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News Briefs

General Developments

MAKING SOUND BUSINESS DECISIONS ON AUTOMATION

AutoMan, a microcomputer program developed at NIST, applies modern mathematical techniques to make factory automation decisions easier. Choosing whether or not to invest in automated manufacturing equipment is a complex problem for shop and factory owners. There are established criteria for making capital investment decisions, but more and more managers are questioning whether these measures alone are adequate for evaluating automation options. AutoMan, developed for the U.S. Navy's Manufacturing Technology Program, allows managers to account for important gains realized by automation, including engineering performance improvements, better control over manufacturing, and improved product quality, as well as harder-to-handle intangible benefits like technology advancement, plant modernization, flexibility, and competitive position. The program for MS-DOS-based machines is available from the National Technical Information Service, Springfield, VA 22161 for $40 plus $3 for shipping and handling. Orders may be placed by phone: (703) 487-4650. Order by PB389-221741. Please specify diskette size 5.25″ or 3.5″.

SOFT-DRINK GLASS BOTTLE STANDARD REVISED

NIST has published a replacement voluntary product standard on glass bottles for carbonated soft drinks. The standard, which supersedes PS73-77, is for manufacturing requirements to improve the safety performance of refillable and nonrefillable glass bottles made from soda-lime-silica glass with nominal capacities up to 36 fluid ounces. It was sponsored by the Glass Packaging Institute Inc., and developed by a standing committee of representatives from soft-drink bottle manufacturers, bottlers, consumers, and others interested in performance requirements, inspection, and testing procedures for soft-drink bottles. NIST, a nonregulatory agency, administers the U.S. Dept. of Commerce Voluntary Products Standards Program in support of private sector standards development. Specific activities are initiated in response to requests from interested parties and subsequent approval by the Secretary of Commerce. To obtain a copy of Voluntary Product Standard PS 73-89, Glass Bottles for Carbonated Soft Drinks, send a self-addressed mailing label to the Office of Standards Management, NIST, A625 Administration Building, Gaithersburg, MD 20899; telephone: 301/975-4023.

EFFECTIVELY DESIGNING COMPUTERIZED WORK STATIONS

The computerized work station often is considered the key to increased office productivity. Yet, work station furnishings and layout seldom are given the same attention and resources as the technology. Instead, space and furniture decisions too often are based on "status" and tradition. To help managers make intelligent choices, researchers at NIST have developed a process for designing work stations based on office activities including reading and writing, talking on the telephone, drafting and drawing, or using a video display terminal. Work station dimensions and configurations then are developed depending on the importance of the activity and the time spent on it. A publication describing this process, Guideline for Work Station Design (NISTIR 89-4163), is available by sending a self-addressed mailing label to Arthur Rubin, NIST, A309 Building Research Building, Gaithersburg, MD 20899. This report is the latest in a series prepared by NIST for the U.S. General Services Administration.

FLUID PROPERTIES OF LENNARD-JONES MIXTURES

The design of chemical process unit operations equipment requires detailed knowledge of the thermophysical properties of fluids and mixtures, often based on mathematical models of their properties and behavior. Many emerging technologies, such as enhanced oil recovery and biotechnology, typically involve materials and fluids not well represented in the current database or which are used in areas of fluid behavior difficult or impossible to study in the laboratory. Computerized models of these systems often benefit from comparison to a model of an idealized mixture. NIST has simulated an idealized mixture (one that obeys the Lennard-Jones intermolecular potential function and has a size ratio of 2:1) over a broad range of temperatures, composition, and energy ratios, and has published the data to be used as a point of comparison for similar real-fluid models. A report of this work, Properties of Lennard-Jones Mixtures at Various Temperatures and Energy Ratios with a Size Ratio of Two (TN 1331), is available from the Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402-9325. Order by stock no. 003-003-02952-1 for $20 prepaid. A computer listing of the data is available on DOS diskette; contact Dr. Marcia Huber, NIST, Div. 584.03, Boulder, CO 80303; telephone: 303/497-5252.

RESIDUAL STRESS MEASUREMENT AND CONTROL DURING FABRICATION OF CERAMIC COMPOSITES

The magnitude of stresses which can inhibit the sintering of ceramic matrix composites can be assessed using a model composite system of unidirectionally oriented fibers. The stress is measured by means of a sandwich compact consisting of a layer of SiC fibers sandwiched between two layers of ceramic powder of different thicknesses. Upon sintering, this configuration produces an asymmetric stress field across the thickness of the specimen, resulting in bending of the compact, which can be characterized by the curvature of the fibers.

Control of the stresses can be achieved by using a colloidal processing route for coating fibers with alumina or other suitable oxides. Coated fibers with small ($d = 0.2$ μm) and large ($d = 0.8$-1.0 μm) particle-size alumina powders have been shown to alter significantly the temperature at which stress initiation begins. For uncoated fibers, bending starts at 1300 °C and increases with increasing temperature. Coating with a 4-μm-thick layer of fine particle-size alumina powder lowered the temperature at which the stress initiates to 1265 °C, and a coating thickness of 16 μm lowered the initiation temperature to 1200 °C. In contrast, the coarse particle coating achieved the desired result of delaying stress initiation to higher temperatures. For a coating thickness of 10 μm, bending of the composite was reduced considerably and, most importantly, stress initiation was raised to 1325 °C. The coarse particle-size coatings appear to reduce the stresses by acting as a buffer layer between the matrix and the fiber. These experiments reflect the importance of the fiber/matrix interface with respect to stress enhancement (small particle-size powder) and stress retardation (coarse particle-size powder) during the sintering of fiber-reinforced composites. Even small interfacial layers of few microns considerably influence the stress state during sintering.

CHARACTERIZATION OF THICK-SECTION COMPOSITES

NIST has completed a survey of methods with potential to characterize the through-thickness variation of properties of thick-section composites. The purpose of the survey is to guide industry's response to the Navy's program to manufacture submarine hulls made of polymer composites. Owing to the performance requirements of submarine hulls, the cross-sectional thickness will be much larger than usually encountered in composites manufacture. Methods are therefore needed which can interrogate the interior of thick specimens nondestructively.

Drawing on a wide range of expertise, NIST scientists identified a wide variety of techniques and the technical barriers to their implementation. The level of development required to bring the techniques to fruition was also evaluated. The most promising methods rely on imbedded sensors. These range from miniaturized dielectric probes to fiber optic sensors. The types of sensor best suited for characterization of properties will also depend on whether thermosets of thermoplastics are selected as the polymer resin.

Industry will use the survey to formulate a research plan that encompasses both the manufacture and inspection of thick-section composites.

SMITHSONIAN AND NIST COLLABORATE ON NEUTRON STUDIES OF PAINTINGS

The Smithsonian Institution (SI), through its Conservation Analytical Laboratory, is collaborating with NIST in applying nondestructive neutron autoradiography to the study of works of art. This is the only facility available in the United States for

neutron-induced autoradiography (NIA) with a large, uniform, highly moderated thermal neutron field.

In this project, the work of art is activated at the thermal column of the NIST reactor in a flux of 3×10^9 n/cm^2/s for 20 min. It is then placed in contact with film, which is removed and replaced to obtain a series of images created by nuclides with different half-lives. Examples of autoradiographs of paintings by Albert Pinkham Ryder (1847-1917), will be included in a 1990 exhibit of that artist's work at the National Museum of American Art. Until the paintings were studied by autoradiography, it was known only that Ryder had a reputation for continually reworking his paintings and not that he was actually engaged in serious reconsiderations of the paintings' compositions. These changes became apparent in the autoradiographs and are now available for study.

MODEL USED TO CONFIRM NEW EXPERIMENTAL METHOD

The NIST-developed ideal mixing of complex components (IMCC) model has been used by Russian high-temperature researchers to confirm experimental data obtained by their new ion-molecule equilibria technique for measuring low O_2 and alkali partial pressures. The IMCC model includes a large database of Gibbs energy of formation functions for complex liquid oxides, including Al-, Ca-, Fe-, K-, Li-, Mg-, Mn-, Na-, and Si-oxides typically found in glass, steel slags, combustion, and other high-temperature processing industrial applications. The model process provides predictive estimates of detailed solid, liquid, and gas phase compositions.

PROCESS CONTROL SENSOR TECHNOLOGY SURVEYED

NIST scientists recently reported to the National Center for Manufacturing Science (NCMS) on the status of sensor technology for monitoring polymer composites processing. NCMS commissioned the report in order to identify areas in which further research and development would lead to significant advances in sensor technology. The polymer composites industry would benefit greatly from the availability of sensors for process monitoring since many problems with polymer composites can be related to inadequate control during processing.

