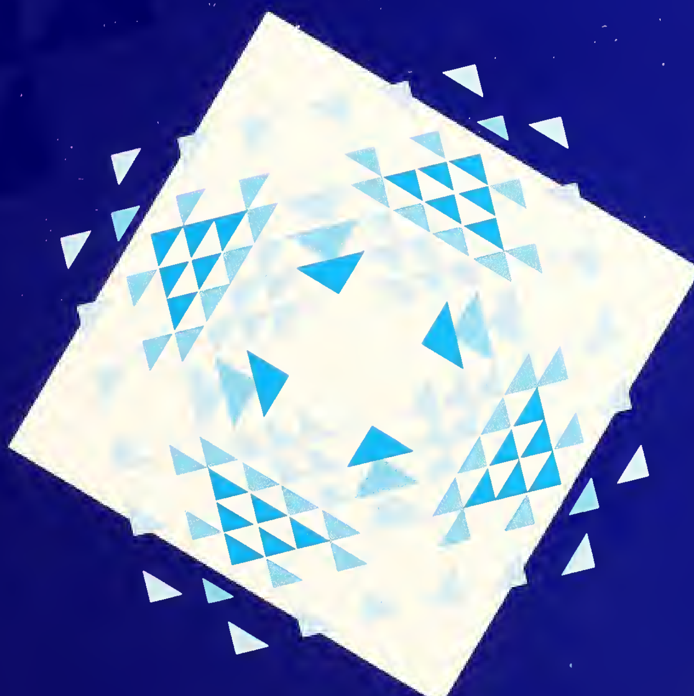
Cooperative Research Opportunities at NIST



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National Institute of Standards and Technology

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The National Bureau of Standards became the National Institute of Standards and Technology on August 23, 1988, under the Omnibus Trade and Competitiveness Act. NIST retains all NBS functions. Its new programs will encourage improved use of technology by U.S. industry.

NIST

Contents

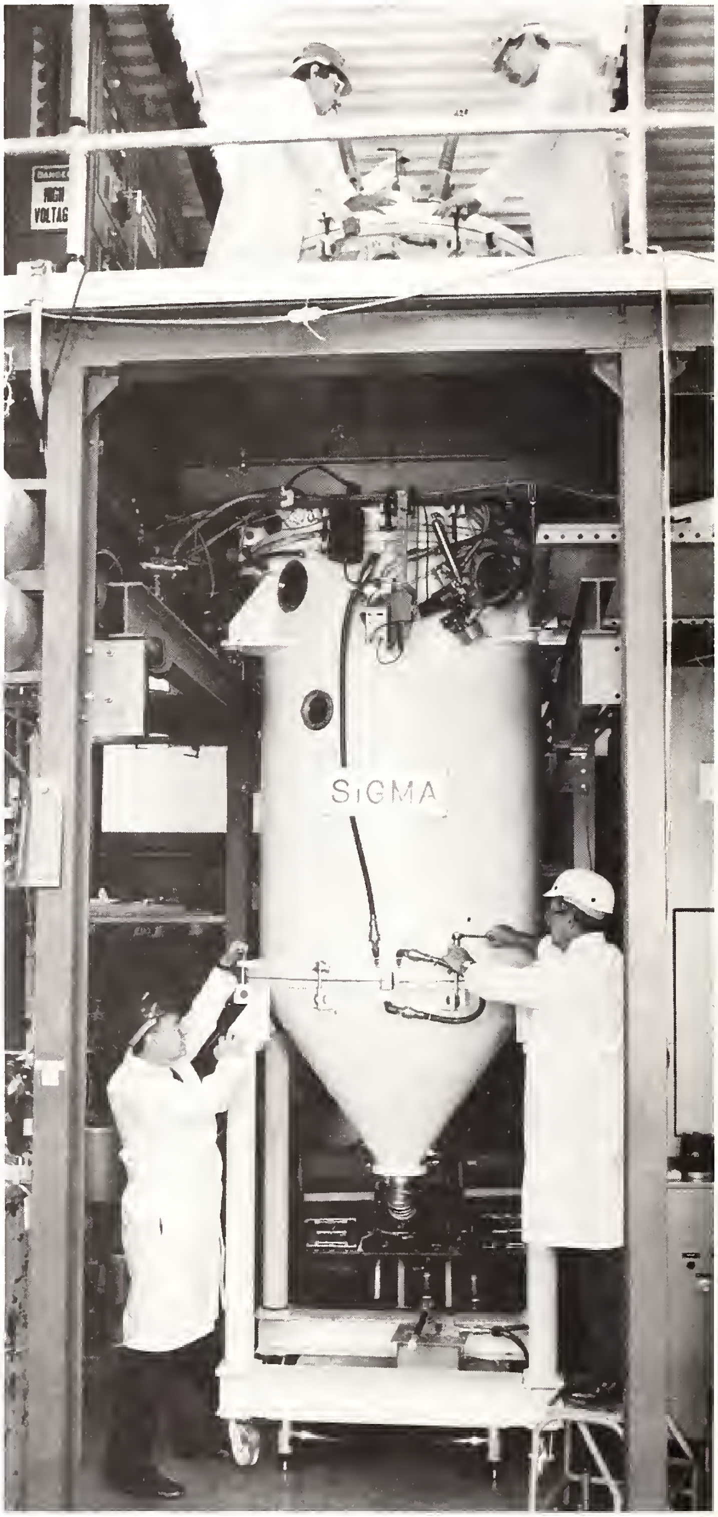
Cooperative Research at NIST

Cooperation has always been part of the Institute's way of doing business. Since its inception in 1901 as the National Bureau of Standards, NIST scientists and engineers have conducted collaborative studies with researchers from industry. Research consortia formed at the Institute were among the first in the nation.

