at different flow velocities and extrapolated to zero velocity, and the resulting value is a basic property of the refrigerant. The uncertainty for difluoromethane is about 5 %. The findings are being published in *Combustion and Flame*, the journal of the Combustion Institute.

#### **NEW PUBLICATION DESCRIBES EFFICIENT NEW SEARCH ENGINE**

Locating relevant information on the World Wide Web is often difficult because of the large amount of information available. NISTIR 5954, *RISQ: A Web-Based Tool for Referencing Information on Software Quality*, describes a new search engine designed to allow the user to do efficient searches for information within a specific domain.

The initial application of the engine is in the domain of high integrity software systems. The Reference Information for Software Quality (RISQ) system was developed by NIST and a private company. The search engine allows searches by taxonomy-based keywords, other keywords, and artifact type. Artifacts can range from simple abstracts, documents, and software to video, audio, and online interactive demonstrations of software tools. The RISQ facility makes available a wide variety of artifacts related to software quality in a highly organized manner. The current RISQ facility is located on the web at <http://hissa.nist.gov/risq/>. By putting the facility on the web, NIST makes the material available to a large and geographically diverse set of potential users.

#### **INFORMATION TECHNOLOGY REPORT**

NISTIR 5938, *Information Technology Laboratory Technical Accomplishments 1996*, describes the programs and achievements of the NIST Information Technology laboratory, gives overviews of its eight technical divisions, and highlights its products, services, and interactions with industry in 1996. The report emphasizes the laboratory's focus of developing tests

for information technology to accelerate the development of quality products, as well as high-quality advanced standards, early in their development cycles. The report is available online at <http://www.nist.gov/itl/lab/nistirs/>, click on NISTIR 5938.

#### **TEN ADDITIONAL FEDERAL IMPLEMENTATION GUIDELINES FOR ELECTRONIC DATA INTERCHANGE ISSUED**

NIST recently published 10 new guideline documents in NIST Special Publication Series 881 for Federal Electronic Data Interchange (EDI) Conventions. Dealing with the procurement and finance areas, the new NIST Special Publications 881-10 through 881-19 bring the total number of ICs issued to date to 19 documents.

NIST was designated as the organization responsible for coordinating the development of Federal Implementation Conventions (ICs) for EDI. ICs are defined by functional-area experts who create and select options from standard EDI Transaction Sets to yield the implementations to be used for practical electronic data interchange. These ICs are made available to Federal agencies and industry by electronic and paper means.

#### **WORLD'S TIMEKEEPERS NOT SECOND GUESSING ON JUNE 30**

Though your summer this year may seem all too short, it will actually be the longest one since 1994. One extra second, a little bonus to allow the world's atomic clocks to be synchronized to the spinning Earth, was added at the end of June. The 21st leap second since 1972 was inserted at 23:59:60 UTC (7:59:60 p.m. EDT) on June 30, 1997.

Leap seconds are needed to keep atomic clocks (such as the NIST-7 in Boulder, CO, and the U.S. Naval Observatory clock in Washington, DC, which are so accurate that they lose or gain less than a millionth of a second in a year) in step with the Earth's rotation, which varies several thousandths of a second per day. Since we cannot speed up the Earth, we have to slow down the clocks to keep them "in sync." In effect, this is done by stopping the clocks every year or two for exactly one second to let the Earth catch up.

For most people, a single second here or there doesn't matter much. But for some, a second is a big deal. Modern television, telephone and other telecommunication systems; marine and aviation navigation systems; computer networks; electric power grids; and multitudes of scientific applications are some of the kinds of activities that depend on very precise time and frequency. Many of these will have to be adjusted for the leap second to maintain synchronism with the rest of the world.

### **NEW ADDITIVE ALLOWS HARD POLYMERS WITHOUT SHRINKING**

Most plastics shrink during the curing process used to make them. The liquid starting materials for making plastic contain short molecules called monomers. The monomers link together in long chains called polymers during curing, and the volume of the plastic shrinks as it hardens. This is very good if you are making shrink wrap for protecting products and very bad if you are making dental restorations. With too much shrinkage, a polymer tooth filling will develop gaps and will no longer adhere to the tooth.

NIST materials scientists have developed an inexpensive "one pot" process for making a chemical additive that can help prevent polymer shrinkage. The chemical is a special kind of monomer that expands as it hardens. The monomer starts out with a ring structure that opens to form long, crosslinked chains during solidification. By adding some of these "spiro orthocarbonate" monomers to traditional dental monomers, the researchers produced a composite material with very low shrinkage and good mechanical strength.

The new monomers also may be useful for making more reliable adhesive coatings and microelectronics packages. For technical information, contact Jeffrey Stansbury, A143 Polymer Building, NIST, Gaithersburg, MD 20899-0001, (301) 975-6790, <jeffrey.stansbury@nist.gov>.

### **NEW REPORT HIGHLIGHTS FIREFIGHTER SAFETY OPTIONS**

Firefighters are just as vulnerable as the occupants in burning buildings; about 6000 firefighters suffer serious burn injuries annually. This grim statistic has not changed in 2 decades despite substantial improvements in protective clothing and equipment.

In June 1996, firefighters, industry representatives, and NIST fire experts met to seek improvements in firefighter safety. The report from that meeting, Firefighter Thermal Exposure Workshop: Protective Clothing, Tactics and Fire Service Personal Protective Training Procedures (NIST Special Publication 911), is now available.

Among the proposals covered in the report are: developing a standardized fire severity scale that could be used to recognize conditions where protective clothing and equipment will not provide adequate protection; identifying the mechanics of heat transfer in which contact with hot surfaces and thermal gases burn even a firefighter wearing protective clothing; designing protective clothing that can be quickly donned or removed; and creating a standard risk analysis method for buildings and contents.

A single copy of NIST SP 911 is available from James Randall Lawson, B366 Polymer Building, NIST, Gaithersburg, MD 20899-0001, (301) 975-6877, <james.lawson@nist.gov>. Multiple copies may be obtained from the National Technical Information Service, Springfield, VA 22161, (703) 487-4650, fax: (703) 321-8547, <orders@ntis.fedworld.gov>. Order by PB 97-153712.

### **INTERNATIONAL MEETING FOCUS: ENTERPRISE INTEGRATION**

NIST is working with the CIMOSA Association, a European organization of firms and research concerns, to help clear the way for an international agreement on actions key to integrating manufacturing and business processes on a global scale.

The partners are organizing an International Conference on Enterprise Integration Modeling Technology (acronym: ICEIMT '97) to be held Oct. 28-30, 1997, in Torino, Italy. The agenda ranges from reports on successful applications of enterprise integration technologies to evaluations of issues impeding the timely capture, analysis, and communication of information within and across manufacturing businesses.

"Despite the talk about agile firms, instantaneous supply-chain communications, and virtual enterprises, confusion abounds," says a NIST spokesperson, "and it's the result of ambiguous terminology and incompatibility among integration technologies. Global cooperation can help industry to scale these obstacles." For more information, contact James Nell, A127 Metrology Building, NIST, Gaithersburg, MD 20899-0001, (301) 975-5748, <nell@nist.gov> or check out the ICEIMT'97 website at <<http://www.nist.gov/workshop/iceimt97/>>.