The report identifies three generic sensor technologies—dielectrics, ultrasonics, and spectroscopy—with the capabilities to monitor polymer composites processing. The report further identifies resin viscosity and degree of cure as the most important properties to be measured. Background information for the report was gathered from literature sources and from review of current work in industrial, university, and government laboratories. Several industrial visits were made to identify process control needs and the current state of implementation of process control sensors.

NCMS, whose members represent a broad range of industries, will use the report to design a research and development program to hasten the availability of sensors for polymer composites manufacture.

URANIUM AND THORIUM ANALYSIS OF POWDERED MILK PRODUCTS

In a NIST study, IAEA (International Atomic Energy Agency, Vienna, Austria), powdered milk and whey samples were assayed for sub-parts-per-billion quantities of uranium and thorium. There is a strong interest in the IAEA powdered milk and whey materials since they were collected shortly after the Chernobyl incident and were known to contain many orders of magnitude higher levels of fission products than pre-Chernobyl dairy products. The uranium isotopic composition was natural and both the thorium and uranium concentrations in these IAEA materials were found to be near ambient levels. The powdered IAEA milk had thorium and uranium levels comparable to the NIST powdered milk (SRM 1549, <500 and 170 parts-per-trillion, respectively), while the concentrations in the powdered IAEA whey (10 and 22 parts-per-billion, respectively) were about two orders of magnitude higher. Studies on locally available fresh milk and on fresh milk collected near the U.S. DOE plant at Fernald, OH, are currently being pursued to determine the distribution of the uranium and thorium between curds and whey.

DISTRIBUTION OF THORIUM DECAY PRODUCTS IN THOROTRAST PATIENT

NIST scientists are collaborating with the research staff at the National Cancer Institute to measure the distribution of short-lived thorium decay products in a variety of organs donated by a former thorotrast patient. This problem is being attacked by measuring the gamma-ray emissions from the radioactive thorium decay products in the donated organs. Thorotrast is colloidal thorium dioxide formerly used to enhance diagnostic medical x-ray images. Patients who were injected with the full dose of thorotrast (equivalent to 12 g of thorium) have

suffered a marked increase in the incidence of cancer to the liver, pancreas, larynx, and esophagus. They also have shown excess leukemia and bone marrow failure. The objective of the study is to quantitate the distribution of the short-lived thorium decay products among organs to further refine human health and safety radionuclide biokinetic models and risk coefficients. Actinium-228, ^{224}Ra, ^{212}Pb, ^{212}Bi, and ^{208}Tl were sought among organs which include eye, larynx, esophagus, breast, kidney, liver, spleen, ribs, red blood cells, and blood serum. Of the materials measured at NIST, it is estimated that over 90 percent of the thorium-derived radioactivity is accumulated in the liver, spleen, and bone.

OPTIMUM FLOW CONDITIONING FOR ORIFICE METERS

A common way to measure flow rates of gases and liquids is to insert an orifice plate flowmeter into a length of pipe and measure the pressure drop across the plate. The accuracy of the measurement, however, is dependent on the condition of the flow, which is adjusted using flow conditioners upstream from the meter. European and U.S. specifications for the location of these conditioners differ, and the location has a substantial impact on measurement accuracy. In work sponsored by the Gas Research Institute, NIST analyzed the effect of varying the distance from conditioner to orifice meter. The results showed that, in general, the conditioner should be located 17 pipe diameters upstream from the orifice plate for tube bundle conditioners. More details are presented in Optimum Location of Flow Conditioners in a 4-inch Orifice Meter (TN 1330), available from the Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402-9325. Order by stock no. 003-003-02961-1 for $4.25 prepaid.

NEW TEST CHAMBER DEVELOPED

Electromagnetic Interference (EMI) has caused a range of problems in military electronic systems—from the inability of pilots to communicate with air-traffic controllers to catastrophic crashes. Researchers at NIST are developing a new type of electomagnetic test chamber to evaluate the ability of operational systems to withstand the effects of radiated EMI. The new chamber combines features of a transverse electromagnetic cell and a broadband reverberating chamber to provide an electromagnetic compatibility test capability for the frequency range 10 kHz to 40 GHz, a frequency range not offered previously by any single facility. A small prototype chamber, which measures $1.3 \times 2.4 \times 3.9$ m, has been constructed by NIST and delivered to another government agency. Initial tests with the chamber have shown the potential for significant cost and time savings. A paper, no. 52-89, describing the chamber is available from Jo Emery, NIST, Div. 104, Boulder, CO 80803; telephone: 303/497-3237.

FRACTURE MECHANICS MODEL FOR WEAR OF ADVANCED CERAMICS

Advanced ceramics materials are being considered increasingly for applications requiring wear resistance, corrosion resistance, and retention of mechanical properties at elevated temperatures. Prediction of wear performance is extremely important for design and selection of ceramic materials for these applications. It has been reported in the literature that the rate of wear suddenly increases by several orders of magnitude as a result of a slight increase in one of the test variables, such as contact load, sliding distance, or sliding speed. A simple contact mechanics model based on linear elastic fracture mechanics was developed to account for this transition. The model predicts that the transition from low to high wear is controlled by crack propagation in the tensile zone at the trailing edge of the contact circle. It also predicts that the wear transition can be prevented by the reduction of either the contact stress or the coefficient of friction, or by increasing the fracture toughness of the ceramic material. Experimental results have been obtained for α-alumina under various test conditions and temperatures ranging from room temperature to 800 °C in confirmation of the model.

NEW MODEL PREDICTS MICROSTRUCTURE DEVELOPMENT IN HIGH-T_c SUPERCONDUCTORS

The compound $Ba_2YCu_3O_7$, the prototype high-T_c material (often denoted the "123" superconductor), contains Cu atoms in "chain" and "plane" sites. Defects such as vacancies and substituents can be introduced in the structure with profound effect on the superconducting properties. The knowledge on a microscopic scale of the atomic configuration of the defects created by metal substitution and/or variation of oxygen concentration is vital not only for understanding the mechanism of superconductivity but also for understanding the evolution of critical microstructures during processing. The latter have a direct effect on mechanical properties;

for example, the density and type of twin boundaries in these materials are directly associated with oxygen content and migration of defects.

NIST neutron diffraction research on high-T_c materials has been extended recently to modeling the motion of vacancies and the configuration of the oxygen atoms and metal impurities in 123-type superconductors. In $Ba_2YCu_3O_{6+x}$ materials, the diffusion of oxygen in the plane of the chains is viewed as a correlated series of jumps of the oxygen atoms into vacant sites in the vicinity of twin boundaries. In $Ba_2YCu_{3-y}M_yO_x$ compounds, the model predicts a rearrangement of the oxygen atoms in order to satisfy the coordination requirements of the substituent metal atoms.

These models qualitatively explain and predict the observed motion and rearrangement of the twin boundaries during diffusion and the symmetry and stoichiometry of the substituted materials. From this, the details of the formation of microstructures which directly affect electronic and mechanical properties may be elucidated. This predictive capability is expected to have a direct bearing on processing strategies to improve materials for technological applications.

BASIC STUDIES OF CHLOROSILANE REACTIONS WITH SURFACES AID UNDERSTANDING OF SILICON FILM GROWTH

NIST and industry scientists have recently observed for the first time how the chlorosilanes $SiCl_4$ and Si_2Cl_6 interact with single-crystal silicon and germanium surfaces. The research, performed primarily at the National Synchrotron Light Source at Brookhaven National Laboratory, and in part at NIST, should further the understanding of how best to use these chemicals as safer alternatives to explosive silane gas during the growth of silicon films for microelectronic applications.

The scientists conducted experiments in ultrahigh vacuum with a variety of surface-sensitive spectroscopies including soft x-ray photoemission and thermal desorption. They discovered that the reactivity of the different chlorosilanes depends on how adsorption occurs on the surface. There is a very low probability that the $SiCl_4$ will stick directly in a single decomposition reaction. In contrast, Si_2Cl_6 first adsorbs in a weakly bound molecular state with near unit probability, and then fragments on the surface. When these surfaces are heated after adsorption, further reactions occur that produce gas-phase $SiCl_2$ and $SiCl_4$, but not Cl_2, indicating that when used as the sole reactant both $SiCl_4$ and Si_2Cl_6 will etch these surfaces. These results explain why an additional reactant that will remove chlorine from the surface is necessary for film growth, and indicate that Si_2Cl_6, with its larger sticking probability, should be the superior source material.