In a given year, about 1,200 scientists and engineers from industry, universities, and other government agencies come to NIST to participate in cooperative research projects, both long- and short-term. Less formal interactions are nearly continuous. For example, more than 15,000 people attend workshops and conferences held at NIST each year, NIST researchers publish about 1,400 papers and reports annually, and one-on-one technical consultations between Institute scientists and those in other organizations occur daily.

Through these collaborations, researchers from industry, universities, and other government agencies get an opportunity to work with NIST specialists, many of whom are renowned experts in their fields, and to use the Institute's premier research and testing facilities. They take newly developed technology back to their organizations to be incorporated immediately into new ideas, new processes, and new products. NIST researchers, in turn, learn firsthand the views and needs of Institute clients and, as a result, NIST is better able to direct its research to meet these needs.

Operated on an annual budget of about $285 million, NIST has been a valuable behind-the-scenes partner of industry and academia, providing the standards and measurement techniques that foster technological advance, domestic and international commerce, and, ultimately, economic progress. With the enactment of the Omnibus Trade and Competitiveness Act in 1988, however, the Institute not only underwent a name change, but was designated the federal government's catalyst for speeding innovation and accelerating the adoption of new technologies and new ideas by U.S. companies. The 1988 law opens more avenues for cooperation between NIST and industry, universities, federal laboratories, state and local governments—any organization that has an active stake in helping U.S. business compete more effectively.



Researchers at NIST are developing automated production techniques for rapidly solidified metal powders.

NIST will work with any company, trade association, university, or other government agency to solve problems of mutual concern. Its highly skilled staff of some 3,000 conduct a wide range of projects, many at the forefront of science and technology. About half of the Institute's scientists and engineers are focusing their efforts on the emerging technologies, including advanced materials, optoelectronics, automation, computing, superconductivity, biotechnology, and thin-layer technology.

One of the most popular ways NIST research and facilities are made accessible to U.S. industry is through the Institute's Research Associate Program. Under this program, companies, trade associations, and technical societies pay their scientists and engineers to work in NIST laboratories with NIST researchers on a specific project.

The longest running research associate program has been a remarkably successful collaboration with the American Dental Association. Started in 1928, the alliance has resulted in the panoramic x-ray machine, composite restorative materials, and the high-speed turbine handpiece, for example, as well as major contributions to dozens of standards for dental materials and hundreds of scientific papers.

In another type of cooperative venture, companies subscribe to a consortium that provides resources for NIST to solve a specific problem facing the industry. This arrangement has advantages when a complex problem—usually development of generic technology or measurement techniques—confronts a particular industry and the research is too costly or not possible for individual companies to undertake.

Companies also donate or loan equipment or software to the Institute when NIST researchers are working on a project that could ultimately improve their products or the way they do business. In such situations, these firms actively consult or advise NIST researchers on the needs and concerns of the industry.

To aid firms in building a competitive advantage, NIST makes available for cooperative research its extensive research and testing facilities at its headquarters in Gaithersburg, Md., and its site in Boulder, Colo. A 20-megawatt research reactor with a cold neutron source, a synchrotron ultraviolet radiation facility, a supercomputer, a large-scale structures testing facility, a metals-processing laboratory, a fire research facility, and a computer network and security facility are but a few of the facilities available. In certain cases, NIST makes its facilities available to companies for proprietary research on a cost-recovery basis, when equal or superior facilities are not otherwise available.

Described below are a few brief examples of different types of cooperative projects and the results they have produced so far. The scope, duration, and structure of the cooperative projects are tailored to the problem to be solved. They can last for a few weeks or a few years and involve one, several, or even hundreds of organizations. The goal is to solve the problem at hand quickly, efficiently, and effectively.

Metal Powder Processing

Crucible Materials, Inc. and the General Electric Corp. are continuing to work with NIST in a consortium to develop automated processing technology for rapidly solidified metal powders. Rapidly solidified metal powders provide a basis for alloys that can exhibit, after consolidation, unique properties, such as high strength-to-weight ratios, excellent fracture toughness and fatigue resistance, unusual magnetic properties, and high corrosion resistance.

Current processes for producing these powders are both labor intensive and lacking in reproducibility; rejection rates are high. The goal of the industry/NIST project is to develop generic research results that will facilitate the automation of different atomization facilities for producing rapidly solidified metal powders, while improving product quality and productivity.

Consortium researchers are designing process models, an expert system, and automated control strategies that will be linked by a computerized control system for the intelligent processing of rapidly solidified metal powders. A major component of the system is an optically based, on-line sensor for monitoring the metal powders while they are being produced.

Magnetic Microscope

NIST has developed an instrument for providing images of the magnetic microstructure of materials with a resolution about a factor of 100 better than conventional imaging techniques. Using a technique called Scanning Electron Microscopy with Polarization Analysis (SEMPA), researchers are able to provide direct images of magnetic microstructure with a resolution of about 0.05 microns.