### **STUDY CITES MEASUREMENT NEEDS OF DEREGULATED INDUSTRY**

Deregulation has given the concept "competitive edge" a new meaning for the U.S. electric power industry, a business sector that impacts the lives of every U.S. citizen and company, has annual sales exceeding \$208 billion and employs more than 440000 people. Many industry observers expect that in the future the most successful competitors in this sector will be those that best use modern technologies to produce less expensive electricity. A new study by NIST, Measurement Support for the U.S. Electric Power Industry in the Era of Deregulation, identifies the measurement capabilities that power producers and distributors will need to meet this challenge.

The study's approach is to characterize: (1) the driving forces behind deregulation's changes in the

electric power industry, (2) the technologies needed to address the changes, and (3) the specific measurement support needed from NIST to assist industry in making these technologies happen. These issues are discussed with four industry concerns in mind: (1) transmission and distribution efficiency, reliability, and stability; (2) equity in trade and international competitiveness; (3) global warming and health effects; and (4) power quality. A single copy of NISTIR 6007 may be requested from James K. Olthoff, B344 Metrology Building, NIST, Gaithersburg, MD 20899-0001, fax: (301) 948-5796, <james.olthoff@nist.gov>. Multiple copies are available from the National Technical Information Service, Springfield, VA 22161, (703) 487-4650, fax: (703) 321-8547, <orders@ntis.fedworld.gov>. Order by PB 97-152508.

### **REVISED DSS FOR FEDERAL AGENCIES UNDER CONSIDERATION**

To broaden the choices Federal agencies have when protecting information, NIST seeks comments on its plans to consider incorporating additional public-key based digital signature methods (such as the RSA and elliptic curve techniques) into its Digital Signature Standard. Digital signatures are used to confirm the identity of the signer and to verify that electronic information has not been altered. If information must be kept confidential, then encryption also is necessary.

This proposal is consistent with the Clinton Administration's overall efforts to promote the use of strong cryptography, by both Federal agencies and those in the private sector, while maintaining societal safeguards.

Digital signatures, used increasingly in electronic business transactions and electronic commerce, also are expected to become an integral part of routine Government business. The DSS, also known as Federal Information Processing Standard (or FIPS) 186, currently requires Federal departments, agencies, and contractors who use digital signatures to do so with the Digital Signature Algorithm. FIPS do not apply to the private sector, but they frequently are used by non-Federal organizations. To comment on the digital signature announcement, write to the Director, Information Technology Laboratory, Planned Revision to FIPS 186, A231 Technology Building, NIST, Gaithersburg, MD 20899-0001, or send electronic mail to <fips186@nist.gov>. Comments must be received by Aug. 11, 1997.

### **U.S.-GCC STANDARDS IN TRADE WORKSHOP**

NIST sponsored a Standards in Trade Workshop Feb. 24-March 6, 1997, for 23 representatives from the Gulf Cooperation Council (GCC) countries (Bahrain, Kuwait, Oman, Qatar, Saudi Arabia, and the United Arab Emirates). This successful workshop was an important step toward cooperation in identifying and eliminating technical barriers to trade between the United States and ongoing trading partners in the Gulf region.

Participants were experts in standardization, metrology, food products safety, international trade, and construction and building products.

The workshop familiarized participants with and built confidence in U.S. technology and practices in standardization, conformity assessment, metrology, and measurement systems. U.S. participants became more familiar with GCC practices. The workshop also strengthened recognition of NIST's representative to the Saudi Arabian Standards Organization (SASO) as an important and knowledgeable technical resource to facilitate the timely transmittal of information on standards and conformity assessment practices between the United States and the Gulf region. Professional contacts were developed and will strengthen technical ties, enhancing trade between the United States and the Gulf countries.

The agenda included briefings and panel discussions with private-sector and government participants, with numerous question-and-answer opportunities. Activities included visits to NIST laboratories and field sites. One highlight was a visit to ASTM headquarters in West Conshohocken, PA, to observe a meeting of standards committee F-15 on consumer products.

U.S. and GCC participants discussed next steps. Future specialized training programs may include sending U.S. experts to the Gulf region, perhaps in 1998.

### **MEMORANDUM OF UNDERSTANDING SIGNED FOR CONSTRUCTION MATERIALS**

The NIST National Voluntary Laboratory Accreditation Program (NVLAP) and a private organization, signed a memorandum of understanding (MOU) on Feb. 18, 1997, to work toward a mutual recognition agreement (MRA) to recognize their respective accreditations of laboratories that test construction materials. The MRA, which will be based on ISO/IEC Guides 25 and 58 and



other appropriate international standards, will aid in the elimination of duplicate accreditations in common areas. The MOU between NVLAP and the organization, is an example of an ongoing effort by NIST under the National Technology and Transfer Act to provide leadership in coordinating standards and conformity assessment activities with government bodies—as well as the private sector—to meet the needs of U.S. industry in the global marketplace.

The Organization provides its more than 2300 state and local government members in the southwest, south, southeast, and on the Atlantic seaboard with a recognized consensus standards program through a model building code. The Organization has more than 15 accredited laboratories to test products related to the construction industry, with primary emphasis on those products and systems used in the design and construction of buildings. NVLAP has approximately 20 laboratories accredited in construction materials testing. There are more than 700 domestic and foreign testing and calibration laboratories in the overall NIST/NVLAP program that are accredited in terms of meeting international standards.

#### **NIST POWER DEVICE MODEL USED TO DEVELOP SIMULATOR COMPONENT LIBRARY FOR INTERNATIONAL RECTIFIER IGBTs**

As part of his continuing effort to apply power semiconductor device models to industry practice, a NIST scientist has collaborated with a software house to extend the component library covered by the company's simulation products. As a result, the library supplied with the recently released version of one of the products includes 30 precharacterized models of insulated-gate bipolar transistors (IGBTs) manufactured by a private company.

To develop this library of models, the scientist made the necessary enhancements to the generic IGBT model and extraction procedure for the advanced structure of the private company devices, the software house extracted the parameters using the NIST extraction procedure, and private company provided the structural information for its most widely used IGBTs. A library of precharacterized IGBT models provides engineers tools for designing power electronic systems without requiring them to develop hardware prototypes or to characterize IGBT devices to obtain needed model parameters.

#### **NIST WORK PROVIDES FIRST CONFIRMATION THAT HIGH-CURRENT QHE DISSIPATIVE STATES ARE QUANTIZED**

Researchers at NIST have carried out a series of experiments and studies to investigate a new quantization phenomenon that arises when quantum Hall effect devices are operated at high currents. The phenomenon involves quantized dissipation within the devices under conditions that normally allow no significant dissipation. The phenomenon was first seen in early experiments at NIST in 1983 and was referred to as “breakdown” of the quantum Hall effect. At that time, there was no satisfactory explanation for it and no indication that the discrete dissipative states were quantized. Later, experimenters at NIST's counterpart laboratory, the Physikalisch Technische Bundesanstalt in Germany, also observed these dissipative states and proposed that they were quantized. New experiments at NIST give the first clear evidence that the states are indeed quantized.