NEW CENTER FOR DENTAL MATERIALS RESEARCH ANNOUNCED

A new Center of Excellence for Materials Science Research has been established to expand the internationally recognized dental and medical materials program at NIST. The center is funded by a 5-year grant from the National Institute of Dental Research (NIDR), one of the National Institutes of Health. The NIDR grant was made to the American Dental Association Health Foundation (ADAHF), which maintains the Paffenbarger Research Center at NIST. Initial research projects will include: developing glass ceramic inserts to strengthen and stabilize composite dental restorations; improving the properties of resin-based composite dental materials to reduce shrinkage; developing protective coatings for both enamel and dentin to prevent caries on exposed roots and to seal restorations; formulating synthetic dentin and bony replacement materials by combining multifunctional monomers with calcium phosphates; and developing new materials that can be readily fabricated into improved shields to protect patients undergoing radiation treatments.

NIST PROPOSES FIPS FOR GOSIP TESTING

NIST is proposing a Federal Information Processing Standard (FIPS) to establish policies, procedures, and criteria for testing networking products for interoperability and conformance with the Government Open Systems Interconnection Profile—GOSIP. After August 1990, federal agencies must use GOSIP (FIPS 146) specifications in procuring networking products. GOSIP defines a set of data communication rules called protocols, which enables computer systems developed by different vendors to communicate, and enables the users of different applications on these systems to exchange information. For further information, contact Jean Philippe Favreau at NIST, telephone: 301/975-3634.

INDEX TO WEIGHTS AND MEASURES PROCEEDINGS REVISED

A new index to the proceedings of the National Conference on Weights and Measures (NCWM) has been published. NCWM is an organization of state, county, and city weights and measures enforcement officials that was established in 1905. NIST, which is a nonregulatory agency, provides technical support to NCWM through its Office of Weights and Measures. NIST Special Publication SP 769, Index to Reports of the National Conference on Weights and Measures from the First to the Seventy-Third (1905-1988), is a subject and speaker index covering the proceedings of the annual meetings of NCWM. SP 769 replaces NBS Special Publication 691, which covered the proceedings from NCWM annual meetings from the first to the sixty-ninth. For a copy of SP 769, send a self-addressed mailing label to the Office of Weights and Measures, NIST, A617 Administration Bldg., Gaithersburg, MD 20899.

TECHNIQUE DEVELOPED TO MEASURE INTERFACE STRENGTH IN POLYMER COMPOSITES

NIST researchers have developed a new technique to estimate the strength of the bonding between polymer matrix resin and reinforcements in polymer composites. Bonding of the resin to the reinforcements is an important engineering property as it strongly influences the mechanical properties of polymer composites. The previously available methods to evaluate the strength of this bond require highly trained personnel, are tedious to perform, and require special test specimens or destruction of the composite. The new test procedure is easy to carry out and correlates well with interfacial strength.

The new method uses a laser to heat a very small, localized region of the sample. The acoustic emission which results from interface debonding is measured. The debonding is a consequence of the widely different thermal expansion of the resin and reinforcement. Since thermal expansion is anisotropic in each ply, the technique also provides a measure of interlaminar bonding in multidirectional laminates. Contacts with industry are being made to seek assistance in adaptation of the new method to industrial test protocols.

ISO WORKING GROUP ON FRACTURE OF HIGH-PRESSURE GAS CYLINDERS

The first meeting of the Working Group on Fracture that was formed under the jurisdiction of International Standards Organization (ISO) Committee TC-58 on Gas Cylinders (Subcommittee SC-3 on Cylinder Design) was held at NIST.

The objective of the working group is to establish test methods and acceptance criteria for high-strength steel cylinders used for transporting compressed gases.

Agreement on a proposed new ISO specification for seamless steel gas cylinders (ISO-DP 9809) was reached at the meeting except for the requirements for tests and acceptance criteria for fracture resistance of cylinders. Significant differences exist between the fracture tests proposed by the U.S. cylinder manufacturers and those proposed by the European cylinder manufacturers.

A test program to evaluate the fracture performance of high-strength steel cylinders was developed by the working group and is to be completed by the working group's next meeting.

SUBMICRON RESOLUTION TWO-DIMENSIONAL X-RAY IMAGING NOW READY FOR MATERIALS SCIENCE STUDIES

An x-ray imaging system with submicron spatial resolution has been developed by the synchrotron radiation group at NIST. Installed at beam line X23A3 of the National Synchrotron Light Source at Brookhaven National Laboratory, the system is used to study the interiors of solids by the techniques of non-destructive x-ray diffraction imaging and microradiography. Important advantages for in-situ imaging accrue from the use of x rays (as opposed to electrons), such as no requirement for vacuum and much less heating of the sample.

The system performance has been evaluated by radiographically imaging palladium lines, as narrow as 0.6 μm, deposited on a silicon wafer. The results give an estimated spatial resolution of 0.5 μm and suggest that the resolution is limited by Fresnel diffraction. Diffraction images of device features and multilayer interfaces have also been observed with this new imaging system. These images are more sensitive to microstructures than microradiography, and are important to detailed understanding of the performance of devices designed from the band-structure engineering approach.

IMPROVED METHOD FOR MEASURING CHEMICAL BONDING ON SURFACES

A knowledge of the geometric structure of a molecule adsorbed on a solid surface is of great importance in understanding the chemistry and reactivity of the molecule with the solid. A technique

called ESDIAD (Electron Stimulated Desorption Ion Angular Distributions), developed at NIST in the 1970s, allows for the direct determination of the local bonding geometry of adsorbed molecules. The technique takes advantage of the fact that atomic and molecular fragments created during electron bombardment may leave or desorb from the surface in the same direction as the chemical bond that was ruptured by the electronic excitation. A major limitation of the original apparatus was that only positively charged desorbed ions could be detected.

Recently, NIST scientists modified the ESDIAD technique to allow for the detection of negatively charged ions and electronically excited neutral species. This has opened up a new direction in the study of the structure of adsorbed molecules and provides new insights into how charged particles desorb from surfaces. For example, in experiments on fluorinated molecules adsorbed on surfaces, they found negative ions came primarily from molecularly intact species whereas the positive ions came mainly from dissociated species. The ability to measure this phenomenon offers the opportunity to study the local structure of complex chemical systems by a comparison of negative and positive ion signals.

MULTILAYERS FOR SOFT X-RAY MONOCHROMATORS

Multilayer structures consisting of alternating layers of ultrathin materials can be efficient, selective reflectors in the soft x-ray region. NIST scientists have recently reported one of the first applications of multilayer optics as a replacement for more conventional (and inefficient) soft x-ray monochromators on a synchrotron radiation beamline. For this application, multilayers were used instead of the usual diffraction elements in soft x-ray monochromators—natural crystals and ruled gratings. In the wavelength range of interest, 6-30 Å, gratings are inefficient, and suitable, robust, natural crystals are scarce. Multilayers are a good alternative because they can provide efficient diffraction with moderate resolution under relatively high power loads, such as produced at the latest generation of synchrotron-radiation facilities.

Operational tests have been performed at the NIST beamline at the National Synchrotron Light Source at Brookhaven National Laboratory. For these studies, multilayers made of tungsten and carbon (40 Å per layer-pair) replaced the two natural crystals in the beamline's primary monochromator. High efficiency was obtained for the multilayer diffraction ($\approx$ 6 percent per multilayer), yielding a flux of $\approx 10^{11}$ photons/s in a bandwidth of $E/\Delta E \approx 100$. No degradation of the multilayer structure with beam exposure was evident. The flux and resolution attained permitted new experiments to be done in a photon-energy range previously inaccessible at the NIST facility.

IONOSPHERIC CALIBRATOR FOR MEASUREMENT OF VARIATIONS IN RADIO SIGNAL DELAY

NIST scientists have recently developed a prototype ionospheric calibrator. The calibrator, which uses GPS (Global Positioning System) satellite signals, provides information on propagation delays through the ionosphere. It monitors the propagation delay for signals at 1.2276 and 1.5754 GHz broadcast from the orbiting GPS satellites. When fit to a $1/f^2$ model of propagation variation, the receiver calculates corrections to the delay of the signal. The added signal delay caused by the ionosphere can be more than 100 ns. The calibrator reduces the uncertainty in that delay to a few ns.

The receiver is codeless, that is, it does not require knowledge of the complex codes used by GPS. The receiver can track up to 12 satellites at once, and it produces a value for the ionospheric correction every 15 s. Each value accounts for the total electron content along the line between the satellite and the receiver. Eventually, the GPS constellation will include 21 satellites providing continuous access to four or more satellites at any location on the Earth.