In cooperation with industry, this "magnetic microscope" is being used to observe details of the magnetic domain structure responsible for the performance of high-technology materials. The ability to see magnetic domains with such clarity is important to the information storage device industry. For example, the storage capacity and fidelity of magnetic tapes and disks depends upon how small magnetic "bits" can be made and the sharpness of the boundaries between the bits. Until now improvements have been limited by the inability to measure magnetic microstructure at the submicron level.

This research has involved extensive collaboration with industry. A number of industrial scientists—from Honeywell, Control Data Corp., Kodak, Westinghouse, Digital Equipment Corp., among others—provided samples for high-resolution analysis. Control Data Corp. and Kodak sent researchers to NIST to help improve the method. Other companies provided some funds for equipment and measurement services. NIST scientists are now working with an industrial consortium—Perkin-Elmer, Control Data Corp., and Honeywell—to develop a second generation, commercially available magnetic microscope. They also are helping several universities to establish SEMPA capabilities.

Open Systems Interconnection Network (OSINET)

For the past several years, NIST has worked with government, industry, and standards groups in support of national and international standardization of Open Systems Interconnection (OSI). International standards for OSI are being developed to overcome common problems that users of computer systems face in integrating large and small computers, networks, workstations, and communications services, and in transferring information between different systems.

To advance this goal, NIST established OSINET, a cooperative government/industry research network that is expediting the development and use of commercial OSI products. With 25 participants and network nodes throughout the United States and in several overseas locations, OSINET is a successful research tool for remote testing of OSI protocols and for vendor interoperability testing.

OSINET also is used by government and industry managers to assess the

NIST computer scientists are working with researchers from private industry to develop security features for "open" computer networks.

applicability of OSI to the needs of their organizations, to monitor the progress of OSI products, and to acquire practical experience in using OSI technology.

Optical Fiber Metrology

As optical fiber metrology moved from the laboratory to commercial applications, NIST worked with the Electronic Industries Association and its associated Telecommunications Industry Association, as well as other organizations, to develop the measurements upon which voluntary industry standards could be based.

The NIST work, which usually involved industry-wide round robins, has provided the measurement basis for 28 industry standards adopted by these voluntary standards groups. For example, the diameter of the core of a fiber affects the loss of light during transmission as well as at connections. NIST, with the cooperation of the industry, conducted comparative measurements of various techniques used to make this measurement, identified the shortcomings of various approaches, and provided the technical basis for a voluntary standard for this measurement.

Radioactivity Measurements

A collaborative project sponsored by NIST and the U.S. Council for Energy Awareness (USCEA) has confirmed the ability of radiochemistry laboratories in the nuclear-power industry to assay several types of radionuclides with sufficient accuracy. In the first year of the program, two USCEA research associates worked with NIST scientists to prepare and distribute special test samples to 12 utilities that operate over 30 percent of the existing generating units in the United States. The company supplying radiochemistry measurement services to the largest number of U.S. power-generating units also was tested.

Additional tests involving gaseous radionuclides, mixtures, and special forms simulating field samples are scheduled with three more utilities planning to participate. A unique feature of the program is the participation of the industry's three major suppliers of commercial calibration and test samples. These companies not only take part in tests prepared for the power-plant laboratories, they also have their measuring ability checked by sending materials they have certified to NIST for verification.

Electronics technician Michael Huff (left) and project chief Kang Lee monitor the Mare Island Flexible Workstation , the first large-scale transfer of flexible and automation technology from the AMRF to a production facility.

Automated Manufacturing

In a cooperative project with the Navy, Westinghouse Corp., and Warner & Swasey Company, NIST researchers have designed and assembled a state-of-the-art manufacturing system for the Navy shipyard at Mare Island, Calif. The flexible manufacturing workstation is capable of operating, largely unattended, 24 hours a day.