In the integer quantum Hall effect, current is passed through a two-dimensional electron gas formed in a semiconductor device cooled to very low temperatures in the presence of a large magnetic field. The quantum Hall voltage across the device remains constant over a range of magnetic field values, forming plateau regions, which are used as representations of the unit of resistance. Normally, the longitudinal voltage drop along a device is very small when the quantum Hall voltage is on a plateau, and there is negligible dissipation within the device. However, the experiments at NIST have demonstrated that when large currents are applied, the longitudinal voltage drops along some devices exist only in discrete, quantized dissipative states when the longitudinal voltage is plotted versus the magnetic field. The ground state and the first 16 excited states were observed in two devices, with the separations between the discrete voltage states being quite large, typically about 5 mV. The phenomenon is interpreted as occurring when electrons are excited to higher Landau energy levels (emitting acoustic phonons to conserve energy and momentum) and then emitting optical phonons while returning to the ground state. The experiments suggest that some 30 % of the conducting electrons typically make transitions, at a rate of  $4 \times 10^{14}$ /s. One NIST experiment provided the first estimate of the maximum value of the electric field across the width of a device: a surprisingly large 1 MV/m. Several previous explanations of the breakdown of the quantum Hall effect at high currents assumed that the longitudinal resistance is quantized, rather than the longitudinal voltage. The range of current was extensive enough in another NIST

experiment to demonstrate that it is the longitudinal voltage that is quantized, which is consistent with the conducting electrons undergoing transitions to higher Landau levels.

### **INTERFACE ROUGHNESS MEASUREMENT VALIDATED FOR ADVANCED SILICON MOSFETs**

A NIST scientist has demonstrated and successfully applied a unique, non-destructive electrical measurement method to measure the roughness of the interface between the gate oxide and silicon channel in a typical commercially relevant silicon metal oxide-semiconductor field-effect transistor (MOSFET) test structure. Interface roughness (IR) is detrimental to MOS device performance (such as switching speed) and reliability; in addition, IR values need to be known for accurate thin-film measurements and standards. As well as being nondestructive, the method validated by the scientist has three other features that are particularly appealing. First, it measures fully processed devices, which means that no ambiguities need be introduced by a requirement for removing layers; second, it yields quantitative IR values; and third, it is model invariant. The method relies upon the physics of a quantum mechanical manifestation known as weak localization (WL). A Hall bar geometry is ideal for WL measurements, but Hall bars are rarely used by industry as test structures.

The scientist has demonstrated that a test structure in common use by the semiconductor industry can be used successfully to measure IR via the WL method. This type of structure is known as a “fatFET,” a large, two-terminal transistor having its conducting channel length equal to its width. Specifically, Richter used 6.5 nm gate-dielectric, silicon fatFETs having silicided low-doped drain junctions, since these devices are typical of advanced silicon MOSFET technology. To demonstrate that the method provided valid results, the fatFETs and specially added Hall bars were fabricated by integrated-circuit manufacturer, and then both types of test structure were measured at NIST at the same time. The NIST scientist found that the results from the WL and Hall bar test structures agreed to within the uncertainty of the measurements; the actual IR values are in the range of 0.1 nm to 0.2 nm. As a result of the scientist’s work, the method is now available for future device technologies. Efforts are under way to improve the resolution of the WL method and to compare its results with image data from atomic force and transmission electron microscopies. The scientist presented his results to the semiconductor community at the 27th IEEE Semiconductor Interface Specialist Conference in December 1996.

### **POLYCAPILLARY LENS SHOWN TO INCREASE EFFECTIVE DETECTION AREA BY FACTOR OF OVER 100 FOR NIST MICROCALORIMETER X-RAY SPECTROMETERS**

NIST scientists, in collaboration with scientists from a private company, have demonstrated that a polycapillary lens can be used to focus x rays in a microanalysis system to enhance significantly the effective area of the detector. The lens, fabricated by the private company consists of tens of thousands of curved glass capillaries that can collect x rays over a large solid angle and focus them on a small spot as a result of multiple grazing-incidence reflections. The use of x-ray optics is especially important for the microcalorimeter x-ray spectrometers developed at NIST, because optimum performance is obtained with small absorber areas (typically 250  $\mu\text{m}$  by 250  $\mu\text{m}$ ). Initial tests show that, even allowing for the increased sample-to-detector distance required by the lens, the effective detector area is increased by a factor of more than 100 over that obtained without the lens. With this large effective area and the previously demonstrated count rates and energy resolution, the combination of the NIST microcalorimeter and a polycapillary lens produces a powerful instrument for x-ray microanalysis, having the energy resolution of a wavelength dispersive spectrometer and the x-ray collection efficiency and parallel energy detection of conventional energy-dispersive systems. This instrument should facilitate greatly identification of particle contaminants of sizes below 0.3  $\mu\text{m}$ , a problem of immediate concern to the semiconductor industry. NIST and the private company have applied for a joint patent on this use of polycapillary lenses in microanalysis.

### **FIRST GOVERNMENT/SRC FELLOWSHIP ESTABLISHED AT STANFORD**

NIST, through the Semiconductor Research Corp. (SRC), is sponsoring a Graduate Research Fellowship at Stanford University. The purpose of the fellowship is to support university research related to and supporting metrology for thin dielectric films important to current or future semiconductor integrated-circuit manufacturing. The SRC currently supports a total of 36 fellowships; this one is the first co-sponsored by a Government agency.

NIST is committed to providing national leadership in developing improved metrology and supporting the measurements infrastructure for thin dielectric films. Current efforts in this area include the development of a materials database for in-situ process metrology, fundamental studies of the properties of dielectric-semiconductor interfaces, and extension of NIST’s

thin-film Standard Reference Materials efforts to include non-artifact-based measurement traceability. The division's thin-film work is done in collaboration with semiconductor manufacturing companies, instrument manufacturers, standards organizations and companies, and universities. The addition of the SRC and Stanford University to this team through this fellowship is expected to expedite the work.

The SRC is a consortium of nearly 50 semiconductor companies and government agencies. It plans, directs, and finances an integrated program of applied research in all areas of semiconductor design and manufacture. The SRC currently sponsors research at more than 50 universities and research institutions across North America.

### QUANTUM ENZYMOLOGY SUGGESTS ROUTE TO NEW ANTIBIOTIC DEVELOPMENT

The recent spread of infectious diseases arising from the rapid evolution of bacterial enzymes has spawned a renewed effort in the biotechnology industry to develop new, improved antibacterial agents. Recently, the therapeutic effectiveness of the penicillins and the cephalosporins has been reduced significantly by the emergence of resistant strains of bacteria that contain new enzymes that are able to break down these compounds before they can carry out their designed role. The limited, qualitative mechanistic information for this class of enzymes has been an obstacle to the development of next-generation penicillins and cephalosporins.

As part of a broad, long-range effort involving protein engineering and rational drug design, NIST and University of Maryland scientists collaborating at the Center for Advanced Research in Biotechnology (CARB) have used new *ab initio* quantum mechanical techniques combined with high-resolution structural information from protein x-ray crystallography to propose a novel, microscopic chemical mechanism for the hydrolysis of  $\beta$ -lactam antibiotics by *Staphylococcus aureus* PC1  $\beta$ -lactamase. This alternative mechanism suggests that the proper structural framework for substrate binding and orientation during catalysis plays a larger role in catalysis than previously appreciated. These insights provide new guidance to the pharmaceutical industry in the development of non- $\beta$ -lactam antibiotics to kill bacteria.