With rising interest in using GPS for accurate surveying and geodesy (observation of motion of land masses), the ionospheric calibrator promises a simple approach to dealing with one of the key ranging uncertainties. This is especially important now that we are near a maximum in solar-radiation-activity level. Time transfer using GPS will also benefit from this advance. The method may also offer a particularly simple means for studying variations in electron content of the ionosphere itself.

NIST RESEARCHER DEVELOPS ROUTING PROTOCOL WITHIN OPEN SYSTEMS INTERCONNECTION (OSI) REFERENCE MODEL

A NIST researcher has developed a model for interdomain or policy-based routing within the OSI reference model for computer communications. Policy-based routing is a key infrastructure element

for deploying significant, operational networks based on OSI.

The model provides the necessary structure to address administrative policy issues, such as selective acceptance of transit traffic across a routing domain or the creation of cooperative, private bilateral routing agreements between independent organizations. A technical report describes the model for policy-based routing, which has been adopted by the European Computer Manufacturers Association (ECMA) and is under consideration by the International Standards Organization (ISO).

GUIDELINE FOR QUALITY CONTROL OF IMAGE SCANNERS PUBLISHED

Federal Information Processing Standard (FIPS) 157, Guideline for Quality Control of Image Scanners, announces the adoption of the American National Standard for Information and Image Management—Recommended Practice for Quality Control of Image Scanners, ANSI/AIIM MS44-1988, as a FIPS guideline. MS44 provides procedures and physical test objects for use by document processing system analysts, designers, and operators in calibrating monochrome, digital image scanners.

NIST ANNOUNCES AVAILABILITY OF STANDARD FLAWS FOR EDDY-CURRENT NDE

NIST has announced the availability of Research Material (RM) 8458, a well-characterized artificial flaw used as an artifact standard in eddy-current nondestructive evaluation (NDE). The RM is the outcome of work carried out to address the need for calibration standards for eddy-current NDE, for example, as used to detect fatigue cracks in aircraft structures. The RM flaw is produced in an annealed aluminum alloy (7075) block by first indenting the block and then compressively deforming the resulting notch until it is tightly closed. The next operation is to restore a flat finish to the block face, after which the block is heat treated to the T6 temper. The problem has been to manufacture artificial flaws that closely simulate the eddy-current response of fatigue cracks. Currently used artifacts include electrical-discharge-machined and saw-cut notches, both of which are relatively poor representations of fatigue cracks as their widths are too great. The new method provides notches that can be made controllably in a variety of geometries, have known dimensions, and with widths that are narrow enough to provide an acceptable representation of fatigue cracks.

DECREASED PERFORMANCE FOR NEW REFRIGERANT DOCUMENTED

NIST researchers completed fundamental calorimetric experiments to document a 20 percent decrease in the heat transfer coefficient for a leading new environmentally safe refrigerant while boiling inside a single tube and over the evaporative boiling regime found in present day commercial office building centrifugal chillers. This decrease closely matches an 18 percent decrease in chiller cooling capacity found by leading manufacturers in field tests of the new refrigerant. Consequently, a cooperative research program has been planned with NIST, universities, and industry to understand and enhance the heat transfer during evaporative boiling of this refrigerant for example, NIST will complete nucleate pool and flow boiling visualization studies of this refrigerant on both smooth and special surfaces designed to enhance the heat transfer rates. High-speed photography will be used to understand and document the components of the heat flux at the interface between the solid and fluid surfaces.

NEW MODEL DEVELOPED FOR SORPTION OF FORMALDEHYDE

NIST researchers have developed a new mathematical model that correctly predicts the adsorption and desorption of formaldehyde gas in the presence of gypsum wallboard. Pressed-wood products are a major source of formaldehyde in indoor environments. Current models correctly predict the equilibrium indoor formaldehyde levels from knowledge of the emission rate of the pressed-wood products. However, the formaldehyde concentration takes days to achieve equilibrium because gypsum wallboard acts as a sink for the pollutant. The new model predicts the nonequilibrium concentration in the presence of wallboard. The model was developed on the basis of mass balances in a building and accounts for building air exchange rates and press-wood product and wallboard areas.

NIST MEASURES PERFORMANCE OF THERMAL BRIDGES IN NEW MOBILE TEST FACILITY

NIST completed its first series of measurements on the performance of thermal bridges in a new mobile test facility housed inside a NIST environmental chamber. Thermal bridges are highly conductive paths for energy flow into or out of a building, usually along structural supports that penetrate insulated exterior walls in office buildings.

These heat flow paths can account for as much as 35 percent of the total heat flow through a wall. Most existing computer codes used by building designers do not account for these thermal bridges. The new facility was built to gather basic data under controlled laboratory conditions on the heat flow along such penetrations. The test room measures $6 \times 2.5 \times 2.5$ m with removable walls and roof and is mounted on a gooseneck trailer for moving. Heat flow transducers and specially built flat and corner calorimeters are used for measuring heat flow rates. To date, measurements have been made on a metal-framed wall typical of use in industrial buildings. The results indicated that measured heat flow rates were as much as 18 percent larger than those predicted due to the multidimensional heat flow paths that exist in metallic framing members.

NIST DEVELOPS NEW SIMULATION MODEL FOR INDOOR AIR MOTION

NIST has collaborated with researchers in Japan to develop a new computer model for predicting indoor airflow distribution. This model will be used to determine effective ventilation distribution for the design of more efficient manufacturing clean rooms and large building air-conditioning systems. The model called "EXACT" solves a nonlinear system of momentum, energy, and turbulence equations to predict three-dimensional nonisothermal flow in either steady-state or transient conditions. The model handles a variety of boundary conditions including air inflows, air outflows, and heat flux or temperature wall conditions. The model has the ability to handle an arbitrary number of obstacles in the flow region to account for furniture and partitions. The computer code for "EXACT" exists in vectorized and nonvectorized versions.

NEW METHOD TO DETECT ALUMINUM IN BLOOD SUBSTITUTE

Patients needing emergency blood transfusions can be given infusions of albumin as an initial replacement for blood loss. This practice eliminates the need for blood typing and can reduce the possibility of disease transfer. However recent studies have uncovered a problem with albumin that could prompt other adverse health effects: trace levels of aluminum. In the past, aluminum was difficult to measure at these low concentrations. But now, at the request of the Food and Drug Administration (FDA), NIST researchers have developed effective methods for measuring aluminum in albumin that combine several chemical analysis techniques. Laboratories in pharmaceutical companies and hospitals can adopt these methods to screen albumin products before they are marketed or used. NIST also has measured aluminum levels in a number of albumin samples the FDA and manufacturers will use to ensure measurement reliability. Apparently a byproduct of the albumin manufacturing process, aluminum at trace levels has been correlated to diseases affecting nerve tissue and bone. Aluminum exposure is a problem for patients with kidney impairment, because they have no way of excreting excess aluminum, and for patients receiving large or frequent albumin doses.

NIST/NASA WORKING ON FIRE SAFETY IN SPACECRAFT

In the not-too-distant future, people may be living in spacecraft for months or even years. Currently, the National Aeronautics and Space Administration strictly limits the type and amount of flammable material in a NASA spacecraft. But, in large spacecraft housing many people over long periods of time, these limitations may not be feasible. To help the space agency have more flexibility in selecting materials, researchers from NIST are assessing the test methods currently used by NASA for determining the fire hazard of materials. One goal of the project will be to help NASA develop broader test methods which can determine a level of hazard for a variety of materials. Current NASA screening tests are limited to either passing or failing a material. The NIST fire researchers also will work with NASA to develop ways to assess on Earth the flammability of materials in an environment with little or no gravity.

NDE EVALUATION OF SHEET METAL FORMABILITY

NIST and private industry have successfully demonstrated a nondestructive, ultrasonic system for evaluating the formability of steel sheet. Consistent formability in the sheet metal stock is necessary in a metal stamping plant to produce reliable, consistent shapes. This is even more important in a highly automated plant, because the automated equipment has difficulty dealing with inconsistent sheets. Current practice is a time-consuming process of cutting a sample from the sheet metal roll, preparing several specimens, and testing them. The new system, designed by NIST in collaboration with a guest researcher from the University of Belgrade, was installed at an industrial plant for evaluation. Tests show that the system, based on

non-contact electromagnetic acoustic transducers and the analysis of ultrasonic wave speeds, can make reliable measurements of the formability directly on the sheet prior to stamping. Various training aids, including a videotaped tutorial, operator's manual, and software, were also developed for the system.