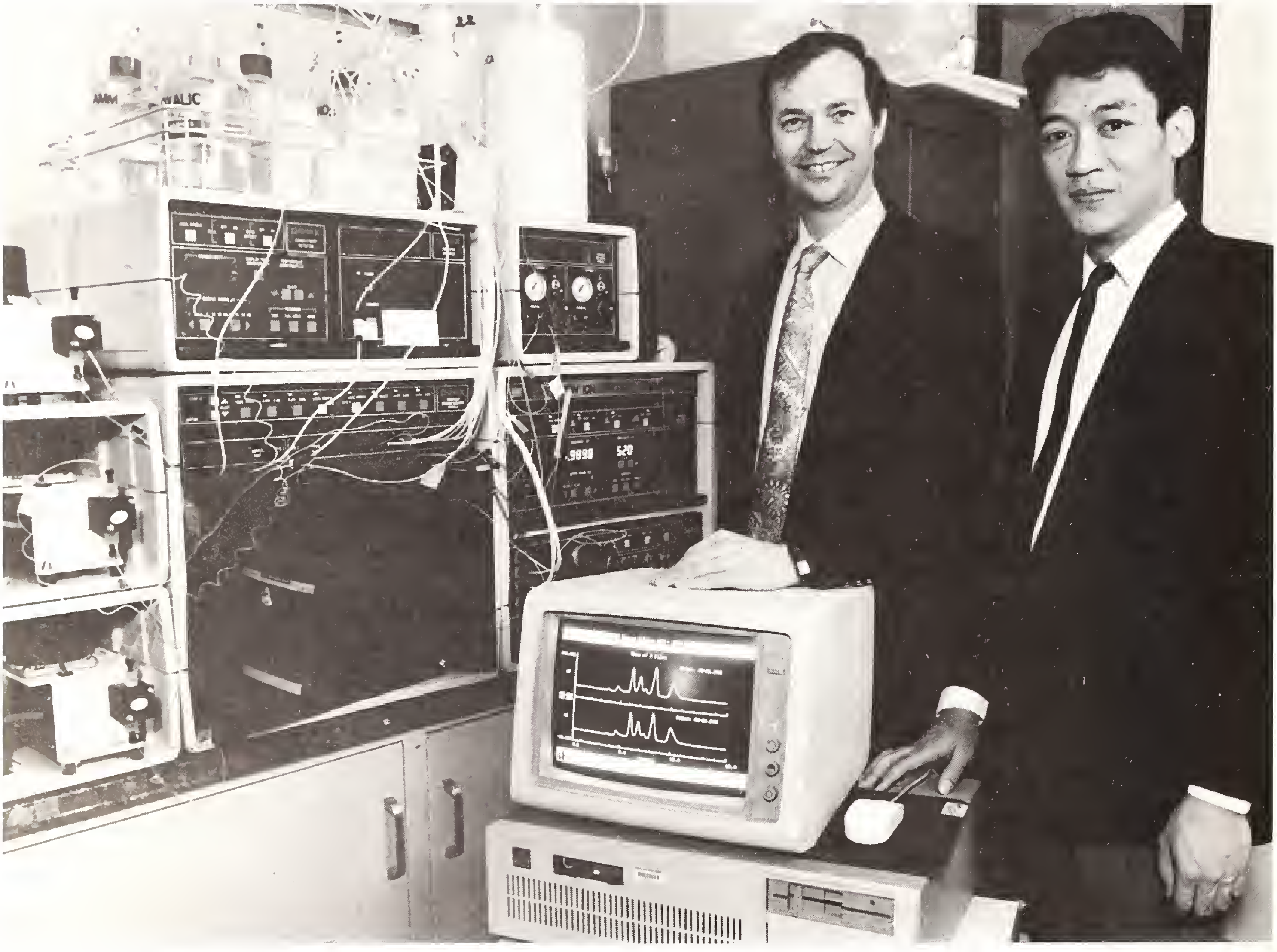
Consisting of an automated multipurpose machining center, industrial robot, automated storage and retrieval system, and various control computers, the Mare Island workstation incorporates several advanced automation techniques, such as chuck jaw changing and tool-condition monitoring. The workstation is designed to produce any of 84 different parts used in nuclear submarines. These parts are not stockpiled, rather they are produced on demand.

Current manual methods require an average of 17 hours to make one such part. The new workstation reduces that to under 30 minutes. The advanced techniques used in the workstation, many of which were developed in NIST's Automated Manufacturing Research Facility (AMRF), are applicable to a variety of manufacturing operations. The AMRF is an experimental facility designed to study the application of advanced robotic and computer-control techniques to small-batch manufacturing.

Research Opportunities

NIST welcomes collaboration with scientists and engineers from industry, universities, and other government agencies on most of its projects. To give those interested in cooperative research an idea of the wide array of NIST programs, a sampling of specific Institute research projects is described on the following pages.

If you are interested in working with NIST on a project, large or small, write or call the NIST Office of Technology Commercialization, 301/975-3085, or one of the contacts given with the project descriptions. (Unless otherwise specified, all contacts are at the National Institute of Standards and Technology, Gaithersburg, MD 20899.)



A collaborative effort between NIST and Dionex Corporation resulted in the development of a chelation ion chromatography system. H.M. (Skip) Kingston of NIST (left) and Archava Siriraks of Dionex are shown with the system, which was named one of the 100 most significant products of 1988 by Research and Development *magazine.*

Analytical Chemistry

Atomic Spectroscopy

Atomic spectroscopy methods are probably the most widely used analytical techniques in industry today. Considerable research is required, however, to keep up with the changing needs of industry. At NIST, research in atomic spectrometry is focused on several different areas. For instance, researchers are working to improve the analytical capabilities of direct current plasma (DCP) and inductively coupled plasma (ICP), as well as experimenting with the glow discharge as an atom reservoir. Additional research concerns the use of spark sampling for the direct analysis of solids, the continued development of laser-enhanced ionization (LEI) in flames, and the evaluation of various types of coupled chromatographic-spectrometric systems to improve the accuracy of spectroscopic measurements.

NIST scientists also are developing a series of neutral density filters that can be issued as Standard Reference Materials for verifying the accuracy of the transmittance and absorbance scales of ultraviolet, visible, and near infrared absorption spectrophotometers.

Contact: Robert L. Watters, B222 Chemistry Bldg., 301/975-4122.

Analytical Mass Spectrometry

Analytical mass spectrometry has played a key role in industries, such as the semiconductor industry, which require accurate measurements of trace elements in their raw materials, products, and product containers. The inorganic mass spectrometry program at NIST is concerned with developing analytical capabilities for making highly accurate determinations of trace inorganics using stable isotope dilution and highly precise measurements of isotopic compositions, as well as the highly accurate measurement of absolute isotopic compositions to redetermine atomic weights. Areas of research include instrumentation in spark source, thermal source, inductively coupled plasma source, and laser source mass spectrometry and chemical separations at the trace level using ion chromatography and other techniques.