### NEW METHODS FOR DNA DIAGNOSTICS

Researchers at NIST are developing improved methods for DNA mutation detection using capillary electrophoresis (CE). Analysis of DNA by single strand conformational polymorphism (SSCP) provides an

efficient means of screening these mutations before the costly and time-consuming task of sequencing is begun. SSCP is a method used to detect single-base changes (mutations) in DNA that introduce conformational changes in the polymer. The finding that these CE-SSCP measurements have specific temperature dependencies provides the basis for developing this technique as an improved method for genetic profiling. For example, in the p53 system under study at NIST, specific mutations may be identified by CE-SSCP. (Mutations in the p53 gene are highly correlated to many forms of cancer.) This work is being done in collaboration with a researcher from a private company.

Preliminary results were presented at the HUGO Meeting on Mutation Detection, May 29, 1997, in Brno, Czech Republic. Complementing these studies, computerized RNA folding analyses are being performed to predict which mutations are detectable by SSCP. In collaboration with other government scientists, preliminary findings have been obtained that have resulted in molecular models of SSCP that are predictive. This information is being used in the design of measurement conditions and standards for SSCP.

### IMPROVED PROCEDURES FOR CALIBRATING THE BINDING-ENERGY SCALES OF X-RAY PHOTOELECTRON SPECTROMETERS

A NIST scientist has made an analysis of the various sources of uncertainty in the proposed procedures for calibration of binding energy (BE) scales in x-ray photoelectron spectroscopy (XPS). The analysis of the uncertainties and the recommendations that were provided should both improve the accuracy of BE measurements in XPS and reduce the time and cost of calibrations. X-ray photoelectron spectroscopy (XPS) is one of the most commonly used techniques of surface analysis. This technique can be used to identify most elements present in the outermost atomic layers of a specimen and can give information on likely chemical state from so-called chemical shifts of the measured core-electron binding energies.

Surveys have shown that the BE scales of many XPS instruments have not been calibrated well enough to measure chemical shifts (often less than 1 eV) with the regulated uncertainty (often about 0.1 eV). The growing adoption of ISO 9000 quality management systems also requires that laboratory equipment be calibrated and that the relevant measurement uncertainties be known. Draft documents for the calibration of the BE scales of XPS instruments are currently under consideration by ASTM Committee E-42 on Surface Analysis and ISO Technical Committee 201 on Surface Chemical Analysis.

In the analysis, some uncertainties, such as the effects of peak asymmetry for different measurement conditions, peak shifts and asymmetry caused by atoms in the outermost surface layer, and different methods of fitting data, can be minimized or eliminated by choice of improved methods of data acquisition and analysis. Uncertainty budgets have been prepared to illustrate the uncertainty contributions associated with a finite number of calibration measurements, non-linearity of the BE scale, and drifts of the BE scale between calibrations. Finally, guidance has been given on appropriate methods of data analysis using commonly available software. All of these will have impact on the measurements and calibrations of the user communities.

### **MASS SPECTROMETRIC MEASUREMENTS CONFIRM PAHS FORMED IN A DIFFUSION FLAME**

In collaboration with a researcher from Brown University, a NIST scientist has analyzed particles by mass spectrometry that were formed and collected on the center line of an ethylene diffusion flame. The purpose of this experiment was to better understand the mechanism by which carbonaceous particles are created in flames and how they evolve into soot. This work impacts many areas of soot research and technology, including health and environmental concerns, fuel combustion efficiency, and forensics.

Previous work by this team has documented the presence of small single sphere-like particles (precursor particles) that are formed at the base of the ethylene flame where the temperatures are relatively low. The precursors undergo a transformation at approximately one-third of the total flame height to particles that are carbonaceous aggregates. These two types of particles are collected by ultrarapid sampling in the flame at selected heights and are later analyzed using laser microprobe mass spectrometry (LMMS) to determine their chemical compositions. LMMS provided evidence for the presence of polycyclic aromatic hydrocarbons (PAHs) in samples containing precursor particles, but the results were not conclusive because of the possibility of mass spectral interferences. To verify the presence of PAHs, a pure deuterated ethylene fuel was burned in the place of normal ethylene to produce particles containing deuterated compounds. The results confirmed the presence of PAHs since the mass spectrum for the deuterated particles shifted in a manner that was totally consistent with the shift expected for the proposed compounds when there is a one-to-one replacement of hydrogen by deuterium. These are the first known experiments to use pure deuterated hydrocarbon fuel to produce particles in which compounds retaining the deuterium signature were

detected as a definitive chemical diagnostic. The PAHs found are those predicted by two NIST scientists in 1985 to be thermodynamically stable molecules in flames that provide a pathway for growth toward larger carbonaceous soot particles.

### **NOVEL SCANNED PROBE FOR OPTICAL CHARACTERIZATION OF NANOSCALE CHEMISTRY**

NIST scientists, have designed and constructed a near-field scanning optical microscope (NSOM) that permits simultaneous measurement of transmitted and reflected light while concurrently recording a topograph of the sample. The instrument has been optimized for chemical problems that require molecular characterization on the nanometer spatial scale.

Near-field scanning optical microscopy is emerging as a powerful technique for obtaining optical images with spatial resolution that exceeds the diffraction limit of light. This enhanced resolution is obtained by scanning a sub-wavelength aperture across a specimen, such that the spatial resolution is determined by the aperture. Most near-field optical microscope designs prohibit simultaneous transmission and reflection measurements, and collection of reflected light is normally inefficient. To accomplish simultaneous measurements in the transmission and reflection modes with high efficiency, a unique optical collection system was designed and implemented. This collection system is based on the 1-to-1 imaging properties of an ellipsoidal cavity. By placing the near-field microscope inside and at one foci of the cavity, light emitted from the microscope's near-field optics is collected and re-imaged at the other foci of the ellipse. This provides a higher collection efficiency since mechanical hindrances, such as the body of the microscope, are now eliminated.

Another improvement over existing NSOM designs is the use of a nonoptical means for shear-force sensing to control the sample/tip spacing. By using one-half of a piezo electric tube to drive and excite the mechanical resonance of a near-field optical probe and the other half of the piezo electric tube to listen and sense the amplitude of this resonance, a change in resonance amplitude can be measured as the probe interacts with a surface. The measurable change in resonance is sufficient to allow for nanometer and sub-nanometer surface variations to be detected and imaged.

As many samples of chemical interest cannot be obtained in thin, optically transparent forms and as the compact shear force concept will expand the use of NSOM to a wider variety of systems, the novel features of the NIST design are expected to have a significant impact on surface microanalysis.

**ELEY-RIDEAL MECHANISM IN THE H ATOM ABSTRACTION OF D FROM Si(100)**

A NIST researcher has used molecular beam studies to demonstrate a novel class of surface reactions that proceeds without energy accommodation of the reactant with the substrate.