NIST UPDATING COMPUTER SECURITY GLOSSARY

In computer parlance, terms like virus and worm refer to malicious software intended to damage or destroy computerized information. But even the experts often disagree on their definition. To help clear up confusion about these and other computer-security related terms, NIST is evaluating existing glossaries for inclusion in a bibliography. The bibliography is to be issued as a Federal Information Processing Standard in 1990. (FIPS are developed by NIST for use by the federal government.) Glossaries can be sent to Samuel P. McCrea, NIST, A216 Technology Bldg., Gaithersburg, MD 20899; telephone: 301/975-5237. If you know of a glossary but do not have a copy to send, please contact McCrea with the title and publisher.

FIRST FIELD TESTS OF RAILROAD WHEEL INSPECTION SYSTEM

The first field trials of a system for inspecting railroad wheels as they roll over a sensor installed in the rail were recently completed by NIST in a research program sponsored by the Federal Railroad Administration (FRA) to improve railway reliability and safety. Over the past 4 years, according to the FRA, railroad wheel failures caused 134 accidents totaling $27.5 million in damages. In the NIST system, electromagnetic acoustic transducer (EMAT) sensors were mounted in rails at the American Association of Railroads' test track in Pueblo, CO, where loaded freight trains were repeatedly driven over them. As the wheels passed over the sensors, ultrasonic pulses were launched into the wheel, and the echoes reflected from cracks in the wheel were detected and analyzed by computer-controlled instrumentation. The track and EMAT system survived the stress of operation and provided clear signals at train speeds up to 15 mph. Further testing will be conducted to calibrate the system and make it more robust, and to evaluate the on-line digital signal processing system. For more details, contact Ray Schramm, NIST, Div. 430, Boulder, CO 80303-3328; telephone: 303/497-3232.

PRIVATE SECTOR PRODUCT CERTIFICATION PROGRAMS

The Office of Standards Code and Information has published an updated directory of private sector product certification programs, replacing NBS SP 703, Private Sector Product Certification Programs in the United States, which was published in 1985. This new edition of the directory lists 132 organizations, 23 more than were listed in the 1985 edition. The product certification activities of these organizations are described by the type and purpose of each organization, the nature of the activity, products certified, standards used, certification requirements, any accreditation or recognition by a U.S. or foreign government agency or by the private sector, availability of services, methods of cost determination, and other relevant details. The information is based primarily on submissions by the organizations and therefore documents the organization's description of its own activities.

This volume is designed to serve the needs of federal agencies and standards writers for information on U.S. private sector certification programs. Manufacturers, engineers, purchasing agents, and others may also find this volume of value. NIST SP 774, Directory of U.S. Private Sector Product Certification Programs, is available for purchase from NTIS and the Government Printing Office.

EXPRESSION OF MEASUREMENT UNCERTAINTY

A draft International Organization for Standardization (ISO) Guide to the Expression of Uncertainty of Measurements was reviewed at a meeting of ISO/Technical Advisory Group (TAG) 4/Working Group (WG) 3 at the Deutsches Institut fur Normung (DIN) in Berlin, West Germany, November 14-17, 1989. The guide is based on a 1981 recommendation by the International Committee of Weights and Measures (CIPM), and the effort is jointly sponsored by ISO, the International Electrotechnical Commission, the International Organization of Legal Metrology, and the International Bureau of Weights and Measures. In addition, ISO/TAG4/WG3 met in Berlin with a counterpart working group of ISO/Technical Committee (TC) 69 on Statistics that is drafting a related standard. The two working groups agreed to collaborate in completing the guide. NIST is coordinating the U.S. input and participation in this work on behalf of the American National Standards Institute. This guide is expected to enhance significantly international harmonization of the expression of uncertainty associated with measure-

ment standards used by testing and certifying laboratories. When completed, it will promote confidence in mutual acceptance among nations of test reports and certificates for affected products in international trade.

DIAMOND FILMS DESIRABILITY

A unique combination of superior properties makes diamond a desirable material for a large number of optical, electrical, optoelectronic, mechanical, thermal, and chemical applications. NIST scientists are obtaining important data relating diamond film processing and structure to properties important to optical and optoelectronic applications. In particular, the group is examining the role of deposition conditions on morphology and the identity and distribution of optically active defects in the films. The films are grown by chemical vapor deposition in a hot-filament reactor. Researchers have recently studied the effects of feed gas composition on growth and properties of the films. The growth rate increases almost linearly with increasing methane content, and the surface morphology becomes smoother as the methane fraction in the feed gas increases. However, the quality of the diamond, as determined by Raman spectroscopy, decreases due to the increased presence of graphitic bonding. Examination of diamond films and particles by cathodoluminescence and photoluminescence reveals the absorption edge at the electronic bandgap, and the presence of dislocations and nitrogen related point defects. The dislocations and point defects are found to be inhomogeneously distributed in the films.

NIST/NIH NANOMETER ANALYSIS FACILITY: IMPLEMENTATION OF PARALLEL DETECTION ELECTRON ENERGY LOSS SPECTROMETRY

The analytical capabilities of the NIST/NIH (National Institutes of Health) Nanometer Analysis Facility, which is based upon a field emission scanning transmission electron microscope located at NIH, have been augmented by the implementation of a parallel detection electron energy loss spectrometer. In electron energy loss spectrometry (EELS), the energy of electrons transmitted through a thin (<50 nm) specimen is measured to reveal characteristic core level energy losses, which can be used to detect and quantify elemental constituents. Generally EELS is more sensitive than energy dispersive x-ray spectrometry for the analysis of thin specimens because the inelastic scattering is strongly peaked in the forward direction, which permits efficient collection of the signal, and because the signal is not partitioned among two or more de-excitation processes as is the case for x-ray emission.

Spectral information present in the fine structure at core edges can be used to determine nearest neighbor atom distributions. Previous EELS systems relied on a scanning single-channel spectrometer. The recent development of suitable spatially resolved detectors for EELS has led to the development of parallel detection. Parallel detection EELS provides an increase in collection efficiency of a factor of approximately 1,000 over single channel collection. The PEELS system is currently being applied by NIST scientists to the study of high T_c superconductors.

DEMONSTRATION OF THE QUANTUM ZENO EFFECT

Quantum mechanics predicts that the act of observing a system influences the behavior of that system. NIST scientists have recently completed the first unambiguous confirmation of one effect of this type—namely, that measurements of the state of a system tend to prevent that system from changing its state. The more frequent the measurements, the stronger the effect. Their particular experiment confirms one aspect of predictions by University of Texas theorists that a continuously observed quantum state can never decay. They referred to this as the quantum Zeno effect, after the paradox conceived by the ancient Greek philosopher, Zeno.

The NIST experiments involved observation of a few thousand $^9Be^+$ ions contained in an electromagnetic trap. Having placed all of the atoms in a particular, long-lifetime state, they noted that the transitions to a second state were heavily inhibited by brief observations made during the period of the transition. All of their ions moved to the second quantum level if they waited 256 ms before making an observation, whereas rapid observations every 4 ms allowed only a few ions to make the transition. The interpretation of the experiments involves a basic prediction of quantum mechanics, namely, that the act of observation projects the system into a particular quantum state. As a given atom progresses toward the second state, it can be described as being in an admixture of the initial and final states. If the system is observed during this process, it must be localized in either the final or initial state. Thus, early observation in the transition process yields a high likelihood of projecting the ion into the initial state where it must start through the transition process all over again.

HIGHEST "Q" VALUE ACHIEVED FOR OPTICAL FREQUENCY MEASUREMENTS

Scientists at NIST have recently reported the highest "Q" ever observed in atomic or molecular spectroscopy. In their experiments a single, laser-cooled mercury ion was stored in a Paul electromagnetic trap and radiated by a probe laser. The natural linewidth of the probed transition, which lies in the ultraviolet region of the spectrum, is extremely narrow, about 2 Hz. Several factors normally prevent one from measuring such a narrow width. A special dye laser (563 nm) was developed to improve the measurement of this narrow transition. This laser, stabilized to a carefully constructed Fabry-Perot cavity, was narrower than any visible laser ever reported. The frequency of this laser is doubled to probe the optical "clock" transition in mercury. The published resonance width (full width at half maximum) of 180 Hz was limited only by the laser linewidth. The most recent results indicate a linewidth of less than 80 Hz, giving a quality factor for the frequency measurement of $Q=\nu_0/\Delta\nu=10^{13}$.

The systematic uncertainties in the mercury transition are estimated to be controllable to about one part in 10^{18}, making it an excellent candidate for an optical frequency standard.