Contact: John D. Fassett, A21 Physics Bldg., 301/975-4109.

Inorganic Electroanalytical Research

Electroanalytical research plays a key role in the development of methods and materials for environmental and clinical determinations. A broad range of electroanalytical and chromatographic techniques, such as voltammetry, coulometry, ion chromatography, and chelation ion chromatography, are used by researchers at NIST for analysis and research. Scientists at the Institute have developed novel methods and instrumentation, such as microwave decomposition equipment and unique laboratory robotic equipment that uses hierarchical computer control. Instrumentation is available for making accurate pH, potentiometric, coulometric, conductometric, voltammetric, and ion chromatographic measurements and for research in analytical laboratory automation.

Contact: H.M. "Skip" Kingston, A345 Chemistry Bldg., 301/975-4136.

Activation Analysis

More than 50 billion chemical analyses are performed annually in the United States. Researchers at NIST help to ensure the accuracy of these analyses by developing new analytical procedures and improving the reliability and accuracy of present methods. One technique under study is activation analysis, a highly sensitive analytical technique not normally available in industrial laboratories. In this research, methods of nuclear analysis are investigated utilizing the 20-MW NIST research reactor. All areas of the technique are researched, including the capabilities of cold-neutron activation, the use of monitor activation, radiochemical separations, the determination of new mathematical procedures for the resolution of gamma spectra, the development of prompt gamma activation techniques, and the use of charged-particle activation techniques.

Contact: Robert R. Greenberg, B108 Reactor Bldg., 301/975-6285.

Liquid Chromatography Electrochemistry

Although liquid chromatography (LC) is one of the most widely used analytical techniques in industrial laboratories, its use can be made even more widespread by improvements in detection methods. NIST researchers are working to develop novel approaches for the electrochemical detection of organic analytes separated by liquid chromatography. For this technique to be applied most effectively, the electrode reaction mechanisms of the compounds to be detected must be investigated using techniques such as cyclic and reverse-pulse voltammetry, coulometry, and LC/ultraviolet spectroscopy. Ongoing NIST work focuses on the use of differential pulse and dual-electrode detection, as well as the development of single- and array-microelectrode detectors. Researchers also are developing new liquid chromatographic separations employing specific chemical interactions, including chelation, ion-pairing, charge transfer complexation, and acid-base equilibria.

Contact: William A. MacCrehan, A113 Chemistry Bldg., 301/975-3122.

To help improve the specificity and sensitivity of biosensing devices, research chemists Anne Plant and Steven Choquette investigate the optical characteristics of fluorescent molecules used in the amplification of biosensor response.

Bioanalytical Sensors

Biosensors are the newest generation of analytical devices with the potential for widespread use in biomedical and industrial monitoring applications. Biosensors will incorporate the latest advances in biotechnology to provide high specificity and sensitivity. Biologically derived substances have great value as components of rapid-sensing devices because of their binding specificity, the strength of their interactions, and their potential for use in a wide variety of amplification schemes. Immunological, enzymatic, and receptor-ligand interactions are being explored as the basis for analytical devices.

NIST researchers are using a variety of optical and electrochemical techniques for detection. Detection can be based on such diverse changes as size and rotational mobility of analytes or binding agents upon interaction, or can be the result of enzymatic activity which occurs due to analyte binding, causing enhanced fluorescence or electrochemical signal. Amplification can be achieved with release to liposome-encapsulated molecules, multi-turnover enzyme reactions, ion-exchange polymer-modified electrodes, and so forth. Combining high specificity for analytes with efficient amplification provides the potential for extremely sensitive devices.

Contact: Richard A. Durst, A113 Chemistry Bldg., 301/975-3118.

Supercritical Fluid Chromatography

Supercritical fluid chromatography (SFC) in both capillary and packed columns offers several advantages over liquid and gas chromatography (GC) for high-efficiency separations of nonvolatile molecules. NIST researchers in this area are investigating the variables that influence the retention, selectivity, and efficiency of SFC systems and the development of SFC as a useful analytical technique to provide high-efficiency separations of complex mixtures. Both packed-column and capillary SFC instrumentation are used for making state-of-the-art measurements. The application of supercritical fluid extraction combined with SFC and GC analysis is under investigation.

Contact: Stephen N. Chesler, 301/975-3102 or Stephen A. Wise, 301/975-3112, A113 Chemistry Bldg.

Liquid Chromatographic Stationary Phases

Liquid chromatography (LC) on chemically bonded stationary phases (e.g., C_{18}, C_8, NH_2, and NO_2) offers unique capabilities for the separation of isomeric compounds or compound classes. However, significant differences in retention and selectivity characteristics, such as relative retention, have been observed among commercial phases produced by different manufacturers and even within different batches prepared by the same manufacturer.