Surface reactions are often described by two ideal mechanisms of energy accommodation between the reactants and the substrate. The Langmuir-Hinshelwood mechanism, where the reaction proceeds with the reactants fully accommodated with surface energy, is thought to describe most catalytic surface reactions. In the other limit, a gas phase species can react directly with an adsorbate, with no energy transfer to the substrate. This Eley-Rideal (ER) mechanism, while proposed nearly 50 years ago, has been observed definitively on metal surfaces only recently. While kinetics studies support an ER process in the H atom abstraction of adsorbates from semiconductor surfaces, conclusive dynamical studies were needed to validate this interpretation.

Experiments were performed using laser photolysis of HI to generate H atoms with well-defined incident kinetic energies in the range of 1 eV to 3 eV. Kinetic energy distributions of the product HD formed from the reaction of these H atoms with D adsorbed on Si(100) were measured with a mass spectrometer detector. For an incident energy of nominally 1 eV, the gas phase product carries away the vast majority of the energy available in this reaction, indicating that the substrate acts predominantly as a spectator. For higher incident H atom energies, the HD product kinetic energy distribution broadens significantly while the mean value remains unchanged, suggesting that substrate participation (i.e., an energy sink) becomes significant and the reaction becomes less ER-like as the incident energy increases.

While these studies indicate that the abstraction of hydrogen adsorbed on Si(100) nominally adheres to an ER-like mechanism, it is apparent that an idealized ER process is not realized, particularly for higher incident energies. This mechanistic insight is necessary for the implementation of accurate modeling algorithms aimed at optimizing semiconductor processing. Given that ER processes are expected to be more important in nonthermal environments, these results will have greater impact in processes where H atom fluxes are high. Specifically, the results address the energy flow of exoergic surface reactions, where it is important to know whether the liberated “chemical energy” remains in the substrate degrading eventually to “heat” or is carried away by the gas phase products.

**MAJOR UPDATE OF THE NIST CHEMISTRY WEBBOOK**

The new February 1997 release of the NIST Chemistry WebBook contains many more properties and data than the initial August 1996 version, which contained thermochemical data and estimates for more than 5000 compounds and gas-phase ion-energetics data for over 10 000 species. The February 1997 release adds additional data for included compounds and provides multiple experimental values if available. In addition, it adds the following new classes of data:

- vapor pressure data for over 5000 compounds,
- antoine coefficient data for over 1200 compounds,
- heats of reaction data for over 1300 reactions,
- mass spectra for over 8000 compounds, and
- IR spectra for over 5000 compounds.

The new proton affinity scale is included with data for over 1600 compounds. The number of species for which ionization energy data is given is now more than 12 000.

Evaluated heats of vaporization as a function of temperature are provided for 400+ compounds. An archive of heats of sublimation for over 1000 compounds as well as liquid-phase heat-capacity data for more than 1300 compounds also have been added.

Enthalpy, entropy, and heat capacity data for over 700 gases, 200 liquids, and 300 solids from the JANAF data compilation are included in equation form.

Some of the estimated and uncertain thermodynamic data included in the August 1996 version have been removed.

For spectral data, if the browser supports JAVA, the user may expand a small wavelength or mass range on their computer.

There are a number of new options for searching, including searching by molecular weight, ionization energy, or proton affinity. Searches now can focus only on molecules for which the database has data; for example, the user can search for compounds with the formula  $C_6H_{10}O$  and for which mass spectra are in the database.

The URL is the same as the original release: <http://webbook.nist.gov>.

**NEW THERMODYNAMIC INFORMATION FOR SILICON NITRIDE**

Recently, NIST has used its one-of-a-kind fluorine bomb calorimetric capabilities to characterize the world's first well-characterized single-phase specimens of  $Si_3N_4$ . Silicon nitride,  $Si_3N_4$ , was discovered about

150 years ago, but only in relatively recent times has it come to be recognized and exploited for its engineering applications. Its physical properties, including chemical stability and wear resistance at high temperatures, make  $\text{Si}_3\text{N}_4$  an ideal material for use in internal combustion engines, heat exchangers, cutting tools, and gas turbines, to name but several applications. Although much has been published concerning the physical and structural characteristics of silicon nitride, a recent critical assessment revealed how little is reliably known about the thermodynamic properties of this material. Such information is crucial to understanding how  $\text{Si}_3\text{N}_4$  behaves under the conditions encountered during industrial processing and operations.

NIST studies have shown that, contrary to some previous hypotheses, the energy difference between the two crystallographic forms of silicon nitride,  $\alpha$ - and  $\beta$ - $\text{Si}_3\text{N}_4$ , is small. This work also has shown that the standard molar enthalpy of formation, one of the fundamental thermodynamic values of  $\text{Si}_3\text{N}_4$ , differs by a very large amount, approximately  $40 \text{ kJ} \cdot \text{mol}^{-1}$ , from the most recent critically assessed and recommended value. This new information provides materials scientists and engineers with a much firmer thermodynamic foundation on which to base studies of the performance of silicon nitride under chemical processing and other conditions.

#### **TEMPERATURE MEASUREMENT FOR RAPID THERMAL PROCESSING**

During the production of semiconductor devices, the surface of a silicon wafer becomes covered with increasingly complex multilayer patterns. These patterns can cause localized changes in absorption and emission of heat during thermal processing, resulting in temperature nonuniformities and difficulty in accurately measuring the wafer temperature.

NIST has initiated a project to develop methods to measure silicon wafer temperatures in a rapid thermal processing (RTP) environment with an uncertainty of  $2^\circ\text{C}$  accuracy in a  $600^\circ\text{C}$  to  $1000^\circ\text{C}$  range. The project will establish reliable contact and optical thermometry traceable to NIST temperature standards. This tracks the Semiconductor Industry Association Roadmap goals for RTP thermometry.

The first advisory group meeting on temperature measurement for rapid-thermal processing was held at NIST on Jan. 30, 1997. Attendees spanned RTP equipment manufacturers, end users, instrument manufacturers, academia, research organizations, and NIST. The outcome of the meeting included: focused research directions for NIST to pursue to fulfill industry needs, improved cooperation with the key

players in the RTP industry, and continued interaction with SEMATECH. The RTP advisory group will meet next at the RTP Conference in New Orleans in September.

#### **NIST RADIOCHEMISTRY INTERCOMPARISON PROGRAM (NRIP)**

NIST, in collaboration with the Council on Ionizing Radiation Measurements and Standards and other interested parties, has initiated a new testing program to evaluate and improve measurement quality in the field of low-level radiochemistry. During a workshop held at NIST Feb. 11-13, 1997, more than 40 participants from commercial and national laboratories, state and Federal regulatory bodies, and NIST established the rationale for the program and began its implementation. The program elements are widely applicable to ANSI standards, to criteria being established for environmental performance testing providers by the National Environmental Laboratory Accreditation Conference, and to good laboratory practices being established under the Multi-Agency Radiological Laboratory Procedures manual. The scope of the program includes chemical separation and purification processes as well as the final radio-metric determination, and it is open to both U.S. and international laboratories.