COMPUTER SECURITY GUIDES PUBLISHED

NIST has published three guides on improving the awareness of executives, managers, and users in computer security requirements and one on establishing computer security training programs. The guides are NIST SP 500-169, Executive Guide to the Protection of Information Resources; NIST SP 500-170, Management Guide to the Protection of Information Resources; NIST SP 500-171, Computer Users' Guide to the Protection of Information Resources; and NIST SP 500-172, Computer Security Training Guidelines. The publications will assist federal agencies in complying with the requirements of the Computer Security Act of 1987 by establishing training programs to improve computer security practice and by improving employee awareness of the threats to computer systems.

NIST ISSUES SOFTWARE GUIDES

NIST Special Publication 500-173, Guide to Data Administration, provides a reference model for the various activities performed by data administration, information resources administration, data modeling tools administration, and database administration. Data administration is the management of information describing the data, functions, operations, and structure of automatic data processing systems and databases. The guide stresses the features of certain computing tools useful for data administration, such as data dictionary systems and computer-aided software engineering tools. NIST Special Publication 500-174, Guide for Selecting Automated Risk Analysis Tools, describes important considerations for developing selection criteria for acquiring risk analysis software and recommends a process for selecting automated risk analysis tools. The document recommends selecting a group of personnel with special skills to participate in the risk analysis studies and describes three essential elements of a risk analysis tool: data collection, analysis, and output results.

MAGNETIC FORCE MICROSCOPE FOR IMAGING MAGNETIC STORAGE MEDIA AND SUPERCONDUCTORS UNDER DEVELOPMENT

NIST recently adapted a scanning tunneling microscope (STM) for imaging the variations in the magnetic field above the surface of a computer disk as a magnetic tip is translated over the surface. The work is aimed at developing new high-resolution methods for imaging very small magnetic domains in materials—such as the "bit" patterns stored in magnetic media or the surface manifestation of the magnetic flux pattern known as an Abrikosov vortex lattice of type II superconductors. In contrast to recent developments reported elsewhere, to date with confirmed resolution of 100 nm, the NIST work has been based on simple force detectors scanned with an STM and is expected to result in a much less costly instrument having a potential resolution of 1 nm.

NIST uses a very-high-compliance magnetic STM tip that is in direct tunneling contact with the sample. The tunneling signal is used to keep the tip from physical contact with the sample. The resulting image is a convolution of surface topography and magnetic field. If the compliance of the magnetic tunneling tip is high enough, then the contribution of topography to the total image becomes negligible. This method has the potential of pushing the limit of magnetic image resolution to below 1 nm because of the close proximity of the magnetic tip to the sample surface. Tips were produced from pieces of a 1-μm Fe film having a spring constant smaller than 0.01 N/m, in order to detect typical tip sample magnetic forces, and a resonant frequency above 10 kHz, to be immune from instrument vibration. NIST is constructing a cryogenic version for superconductor flux lattice studies.

NIST DELIVERS HIGHLY ACCURATE SENSOR SYSTEM

NIST recently delivered a sensor system to a government manufacturing facility which produces precision turned metal parts. The sensor system requirements were that it measure part thickness from one side, in process, rapidly (about 30,000 measurement locations per part), and with high accuracy (better than 100 μin). The system has been demonstrated at NIST to meet all the measurement requirements. The system uses pulsed ultrasound and a measurement of transit time between the front and back surface of the part to determine local part thickness. The ultrasound is coupled to the part by a laminar stream of coolant/lubricant already in use in the process. The measurements are made in process so that any necessary corrections to the machining path can be made before dimensional control is lost. Plans are under way to enhance the system so that surface finish and shape profile can also be determined in process.

STANDARD E1321 TEST METHOD FOR DETERMINING MATERIAL IGNITION AND FLAME SPREAD PROPERTIES

A new test method for ignition and flame spread successfully passed the American Society for Testing and Materials (ASTM) society ballot. This is the last step to becoming an official standard. The acceptance was formalized at a recent meeting of ASTM E-5. This is the first fire test standard to provide measurement data consistent with theories of ignition and flame spread. Specifically, it provides data for radiative ignition on a vertical surface and data for lateral flame spread in terms of radiant heating, and surface temperature. Material properties can be deduced which can aid manufacturers in assessing the performance of their products in terms of specific components or additives. NIST scientists developed the test method and chaired the ASTM task group that guided the development of the standard. The test is also being considered by the International Standards Organization.

SHEARING APPARATUS FOR SMALL-ANGLE NEUTRON SCATTERING

A couette-type concentric cylindrical apparatus to investigate liquids at equilibrium and under shear by small-angle neutron scattering (SANS) has been developed by NIST scientists. This apparatus is the first of its type designed and built to be a general-purpose tool available to all researchers at a user-oriented neutron scattering facility in the United States. Design features include: a versatile yet rugged construction; a wide range of shear rates (up to 2000 Hz) and operating temperatures; and fully automated operation via a dedicated computer control system.

The cell consists of a stationary cylindrical quartz stator surrounded by a cylindrical quartz rotor with a 0.5 mm gap for the sample. Thermostating fluid is circulated within the stator for temperature control. The outer cylinder is directly coupled to a direct current brushless servo motor whose direction, velocity, and acceleration can be programmed to execute any combination of motion changes.

The cell has been used successfully to observe changes in the interparticle structure associated with the shear melting of charge stabilized colloids of spherical polystyrene latex particles. Other anticipated uses for the apparatus include: the alignment of anisotropic macromolecules by shear flow in order to determine their aspect ratio and orientational relaxation rates, tests of non-Newtonian behavior in both simple and complex fluids, and measurements to relate macro-molecular interactions to bulk rheological properties. Recently, a shear cell has also been developed by NIST scientists for polymer applications.

NIST AND MIT DEVELOP NEW METHOD FOR MEASURING SKIN DOSE FROM HOT PARTICLE EXPOSURE

In a joint project between NIST and the Massachusetts Institute of Technology (MIT), a new method for measuring skin dose from radioactive "hot" particles has been developed. Particles which are found in and around nuclear reactors, and those identified in fallout from the Chernobyl nuclear accident, have resulted in an increased need for more accurate measurement of skin dose. These particles are very small (less than 200 μm in diameter), have high beta-particle activities, and deliver high-dose rates to very small areas of the skin. In the past, dose estimates have been based on radionuclide identification and calculations.

Well-characterized spherical metal particles were fabricated and irradiated at the MIT reactor (to produce mainly ^{60}Co) and sent to NIST for shallow dose rate measurements using radiochromic dye films. A series of exposures was made with each particle, and the films were read on a laser scanning densitometer with a resolution of 40 μm. By combining the film images, dose rate information can be obtained for areas as wide as several mm in radius, which allows dose averaging

over the 1-cm^2 area recommended for dose reporting. Preliminary results show good agreement with other experimental methods and point up shortcomings in currently used dose calculation algorithms.

FLUID-STRUCTURE INTERACTION STUDY COMPLETED IN CCT WATER TUNNEL

An experimental study of the interaction between a high Reynolds number boundary layer and a passive compliant surface has, for the first time, succeeded in producing flow velocity and surface displacement measurements for small amplitude, stable surface waves. This 3-year program was a collaborative effort involving the Office of Naval Research, NIST, and Johns Hopkins University. The program included flow measurement surveys for both noncompliant and two compliant surfaces. Measurement techniques included single component hot-film anemometry and laser-based surface displacement detection. Still photography and videotapes were used to make visual records of the compliant surface motions. Spectral analyses of these results were used to quantify the characteristics of the flow-structure interaction. Based on the results described above, it was concluded that actively controlled surfaces could play a decisive role in fluid-structure interactions. If fluid-structure interactions can be altered in such ways, it may be feasible to modify drag characteristics, acoustic properties, and heat and mass transfer rates. Potential application areas would include mixing processes, drag reduction for surface and underwater vehicles, sound absorption, vibration reduction, and noise shielding.

NEW COMPUTER SIMULATION DESIGN TOOL

Computer simulation of the dynamics of molecules is a powerful and widely used technique for studying the thermal properties of a wide range of materials, including liquids, crystals, and polymers. An important question about these simulations is: "How long must they be run so that reliable results are obtained?" The problem is knowing when the simulation has fully sampled the possible states of the system. To date, the methods used to estimate the time needed for the sampling to converge to the correct answer have all been empirical. Recently a quantitative method to determine convergence times for specific properties has been developed at NIST. The method predicts convergence times using the equivalence of long time interval averages and statistical (ensemble) averages for systems in thermal equilibrium (or in stationary, nonequilibrium states) along with the results of a short time interval simulation. The method is quite general and will be extremely useful in a wide variety of simulations of complex systems.