NIST researchers are working to understand which factors influence LC retention on these various stationary phases to predict, improve, and control the separation selectivity. In reversed-phase LC on C_{18} phases, polycyclic aromatic hydrocarbons have been used as model nonpolar solutes to study retention mechanisms and selectivity. The scientists have studied various physical parameters of these solutes to determine their influence on retention and selectivity in LC. Their investigations have focused on both the physical and chromatographic characterization of these stationary phases. A variety of methods are available at NIST for physical characterization of these materials, including carbon analysis, gas adsorption surface area techniques, infrared and nuclear magnetic resonance spectroscopy, and small-angle neutron scattering techniques. Currently, NIST scientists are attempting to develop chromatographic test mixtures to evaluate LC stationary phase characteristics and chromatographic performance. Such "performance" standards would allow direct comparison of the various LC phases produced by different manufacturers and provide insight into the development of improved stationary phases for specific separations.

Contact: Stephen A. Wise, 301/975-3112 or Lane C. Saunders, 301/975-3117, A113 Chemistry Bldg.

Multidimensional and Very High-Resolution Gas Chromatography

Analysts are able to use multidimensional (dual column) and very high-resolution (100,000 plates) gas chromatographic methods to perform difficult separations to facilitate species-specific quantitation. These high-resolution techniques are being investigated at NIST to develop highly specific analytical procedures to quantitate pg/g organic constituents contained in complex environmental and clinical matrices. Research in this area focuses on optimizing multidimensional gas chromatographic experiments in which two capillary columns, each possessing individual and different retention mechanisms, are serially connected by a pneumatic switch. In addition, scientists at NIST are using and developing tailored, very high-resolution capillary columns. An independently controllable, dual-oven gas chromatograph is available for multidimensional research. Additional facilities and equipment include state-of-the-art sample preparation and gas chromatography laboratories, eight capillary gas chromatographs with multiple specific and nonspecific detectors, and a large laboratory information management system (LIMS).

Contact: Stephen N. Chesler, 301/975-3102 or Franklin Guenther, 301/975-3105, A113 Chemistry Bldg.

Nuclear Magnetic Resonance Spectroscopy of Bio-organics

A major task in the industrial production of organic fine chemicals, drugs and antibiotics, and biomolecules is the characterization of the product for both compositional analysis and quality control. Nuclear magnetic resonance (NMR) spectroscopy has proved to be a powerful and widely used tool for these and related purposes.

One NIST program in this area involves the development of new and improved methods for the structural, quantitative, and conformational analysis of materials of chemical and biotechnological importance. The principal techniques being investigated include multinuclear, two-dimensional NMR and its combination with multiple quantum methods and polarization transfer techniques (DEPT and POMMIE). A specific goal of this work is the development of new two-dimensional spectrum editing and filtering techniques and their application to structural and conformational characterization via correlations with multinuclear chemical shifts, coupling constants, relaxation times, and nuclear Overhauser effects. Scientists at NIST use a high-field (400-MHz) multinuclear NMR spectrometer equipped with a process controller, a high-capacity data acquisition system, an array processor, and an off-line data processing station.

Contact: Bruce Coxon, A361 Chemistry Bldg., 301/975-3135.

Protein Characterization by Two-Dimensional Electrophoresis

NIST researchers are using a two-dimensional electrophoresis system to characterize proteins and peptides. They are probing the influence of size, shape, and charge on migration characteristics in the electrophoretic medium. Although well-defined protein "markers," especially of high molecular weight, are required to allow standardization of polyacrylamide gel electrophoretic systems, charged polymeric materials other than proteins may be considered for markers. Because staining and detection of such markers is of special interest, the researchers plan to examine the mechanisms of silver stains using neutron activation techniques. Additional studies will be directed toward understanding the interactions of proteins with metal ions.The researchers will use image processing by state-of-the-art instrumentation to form meaningful databases. As part of this program, NIST plans to issue well-characterized mixtures of proteins as Standard Reference Materials (SRM's) that will be used to assess the abilities of existing and new electrophoretic techniques to separate and detect proteins.

Contact: Dennis Reeder, A361 Chemistry Bldg., 301/975-3128.

Capillary Zone Electrophoresis

The new technique of electrophoresis in small bore capillaries promises to revolutionize the separation of charged molecules. However, since the highest efficiencies are obtained with small sample sizes (nL) in narrow bore (≈10 µm) columns, this presents a challenge in microdetection technology. Detection schemes being investigated at NIST include conductivity, amperometry, UV absorbance, fluorescence, and mass spectrometry. Much work is needed to design the chemistry of the mobile phase and capillary column to suit the analytical need. Ion-pair, complexing, and micellar agents, as well as pH manipulation, can be used to enhance the selectivity of the separations of ionic and neutral molecules. Derivatization of the capillary surface can control the bulk electro-osmotic flow and prevent the adsorption of the analyte molecules. NIST researchers will use the technique to investigate the fundamental property of the electrophoretic mobility and to determine important analytes such as proteins, peptides, DNA fragments, and trace metals.

Contact: William A. MacCrehan, A113 Chemistry Bldg., 301/975-3122.

Microbeam Compositional Mapping

Interpreting the relationship between the physical and chemical microstructure of materials is important in understanding their macroscopic behavior and in extending their in-service performance. Conventional microbeam techniques for elemental/molecular compositional analysis on the micrometer scale, such as the electron microprobe and ion microscope, have been restricted to quantitative analysis at individual locations. Mapping of the distribution of constituents has been possible only at the qualitative or semiquantitative level. However, recent NIST research developments have led to the production of the first true quantitative elemental compositional maps. Quantitative compositional mapping with the electron microprobe has been demonstrated down to levels of 0.1 weight percent, while quantitative isotope ratio measurement in images has been demonstrated with the ion microscope.