Two committees were created at the workshop. An interim NRIP steering committee is charged with establishing the long-term test sample priorities, defining test material quality criteria, and defining protocols for out-of-control test measurement results. The steering committee also will be a forum for discussion and resolution of radioanalytical problems discovered through the testing program. A second committee was created to develop performance criteria for radiochemistry. This committee will establish minimum acceptable quality assurance and quality control requirements, traceable performance testing criteria, and protocols for on-site assessments. It also will develop criteria for a future low-level radiochemistry accreditation program.

#### **DETERMINING REACTOR PRESSURE VESSEL NEUTRON FLUENCE**

During the operational lifetime of a nuclear power plant, fast-neutron irradiation of the reactor pressure vessel (RPV) will degrade certain mechanical properties important to maintaining its structural integrity. Specifically, fast-neutron-induced embrittlement brings about a reduction in the fracture toughness of the RPV, and hence defines the service life of the vessel. Because of the obvious safety implications, the U.S. Nuclear

Regulatory Commission (USNRC) has issued regulations designed to help ensure that the structural integrity of reactor pressure vessels is not compromised. Operators of all commercial nuclear power stations are required to determine the RPV fast-neutron fluence by a calculation that considers the transport of neutrons from the reactor core out to the vessel and vessel cavity.

NIST scientists are helping to prepare USNRC Draft Regulatory Guide: DG-1053, Calculational and Dosimetry Methods for Determining Pressure Vessel Neutron Fluence. This document provides a methodology acceptable to the USNRC for demonstrating compliance with the regulatory requirements. The methods described in the guide address the calculation of neutron fluence and the techniques to validate these calculations via comparison with in-vessel and ex-vessel measurements of the neutron fluence. DG-1053 has been developed with extensive input from industrial representatives; NIST recently hosted a public meeting in which these representatives shared their ideas and concerns with the NRC and the document's principal authors.

As the first generation of nuclear power plants reach the end of their design lives, accurate assessments of the extent of RPV embrittlement become increasingly important to the U.S. nuclear industry, not only from a safety perspective but also from an economic standpoint.

### **COHERENT CONTROL OF WAVE PACKET DYNAMICS**

The ability to prepare coherent combinations of quantum mechanical states has many applications for the manipulation of information coded into the time evolution of quantum mechanical systems. Applications include the ability to affect the direction of photocurrents in semiconductor quantum wells and to use phase control to encode information, such as in quantum computing. Typically in this type of experiment, ultrafast laser pulses are used to excite a target, which is then studied. However, all the atoms or molecules of ordinary targets are in different quantum mechanical starting states, which can blur the experimental results.

In recent work at NIST a continuous-frequency single-mode laser was used to prepare a specific intermediate state of a molecular target. Then, that specific state was excited by the ultrafast laser, forming a "wave packet," a coherent superposition of states. This two-step process was shown to allow much more precise control of the wave packet information. This technique is being used as an advanced measurement tool for molecular spectroscopy and photonic applications.

### **NEW GRINDING FLUID CHEMISTRY PROTECTS DIAMOND TOOLS**

For a long time, diamond tools have been used to machine hard materials. Researchers at NIST have found that certain substances, when used in grinding fluids, help to protect the diamond from rapid oxidation and wear. During grinding, diamonds are subject to high surface temperatures as well as surface bond disruption. Under these conditions, the diamond oxidizes rapidly producing a soft surface layer, which is removed by the rubbing process. This process produces blunt diamond tips, which, in turn, reduce the penetration depth of the diamond grit into the materials that are being ground. In this fashion, the machining rate decreases rapidly, and the surface temperatures at the grinding interface rise exponentially. High surface temperatures accelerate the oxidation kinetics of the diamond, and more diamond is lost.

By introducing molecules that bond tightly with the diamond surface under grinding conditions, a tenacious film is formed on the diamond surface; these molecules are oxidized preferentially instead of the diamond surface, thus preventing the diamond from wearing oxidatively. This discovery has been demonstrated through work with an industrial partner. The substances were introduced into an industrial production facility producing cemented tungsten carbide cutting inserts for the automotive industry. Diamond wheels are used to machine (sharpen) the tungsten carbide cutting inserts. However, the diamond wheels need to be dressed (sharpened) after machining 30 inserts. The improved chemistry permits the machining of a maximum of 500 inserts before diamond dressing is required again. A patent on these fluids is being filed.

### **MODEL DEVELOPED TO PREDICT ALPHA CASE IN TITANIUM CASTINGS**

A model to predict the thickness of the oxygen contaminated layer in titanium castings has been developed at NIST and implemented into a commercial programming code for modeling of castings. This activity is part of the NIST Consortium on Casting of Aerospace Alloys.

The surfaces of Ti investment castings become contaminated with oxygen because of reaction with the oxide mold material. This brittle surface layer, called alpha case, must be removed before use. Prediction of the thickness of the contaminated layer allows adjustment of mold design and gating to modify the alpha case thickness. Moreover, investment casters can determine from these predictions the optimal extra dimension to be added to Ti castings to allow for alpha case removal.

The oxygen penetration normal to the surface is predicted by a NIST developed diffusion-based model, which uses temperature-time histories at points along the surface of a casting as obtained from a thermal solidification analysis. The model was tested by comparison to experimentally measured alpha-case thicknesses obtained from a step wedge casting fabricated by a consortium member. Excellent agreement was found between the predicted and measured  $\alpha$ -case thickness, which ranged from 0.2 mm to 0.8 mm.

#### **NIST PATENTS NEW METHOD OF DETECTING NATURAL GAS PIPELINE FLAWS**

Scientists at NIST recently received a patent for a new method of measuring wall thickness and detecting flaws (such as cracks, delamination, scaling, and corrosion) in natural-gas pipelines by using ultrasound. Use of ultrasound inspections is common for oil pipelines but has been less effective for the natural-gas variety. Gas is a poor coupling agent for the ultrasonic signals emanating from the transducer to the pipe wall.

The researchers showed that use of wide-band, well-dampened ceramic transducers and high-dynamic-range receiver amplifiers can overcome signal losses. They also demonstrated that by using a diplexer, the same transducer can be used to generate and detect the ultrasonic signals. "This method is inherently suitable for the task, because it relies on the use of the natural gas as the coupling fluid for transmitting the probing ultrasonic signals into and out of the pipe wall," the patent states.

NIST is working currently with the Southwest Research Institute, under contract with the Gas Research Institute, to show the practicality of the technology.

#### **NIST ECONOMIST ON U.S. DELEGATION TO OECD CONFERENCE**

A NIST economist was an invited member of the U.S. delegation to the Organization for Economic Cooperation and Development (OECD) conference, International Conference on Greener Public Purchasing, recently held in Biel, Switzerland. The U.S. delegation, led by the Environmental Protection Agency (EPA), consisted of experts from industry, government, and academia, all with an interest in Executive Order 12873, which directs U.S. Federal agencies to incorporate environmental preferability into their decisions to purchase nearly \$200 billion in products and services each year.