NIST SPONSORS HYPERTEXT STANDARDIZATION WORKSHOP

A Hypertext standardization workshop to address formally standardization issues was sponsored by NIST in January. Hypertext technology is an approach to information management in which data is stored in a network of nodes connected by links. The nodes, which may contain text, graphics, audio and video, source code, and other data, are viewed through an interactive browser and manipulated through a structure editor.

Papers presented at the workshop focused on requirements, reference models, and candidate specifications. Several well-known researchers and different industry groups already informally involved in some aspect of Hypertext standardization contributed their results to the workshop with the expectation that it could evolve into a more public forum for the planning and development of Hypertext standards.

FUNCTIONAL REQUIREMENTS OF NETWORK MANAGEMENT BASED ON OPEN SYSTEMS INTERCONNECTION (OSI) PUBLISHED

To provide for the management of future interoperable multivendor networks, the International Organization for Standardization (ISO) and other international organizations are developing management standards for communications networks based on the OSI reference model. NIST Special Publication 500-175, Management of Networks Based on Open Systems Interconnection (OSI) Standards: Functional Requirements and Analysis, examines current and proposed network management systems to determine both user and functional requirements for network management.

The report compares the derived functional requirements to emerging standards to determine where and how requirements are being met. Deficiencies are noted in cases where requirements are not being met. The examination of requirements focuses on those necessary for interoperability in the following broad areas: architecture, configuration management, fault management, security management, performance management, and accounting management.

FEDERAL INFORMATION PROCESSING STANDARD (FIPS) 127, DATABASE LANGUAGE STRUCTURED QUERY LANGUAGE (SQL), REVISED

A revision to FIPS 127 was recently approved. The revision incorporates Database Language Embedded SQL (ANSI X3.168-1989), recently published by the American National Standards Institute (ANSI). Embedded SQL adds programming language access alternatives to existing FIPS 127 specifications. Revised FIPS 127 also consists of Database Language SQL (ANSI X3.135-1989), which ANSI will soon publish. In addition, NIST released version 2.0 of the SQL test suite, which helps users and vendors determine compliance with FIPS 127, Database Language SQL. This version of the test suite includes tests for features to be available in the revision of FIPS 127, as well as tests for direct invocation of SQL commands (interactive SQL) and utility software to support the validation process. Version 2.0 replaces version 1.2 of the SQL test suite released in May 1989 and will be used in the SQL testing service that will start in April 1990. Over 40 organizations presently utilize the SQL test suite.

NIST CONTRIBUTES TO ASSESSMENT OF "LEAD IN PAINT" DETECTORS

The Department of Housing and Urban Development (HUD) is in the process of implementing a lead abatement program in public housing. To decide whether abatement is needed, they must determine the lead concentration in paint on walls, rails, cabinets, and so forth. HUD requested NIST to assess methods for measuring lead concentration in paint. NIST has provided the necessary statistical guidance. As part of the overall project, NIST scientists examined x-ray fluorescent (XRF) lead detectors because they are nondestructive and relatively simple to use. In order to assess the measurement quality of two types of commonly used lead-specific XRF detectors under a variety of conditions typically seen in the field, NIST proposed running a statistically planned experiment. This ensured that a balanced set of conditions were studied for each XRF detector and allowed independent evaluation of each source of uncertainty. After running the experiment, graphical and analytical statistical techniques were used to analyze the data. Results indicated that the nondestructive detectors examined were not capable of quantitatively measuring lead concentrations near the regulatory limit of 1 mg/cm^2. The study clearly established that improved techniques are needed.

NIST-MIT RESEARCH IDENTIFIES SOURCE OF WEAK-LINK BEHAVIOR IN CERAMIC SUPERCONDUCTOR

NIST and Massachusetts Institute of Technology scientists have identified the source of weak links in a ceramic superconductor. The superconductor in question is $BaPb_{1-x}Bi_xO_3$, which has a cubic structure and a relatively low critical temperature of 13 K. In spite of its isotropic structure and long coherence length of about 75 Å, this material's grain boundaries behave as weak links. The presence of weak links (unintentional junctions of superconductor-normal material-superconductor or superconductor-insulator-superconductor exhibiting Josephson-effect behavior) in a superconductor restricts its usefulness, as weak links are thought to limit the transport current even at low-magnetic fields. The team found that the weak links are due to Pb-Bi-O rich phases at the grain boundaries which result from melting during annealing. Transport critical current density measurements on samples prepared at low temperatures (below 600 °C) show that weak links are still present, and Auger spectroscopy and scanning transmission electron microscopy reveal a corresponding composition variation at the boundaries. Currently, work is under way to establish the solidus temperature, below which no liquid phase is formed, in this system. The team also is carrying out transport critical current density measurements, as a function of both temperature and applied field, in order to show that the grain boundaries containing second phase behave as superconductor-insulator-superconductor junctions.

NIST REDUCES UNCERTAINTIES IN MEASUREMENTS OF PEAK IMPULSE VOLTAGE

NIST scientists have reduced the uncertainties to ± 0.1 percent in measurements of impulse voltage peaks based on the use of analog oscilloscopes. NIST needs the improved measurement methods for the calibration of voltage dividers to respond to needs of the pulse-power community. Typical oscilloscope uncertainties in the measurement of peak voltages of microsecond impulses have been of the order of ± 1 percent. Researchers previously developed measurement methods that employed dc reference levels and offsets to facilitate measurement on more sensitive oscilloscope scales, with resulting uncertainties of ± 0.3 percent. Building on this work, they have achieved the new reduction by using dc reference voltages applied in the form of voltage steps to reduce the measurement errors

arising from differences in the oscilloscope amplifier's response to pulsed and to dc inputs. The researchers have verified the method using a 5-V standard voltage step maintained by the division and have already applied the method to the calibration of high-voltage impulse dividers.

NIST PROVIDES EPA PRELIMINARY EVALUATION OF THE PERFORMANCE OF VARIOUS REFRIGERANT MIXTURES FOR CONVENTIONAL REFRIGERATORS

At the request of the Environmental Protection Agency (EPA), researchers at NIST developed a vapor compression refrigeration cycle model which was used to evaluate the performance of conventional refrigerators using various refrigerant mixtures. Mixtures of refrigerants that do not damage the ozone layer of the upper atmosphere are considered viable replacements to the refrigerants currently used in household refrigerators. NIST developed CYCLE11, which models the thermodynamic cycle of a household refrigerator and is a modification of the existing CYCLE7 model developed previously by NIST to simulate the cycle in air conditioners and heat pumps. Eleven different binary refrigerant mixtures were evaluated, and the results were presented to EPA. Several of the mixtures improved the steady-state efficiency of the refrigerators between 5 and 10 percent compared to the use of R-12. Future research will focus on modification of the basic refrigeration cycle to get further enhanced performance with refrigerant mixtures.

Standard Reference Materials

NIST ANNOUNCES NEW PORTLAND CEMENT STANDARDS

A new series of Standard Reference Materials (SRMs) has been developed by NIST for the producers and users of Portland cement. SRMs 1884-1889 are used in analyzing the composition of Portland cement by instrumental and chemical analysis. The new series of SRMs replaces the 630 series of materials and covers the same nominal range of concentrations of certified constituents. Information on each of the new SRMs and their certified constituent properties and percent by weight is available from the Office of Standard Reference Materials (OSRM). Available for $98 a unit, each SRM consists of three sealed vials, each containing approximately 5 g of material. To order SRMs 1884-1889, contact: OSRM, NIST, Rm. 204, Bldg. 202, Gaithersburg, MD 20899; telephone: 301/975-6776, FAX: 301/948-3730.

ACCURATE EMISSIONS ANALYSES ARE AIM OF GAS STANDARDS

Enforcement agencies at the federal, state, and local levels regularly survey outdoor pollution levels by measuring exhaust emissions from cars, trucks, and other vehicles. Environmental concentrations of the gases propane, carbon monoxide, and carbon dioxide are key components of such a survey. The reliability of these studies depends on how well laboratory instruments work and how accurate analytical methods are. NIST is now offering four different standard reference materials (SRMs) that can help ensure measurement reliability. Each certified to contain a specified concentration of the three gases in nitrogen, these SRMs can be used to calibrate analytical instruments and to check laboratory methods. By running a sample from one of the SRMs through an instrument, a chemist can compare the results with the concentrations listed for the SRM to determine instrument accuracy. The SRMs, numbers 2725-2728, are available for $870 each from the Office of Standard Reference Materials, NIST, Rm. 204, Bldg. 202, Gaithersburg, MD 20899; telephone: 301/975-6776.