Current research activities at NIST include extending compositional mapping to analytical electron microscopy, laser Raman microanalysis, and laser microprobe mass analysis. Potential projects could involve applying the compositional mapping instruments to materials characterization problems, developing new techniques for compositional mapping on other microanalysis instruments, and investigating basic topics in elemental and molecular quantitative analysis with microbeam instrumentation.

Among the equipment available at NIST is an electron microprobe, an analytical scanning electron microscope, 200- and 300-kV analytical electron microscopes, an ion microscope (secondary ion mass spectrometry, SIMS), a time-of-flight SIMS, a laser microprobe mass analyzer, two laser Raman microprobes of NIST design, and extensive computer facilities, including a VAX 11/780 computer, micro-Vaxes, and a DeAnza image processor.

Contact: Dale E. Newbury, B364 Chemistry Bldg., 301/975-3921.

Trace Gas Measurement Techniques

Accurate measurement of gaseous species is of great importance to many industries for a number of applications ranging from the quantification of pollutant and toxic gas emissions to the quality control of products. The validity of data derived from such measurements is tied directly to the availability of useful gas measurement techniques and to the degree of understanding of their capabilities and limitations. Although a variety of techniques have been applied to trace gas analysis, more research is needed to improve the present state of the art. This research is particularly important due to the growing need for the analysis of specific gas species in multicomponent gaseous mixtures; it also is necessary to extend accurate analyses to below the parts-per-million and parts-per-billion levels. Current NIST research focuses on new detection systems using chemiluminescence, electrochemistry, infrared diode laser systems, capillary gas-liquid and gas-solid chromatography coupled to mass spectrometry, and isotope-dilution mass spectrometry. Institute scientists also are examining the use of class-specific detectors for gas chromatography and evaluating electronic circuitry to optimize signals and reduce instrumentation noise and drift.

Contact: William D. Dorko, B364 Chemistry Bldg., 301/975-3916.

Instability of Compressed Gas Mixtures

Inorganic and organic compressed gas mixtures are employed extensively throughout industry to calibrate equipment used to assess the quality of products and the effectiveness of emission controls. Although the stability of these mixtures is critical to their successful use, a number of instances have been noted in which instability has been observed, particularly in mixtures containing low levels of reactive gaseous species, such as nitrogen oxides, sulfur dioxide, and hydrocarbons. The reasons for instability may differ somewhat for different gaseous species, but they are related to at least two possible phenomena: gas-phase reactions and gas-metal interactions with the internal surface of the cylinder. NIST researchers are working to improve the understanding and predictability of these phenomena. Their techniques involve those employed in surface science studies and other approaches, such as Fourier-transform infrared, diode laser, and other spectroscopies; mass spectrometry; metal analysis; trace water and oxygen analysis; chemiluminescence analysis; and the use of specifically doped mixtures and homogeneous gas phase kinetics.

Contact: Walter L. Zielinski, Jr., B364 Chemistry Bldg., 301/975-3918.

Applied Mathematics

Performance of Parallel Computers

In a project designed to measure the performance of parallel computers, NIST researchers are focusing on two major questions: How can codes be improved? and What types of codes should be run on a given machine? They are evaluating the performance of algorithms on parallel computers by using data motion as the principal determining factor. Their approach to performance measurement is to develop a taxonomy of algorithmic paradigms based on how the data move during a calculation, rather than on what the specific computation steps are.

The scientists will implement benchmark codes typical of applications in each class of the taxonomy on two different parallel computers in order to obtain detailed measures of performance. The target machines for measurements are representative of the two main classes of MIMD parallel architectures: loosely coupled, message-passing machines and tightly coupled, shared-memory machines.

Contact: Francis Sullivan, A438 Administration Bldg., 301/975-2732.

Design for Quality

Through its Design for Quality program, NIST supports collaborative research within NIST and with industry, technical societies, and universities to develop and refine effective and efficient statistical, mathematical, and computer-based techniques for quality improvement. These techniques are designed for ease of use by industrial scientists and engineers and are disseminated through research collaborations with industry, tutorials, and workshops.

Statistically planned experiments (SPE's), effective and efficient techniques for improving quality, are being used to accelerate the development of new and improved industrial process designs. At NIST, researchers are employing these techniques to improve fabrication of advanced ceramics for cutting tools and of superconducting ceramics. SPE's are also being used to develop a reliable and cost-effective method to measure the size distribution of silicon nitride powders. Collaborative research opportunities for developing other SPE's exist in the following areas: polymers and other composites processing, dental and medical materials fabrication, automated flexible manufacturing, integrated circuit fabrication, optoelectronics, and bioprocess engineering.

Contact: Raghu N. Kacker, A337 Administration Bldg., 301/975-2109.

Measurement Assurance

Quality assurance for physical and chemical measurements supporting technology transfer and on-line quality control demands statistical methods applicable to complex models. NIST researchers critique methods for their resistance to outliers and their capacity to detect autocorrelation in highly precise measurement systems.