The NIST economist presented her BEES (Building for Environmental and Economic Sustainability) methodology at the conference. The BEES methodol-

ogy, to be published December 1997 in the form of Windows-based decision-support software, balances the life-cycle environmental and economic performance of building products. The life-cycle environmental approach, following ISO 14000 draft standards, measures and synthesizes environmental impacts (e.g., global warming, acid rain, resource depletion, solid waste) across all stages in the life of a product, from raw material extraction through manufacture, use, and ultimately disposal. The life-cycle economic approach, following ASTM life-cycle cost standards, measures the dollar costs of owning, operating, maintaining, and disposing of a product over a fixed period of time. These life-cycle approaches received overwhelming international support at the OECD conference.

The NIST economist recently began a four-year project under EPA sponsorship to extend her BEES methodology to include product technical performance. The methodology will be implemented in new decision-support software for the federal procurement community for selecting products that achieve the most appropriate balance between life-cycle environmental, economic, and technical performance.

#### **LIBRARIANS BURN BOOKS IN LARGE FIRE RESEARCH FACILITY**

Personnel from the large fire research group at NIST gave members of the NIST Office of Information Services and their colleagues from other Federal Government libraries the opportunity to learn firsthand how to salvage books damaged by fire, smoke, and water. When disaster strikes, prompt action can sometimes limit the extent of damage. This is especially true for a library after a fire has occurred. Damaged books can be recovered if quick action is taken. Training helps to ensure that the response to a library fire will be effective. However, the opportunity for hands-on training in book recovery is rare.

As part of a conference on book recovery being held at NIST, a simulated library fire was staged in the Large Fire Research Facility. A fire was started by a cigarette discarded in a recycling container between two rows of bookshelves. The fire was allowed to burn for several minutes before being extinguished using a single sprinkler. Conference attendees spent several hours carefully working to "recover" the damaged materials.

According to a spokesperson from the NIST Office of Information Services who organized the event, only books slated for disposal were used in the test. Other agencies participating in the activity included the National Library of Medicine, the National Archives and Records Administration, and the Department of Agriculture.



### **NIST AND SOFTWARE COMPANY WORK TOGETHER TO APPLY MULTIKRON SYSTEM**

A software company has expressed an interest in exploring the use of NIST-developed MultiKron boards to examine the performance of systems in general. The MultiKron series of very large scale integration instrumentation chips and interface boards are measurement tools that promote the development of high-performance computing and flexible, scalable systems. The software company wants to apply the board to normal applications on multiprocessor machines, to video servers where peripheral component interconnect utilization and synchronization are important, and to client server and cluster performance applications where a synchronized timebase is important. NIST will provide two MultiKron boards to the software company and will work with the company in enhancing the functionality of the technology, particularly in the area of clustering.

### **NEW RELEASE OF NIST FORM-BASED HANDPRINT RECOGNITION SYSTEM PUBLISHED**

NISTIR 5959, NIST Form-Based Handprint Recognition System (Release 2.0), describes a new release of a standard reference form-based handprint recognition system for evaluating optical character recognition. As with the first release, NIST is making the new recognition system freely available to the general public on CD-ROM. This source code testbed, written entirely in C, contains both the original and the new recognition systems; the new system is an embellishment to the old one.

Since the release of the first handprint recognition system in August 1994, NIST has distributed more than 700 copies of the technology to more than 40 countries around the world. The system serves as a vehicle for transferring recognition and performance assessment technology from NIST to system developers and researchers in the private sector.

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## **Standard Reference Materials**

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### **NIST RESEARCHERS DOCUMENT SRM 1450c FOR THERMAL INSULATION TEST METHODS**

NIST researchers have completed the development of the renewal of SRM 1450c, Fibrous Glass Board. The SRM 1450 Series has been the industry's choice for the calibration of standard test methods used for determining the steady-state thermal transmission properties of thermal insulation. Manufacturers of commer-

cial heat-flow-meter equipment that conform to ASTM Test Method C 518 typically will include a specimen of the SRM with the sale of their apparatus, thereby providing the user with a means of establishing traceability. Predicted values of thermal conductivity and certified values of thermal resistance of SRM 1450c were determined from thermal conductivity measurements obtained with NIST's 1 m guarded hot plate apparatus. Thermal conductivity measurements were determined following a randomized full factorial experimental design for two independent variables, bulk density, and mean temperature. Certified values of thermal resistance for SRM 1450c have been tabulated for bulk density from 150 kg/m<sup>3</sup> to 165 kg/m<sup>3</sup> and mean temperature from 280 K to 340 K. A summary of the experimental results has been published in NIST Special Publication 260-130.

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## **Standard Reference Data**

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### **STANDARD REFERENCE DATABASE ON HIGH-TEMP SUPERCONDUCTORS UPGRADED**

Materials researchers will be interested in the upgraded version of NIST Standard Reference Database 62: High-Temperature Superconductors, now available from NIST. Version 2.0 of the database provides evaluated thermal, mechanical, and superconductor property data for the class of materials commonly called high-temperature superconductors, including cuprates, bismuthates and the relatively new borocarbides.

The materials are described by specification and characterization information, including processing details and chemical compositions. Physical characteristics such as density and crystal structure are given in numeric tables.

The updated database also houses a collection of data from the Science and Technology Agency of Japan that has not been available previously in English. This unique collection of property and characterization data for single batches of materials resulted from a Japanese study of the processing and properties of high-temperature superconducting materials. The data were provided to NIST as part of an agreement with Japan's National Research Institute for Metals.

Copies of SRD 62, Version 2.0, are available for \$265 by contacting the SRD Program, Rm. 113, Building 820, NIST, Gaithersburg, MD 20899-0001, (301) 975-2208, fax: (301) 926-0416, <srdata@nist.gov>. The SRD catalog can be accessed on the World Wide Web at <<http://www.nist.gov/srd>>.

# Calendar

August 12–15, 1997

## LASER MEASUREMENTS SHORT COURSE

Location: The Broker Inn  
Boulder, CO

**Sponsors:** National Institute of Standards and Technology (NIST) and the University of Colorado.

**Audience:** Scientists and engineers involved with laser measurement.

**Format:** Training and site visit

**Purpose:** To provide training on laser measurement theory and techniques. This course will emphasize the concepts, techniques, and apparatus used in measuring laser parameters and will include a visit to the NIST laser measurement laboratories

**Topics:** Optics for laser measurements, attenuation techniques, laser operation, basic laser power/energy standards, laser power/energy measurement techniques, optical fiber power measurements, pulse measurements, transfer standards, beam profile measurements, diode lasers, laser measurement for optical communications, statistics and error analysis, laser safety, and detectors.

**Technical Contact:** Thomas Scott, NIST, 325 Broadway, Boulder, CO 80303-3328, phone: 303/497-3651, fax: 303/497-3387, email: scott@boulder.nist.gov.

September 9–11, 1997

## MEASUREMENT QUALITY CONFERENCE

Location: National Institute of  
Standards and Technology  
Gaithersburg, MD

**Sponsors:** NIST and American Society for Quality Control/Masurement Quality Division.

**Audience:** Metrology and quality assurance professionals involved in measures of quality.

**Format:** Lectures and papers, single track.

**Purpose:** To provide a forum for presenting and discussing ideas and current topics on the quality of measurements and measurement of quality for quality professionals.