NIST HELPS INDUSTRY WITH VEHICLE EMISSION MEASUREMENTS

With federal limits on vehicle emissions more stringent than ever, car manufacturers need to ensure that measurements are reliable and comparable between in-house labs and with regulatory agencies. Currently, some standards are available for certain emission pollutants that allow chemists to check the accuracy of analytical instruments. Now NIST, in partnership with the Motor Vehicle Manufacturers Association, is developing seven previously unavailable standard reference materials (SRMs) intended to be national standards that will add to the accuracy base of emission measurements. These bottled gas mixtures—nitric oxide in nitrogen and methane in air among them—represent levels of these pollutants typically found in auto exhaust and have been rigorously certified for their concentrations. Since the amount of a given component in these SRMs will be known, chemists can run a sample through their equipment as a reference to calibrate instruments and methods. The materials also will be useful to specialty gas manufacturers who produce the day-to-day standards used by the motor vehicle industry. NIST expects the SRMs to go on sale by fall of 1990.

MICROPOROUS FUMED-SILICA INSULATION

Microporous fumed-silica insulation consists principally of extremely fine particles (~10 nm) of amorphous silica and fine ceramic fibers, forming a light rigid board of extremely low thermal conductivity [of the order of 20 mW/(m×K]. The low conductivity is a result of the very small pore size and tortuous conduction paths of both solid and gaseous components of the bulk material. This material has been previously issued as a NIST standard reference material for thermal resistance at temperatures below 330 K, and will be certified for its apparent thermal conductivity at temperatures from 318 to 733 K (45 to 460 °C) and air pressures from 26.7 to 83.5 kPa (200 to 626 Torr). A report describing these studies, Microporous Fumed-Silica Insulation as a Standard Reference Material of Thermal Resistance (NISTIR 89-3919), is available from the National Technical Information Service, Springfield, VA 22161. Order by PB #90-130311/AS for $17 ($8 for microfiche).

MATERIALS DESIGNED TO HELP MONITOR WATER POLLUTION

Environmental agencies, as well as others studying pollution in the nation's waterways, need materials containing an accurate composition of various compounds as a check to verify the reliability of laboratory instruments and methods. Now NIST has developed a bottled standard reference material (SRM) for this purpose. It contains marine sediment with a wide range of pollutant compounds of interest to environmental scientists. The sediment material, which has certified values for 11 polycyclic aromatic hydrocarbons (PAHs), was collected from the Chesapeake Bay area near Baltimore harbor. It is in dry powdered form which can be reconstituted into wet form so that the compounds can be extracted by solvents for organic analysis. The material also contains noncertified values for other PAHs, polychlorinated biphenyls, and chlorinated pesticides. It is available for $241 from the Office of Standard Reference Materials, NIST, Room 204, Building 202, Gaithersburg, MD 20899; telephone: 301/975-6776.

NIST INVESTIGATES RELATIONSHIP BETWEEN BONDED PHASE MORPHOLOGY AND CHROMATOGRAPHIC SELECTIVITY IN REVERSED-PHASE LIQUID CHROMATOGRAPHY

A major problem confronted by liquid chromatographers worldwide is the unexplained differences in retention behavior among columns that are generically identical, but prepared by different manufacturers or by the same manufacturer at different times. As a result of careful studies of the reversed-phase separation process, scientists at NIST have developed a model that explains the effect of subtle differences in bonded phase morphology on relative retention (selectivity) for structurally similar compounds.

Three molecular probes have been identified whose retention behavior provides the basis for classifying columns according to bonding phase morphology (i.e., those exhibiting behavior characteristic of monomerically or polymerically bound ligands). The elution order for these probes is useful in predicting the efficacy of columns for the difficult separation of isomers. Isomeric separations are becoming increasingly important in nutrition, cancer chemoprevention, and environmental/human health studies.

These efforts have provided the first evidence that temperature influences other parameters besides absolute retention and efficiency (the sharpness of bands). By performing separations of key probe molecules at various temperatures (−30 to 100 °C), it was observed that elution orders can change with temperature and that "monomerically bound" reversed-phase columns that normally provide little selectivity for the separation of isomeric compounds could be made to acquire "polymerically bound" behavior and provide separations of isomers as the temperature is lowered to the appropriate point. Conversely, columns with "polymerically bound" ligands can be induced to acquire "monomerically bound" character by increasing the temperature to the appropriate point.

Columns using "monomerically bound" ligands are used for the vast majority of separations in liquid chromatography. These results provide chromatographers with a tool for fine tuning the selectivity of columns obtained from various sources to meet specific separations needs. The three component probe mixture is being issued as SRM 869 and will be used by both manufacturers and bench scientists worldwide for column classification and quality control.

RADIOCHROMIC DYE STANDARD REFERENCE MATERIAL FOR HIGH-DOSE DOSIMETRY

NIST announces the availability of a new Standard Reference Material (SRM 4500) for the radiation processing industry. SRM 4500 is a radiochromic dye solution which can contribute to the standard-

ization of measurements of absorbed dose in many radiation processing applications, including sterilizing medical devices, curing polymers and elastomers, testing electronics, and extending the shelf life of foods.

These standards can be used to calibrate cobalt-60 or cesium-137 sources of gamma radiation for absorbed dose in the range 50 Gy to 5 kGy (5–500 krad). Once the solution is irradiated, a blue chromophore is formed whose color intensity is linearly related to absorbed dose. The intensity is measured at 600 nm and the corresponding absorbed dose is calculated from the well-established values of the radiation chemical yield of the dye molecules in solution and their linear molar absorption coefficient at 600 nm.

SRM 4500 consists of a set of six flame-sealed amber glass ampoules. Each ampoule contains 5 mL of solution of a radiochromic dye in a solvent composed of 15 percent dimethyl sulfoxide (DMSO) and 85 percent n-propanol. The notes on the use of the SRM provide details on the characterization of the material for stability, dose rate dependence, dose range, and temperature coefficient.

CERTIFICATION OF COCAINE IN URINE SRM COMPLETED

NIST has an ongoing program in cooperation with the College of American Pathologists to provide the drugs- of-abuse testing community with urine-based reference materials. The first such material was SRM 1507, a freeze-dried urine pool certified for the principal urinary metabolite of marijuana (20±2 ng/mL). Scientists at NIST have recently completed work on SRM 1508, a freeze-dried human urine pool with certified concentrations of cocaine and its principal urinary metabolite, benzoylecgonine (BE). Each unit of this SRM consists of four bottles of freeze-dried urine: one bottle for each of three levels of cocaine and BE, plus one bottle of blank urine.

The SRM was certified using two independent methods that agreed within a statistical tolerance. One of the methods was based on a gas chromatography/mass spectrometry (GC/MS) procedure and was similar to those used in drug testing laboratories to confirm positive results from preliminary screening analyses. Information values are provided for the methyl ester of ecgonine, another important metabolite of cocaine in each of the three levels.

The certified concentrations (in ng/mL) in SRM 1508 are as follows: Level 1—cocaine 90±10, BE 104±7; Level 2—cocaine 254±10, BE 261±16; and Level 3—cocaine 425±10, BE 515±32. These concentrations bracket the cutoff level set by the National Institute on Drug Abuse (NIDA) for establishing cocaine abuse, thereby providing laboratories a basis for validating the accuracy of their measurement methods throughout the legally critical concentration range. This SRM should also be of benefit to laboratories making measurements concerning scientific and health-related questions regarding cocaine abuse.

Standard Reference Data

NEW DATABASE ON ELECTRON AND POSITRON STOPPING POWERS AND RANGES AVAILABLE FOR PC USERS

Medical and health physicists, laboratory researchers, and industrial users of high-energy radiation equipment will benefit from a new personal computer (PC) version of an important database developed by NIST. The database also provides for rapid calculations on the collision, radiative, and total stopping powers of materials, their continuous-slowing-down approximation (CSDA) ranges, and the radiation yields for electrons or positrons with kinetic energies from 1 keV to 10 GeV.

The new PC resource, NIST Standard Reference Database 7A, Electron and Positron Stopping Powers and Ranges, was developed from a database that is available for lease on magnetic tape. Unlike the tape version, which can only supply information on the performance of materials in tables of stopping powers and ranges, the PC program gives these quantities for any material that can be described by chemical formula using standard symbols.

The new PC version of the NIST database is available on 3-1/2 in or 5-1/4 in disks for $360. The program can be stored on a hard disk of any AT or XT-Class PC.

To order NIST Standard Reference Database 7A, contact the Office of Standard Reference Data Programs, A323 Physics Bldg., National Institute of Standards and Technology, Gaithersburg, MD 20899; telephone: 301/975-2208.