**Topics:** Quality measurement, software for quality, data analysis, uncertainty determination, management process statistics, and physical measurement technology.

**Technical Contact:** Norman Belecki, NIST, Building 220, Room B146, Gaithersburg, MD 20899-0001, phone: 301/975-4223, fax: 301/926-3972, email: norman.belecki@nist.gov.

September 17–19, 1997

## FOURTH INTERNATIONAL SYMPOSIUM ON ROOFING TECHNOLOGY

Location: National Institute of  
Standards and Technology  
Gaithersburg, MD

**Sponsors:** NIST, U.S. National Roofing Contractors Association (NRCA), Canadian Roofing Contractors' Association, National Research Council of Canada, International Waterproofing Association, International Council for Building Research Studies and Documentation, and International Union of Testing and Research Laboratories for Materials and Structures.

**Audience:** Roofing contractors, consultants, design professionals, and individuals involved in research and development, technical services, or marketing of roofing products.

**Format:** Five sessions of papers, each session followed by a period of questions and answers.

**Purpose:** To present the results of the latest roofing research and advances in technology as well as recommendations for their implementation.

**Topics:** Performance of synthetic single-ply and polymer-modified bitument roof systems, advances in roof system analysis, advances in application technology and wind performance of roofing.

**Technical Contact:** Walter Rossiter, Jr., NIST, Building 226, Room B348, Gaithersburg, MD 20899-0001, phone: 301/975-6719, fax: 301/990-6891, e-mail: walter.rossiter@nist.gov. WWW Homepage: <http://ciks.cbt.nist.gov/roofing97>.

September 29–October 3, 1997

**INTERNATIONAL CONFERENCE ON ATOMIC AND MOLECULAR DATA AND THEIR APPLICATIONS**

Location: National Institute of Standards and Technology  
Gaithersburg, MD

**Sponsor:** NIST.

**Audience:** Users and producers of atomic and molecular data and database developers.

**Format:** Invited talks (mornings) panel discussions, working groups, and poster papers (afternoons).

**Purpose:** To establish a forum for direct interaction of major atomic and molecular data producers, atomic and molecular data centers, and database developers with the data users in various fields of science and technology.

**Topics:** Data needs in nuclear fusion research, lighting applications, gaseous discharge (plasma) technology, spectrochemistry, etc.; atomic and molecular database development, and data assessment.

**Technical Contact:** W. L. Wiese, NIST, Building 221, Room A267, Gaithersburg, MD 20899-0001, phone: 301/975-3201, fax: 301/990-1350, email: wolfgang.wiese@nist.gov, WWW Homepage: <http://physics.nist.gov/icamdata>

October 6–7, 1997

**REFRIGERANTS FOR THE 21ST CENTURY**

Location: National Institute of Standards and Technology  
Gaithersburg, MD

**Sponsors:** NIST and American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc. (ASHRAE).

**Audience:** Refrigeration research and development engineers.

**Format:** Presentations by invited speakers.

**Purpose:** To educate the U.S. industry on refrigerant choices for the 21st century.

**Topics:** Montreal protocol, global warming, HFC refrigerants, carbon dioxide, hydrocarbons, ammonia, barriers to implementing hydrocarbon refrigerants in the United States.

**Technical Contact:** Bill Seaton, ASHRAE, 1791 Tullie Circle, NE, Atlanta, GA 30329, phone: 404/636-8400, fax: 404/321-5478, WWW Homepage: <http://www.ashrae.org>.

October 6–9, 1997

**20TH NATIONAL INFORMATION SYSTEMS SECURITY CONFERENCE**

Location: Baltimore Convention Center  
Baltimore, MD

**Sponsors:** National Institute of Standards and Technology (NIST) and National Computer Security Center of the National Security Agency.

**Audience:** The audience represents a broad range of information security interests spanning government, industry, commercial, and academic communities.

**Format:** Tutorials and exhibits.

**Purpose:** To address today's hottest information systems security issues.

**Topics:** International electronic commerce, legal and privacy issues, warding off computer crime, security on the WWW, firewall technology, internet security, virus protection, cryptography, and handling of security incidents.

**Technical Contact:** Tim Grance, NIST, Building 820, Room B426, Gaithersburg, MD 20899-0001, phone: 301/975-4242, fax: 301/948-0279, email: [tim.grance@nist.gov](mailto:tim.grance@nist.gov), WWW Homepage: <http://csrc.nist.gov/nissc>.

October 20–24, 1997

**PRECISION THERMOMETRY WORKSHOP**

Location: National Institute of Standards and Technology  
Gaithersburg, MD

**Sponsors:** NIST.

**Audience:** These workshops are intended for calibration laboratory personnel and others who wish to undertake precision temperature measurements. Applicants should possess undergraduate training in physics or engineering and should have some laboratory experience in metrology. Participation is limited to 16 people, and pre-registration is required.

**Format:** Classroom and laboratory instruction.

**Purpose:** To provide advice and assistance on measurement and calibration problems, tracing to NIST the accuracies of measurement standards needed for research work, factory production, or field evaluation.

**Topics:** Temperature scales, platinum resistance thermometry, vapor pressure and gas thermometry, low temperature calibrations, thermistor thermometry, liquid-in-glass thermometry and thermocouple thermometry.

**Technical Contact:** Andrea Swiger, NIST, Building 221, Rm. B128, Gaithersburg, MD 20899-0001, phone: 301/975-4800, email: [andrea.swiger@nist.gov](mailto:andrea.swiger@nist.gov).

October 30–31, 1997

**THIN DIELECTRIC FILM METROLOGY**

Location: National Institute of  
Standards and Technology  
Gaithersburg, MD

**Sponsor:** NIST.

**Audience:** Industry, government, and university thin-film metrologists for semiconductors.

**Format:** Invited speakers and discussion groups, several 30 to 60 minute presentations, open discussion period, and round table panel discussions.

**Purpose:** To establish traceability to NIST for optical metrology of thin dielectric films used in microelectronics—the evolution of reference materials for thin dielectric films.

**Topics:** Issues pertinent to the set-up and calibration for metrology tools, use of standards, traceability of standards to NIST, and ways to address related evolving industry requirements for thin dielectric films.

**Technical Contact:** Barbara Belzer, NIST, Building 225, Room B310, Gaithersburg, MD 20899-0001, phone: 301/975-2248, fax: 301/948-4081, email: barbara.belzer@nist.gov.

May 4–5, 1998

**METROLOGY FOR ELECTRONIC  
PACKAGING AND INTERCONNECTION**

Location: National Institute of  
Standards and Technology  
Gaithersburg, MD

**Sponsor:** NIST.

**Audience:** Industry, university, and government experts in electronic packaging and interconnection.

**Format:** Technical presentations and working groups.

**Purpose:** To revise NIST's strategic planning in electronic packaging and interconnection based upon 1997 editors of leading industrial roadmaps.

**Topics:** Electronic packaging, metrology, interconnection, printed wiring boards, on-chip interconnects, semiconductor packaging, and materials.

**Technical Contact:** Michael Schen, NIST, Building 224, Room B320, Gaithersburg, MD 20899-0001, phone: 301/975-6741, fax: 301/869-3239, email: michael.schen@nist.gov.