In multivariate settings, such as electronic test systems, estimation of uncertainty and statistical tolerance limits can be complicated by variance components from multiple sources. Researchers also are investigating the applicability of artificial intelligence to complex analyses. Calibrations, where instrument response depends on stimuli over a regime, support critical measurement areas such as radiation dose measurements. NIST research in this area is focused on optimal procedures to accommodate real-life models such as random changes in instrument response over time and gradual instrumental drift.

Contact: Carroll Croarkin, A337 Administration Bldg., 301/ 975-2849.

Computational Mechanics

At NIST, researchers are designing comprehensive software for modeling and database applications in materials science and engineering. NIST research on computer-aided modeling of the behavior of structural materials and components ranges from microscopic feature analysis of fatigue, fracture, phase change, creep, and polymer crystallization to the stress-life prediction of structural reliability of critical components based on mechanical and flaw-detection testing. In these studies, NIST researchers emphasize the interplay among the choices of data representation, appropriate physical principles, incisive mathematical and computational tools, and integrated software for graphics and databases. In addition, they are interested in mathematical theories of elasticity, plasticity, viscoelasticity, as well as mathematical methods using matrix theory, finite-element algorithms, bifurcation analysis, statistical distribution concepts and sampling theory, and stochastic differential equations.

Contact: Jeffrey T. Fong, A302 Administration Bldg., 301/975-2720.

Nonlinear Mechanics

Mathematical analysis, used with symbolic computation, leads to efficient analytical approximations by computers. Perturbation algorithms applied to nonlinear differential equations, especially in celestial mechanics, result in analytical developments where the complexity grows exponentially with the order of the approximation. Several different avenues are being explored by scientists at NIST to simplify literal developments generated by perturbation algorithms applied to nonlinear systems. These include identification of algebraic structures on the domain of the normalization, smoothing transformations to eliminate perturbation terms outside the kernel of the Lie derivative, preparatory transformations of a geometric nature, and the creation of natural intermediaries. Problems being examined at NIST are resonances at an equilibrium, perturbed pendulums, and the major theories of celestial mechanics. NIST researchers, using a LISP computer, are focusing their studies on algorithms amenable to computer automation through symbolic processors.

Contact: Andre Deprit, A302 Administration Bldg., 301/975-2709.

Vector Algorithms and Mathematical Software

To make effective use of vector computers, new algorithms appropriate to the special architecture of these machines need to be designed and incorporated in high-quality mathematical software for general use. Very successful vector algorithms have been developed for computations in numerical linear algebra (e.g., computation of the discrete Fourier transform), but few are available for combinatorial problems. One area of NIST research is concerned with developing vector algorithms appropriate to the combinatorial problems encountered in molecular dynamics simulations, particularly three-dimensional simulations with very large ensembles of particles. Other areas of interest include methods for solving highly nonlinear elliptic and parabolic partial differential equations as well as nonlinear constrained and unconstrained optimization problems and the solution of nonlinear systems of equations. NIST researchers also are working on the solution of integral equations and numerical evaluation of integrals. Software development goals include portable, interactive packages, which integrate modern graphics with numerical algorithms.

Contact: Paul Boggs, A151 Technology Bldg., 301/975-3800.

Scientific Visualization

Researchers at NIST are developing and applying advanced methods for the use of state-of-the-art, computer-based scientific graphics for visual rendering of complex experimental, computational, and analytic results in physics and chemistry. Researchers take advantage of a collection of vector and raster workstations, photographic and video hardware, high-speed networking for transmitting large graphics data sets between computers and graphics devices, and computational geometry algorithms and software for the analysis of two- and three-dimensional data sets. Recent activities include the development of easy user interfaces to manipulate static objects and of techniques to manipulate dynamic objects in automated design and manufacturing systems, the display of quasicrystal structures with icosahedral symmetries, the display of scanning electron tunneling microscopy data with polarization analysis, and the study of models of turbulent combustion showing the dependence of solutions on time and fuel-oxidizer mixture parameters.

Contact: Sally E. Howe, B146 Technology Bldg., 301/975-3807.

Atomic, Molecular, and Optical Physics

Studies of Semiconductor Materials

The growth of gallium arsenide (GaAs) semiconductors on silicon substrates has generated considerable interest due to the excellent mechanical strength and thermal properties of the substrates—qualities not provided by the GaAs material alone. A major difficulty in growing GaAs on silicon has been the mismatch of lattice constants and the concomitant incorporation defects. However, new studies show that a better match of the lattices can be achieved if the silicon substrate is cut at a small angle to the crystal plane. NIST scientists are investigating the interaction of relevant semiconductor materials with silicon substrates, using sensitive, tunable laser sources to detect the individual states of the atoms and molecules as they interact with the growth substrate and growing material. Complete surface diagnostics and ultrahigh vacuum conditions are used in this work. The researchers are determining the sticking coefficients and adsorption energies of individual spin-orbit states of gallium atoms and other dopant atoms plus the effects of vibrational excitation of arsenic dimers on the growth of GaAs semiconductor materials.

Another study involves the deposition of thin films of amorphous silicon, which are used in photosensitive devices and in photovoltaic cells. Scientists are examining mechanisms involved in silane discharge and thermal chemical vapor deposition (CVD) production of such films. Mass spectrometry is used to study gas discharge processes, gas chemistry, and surface chemistry and their effect on film growth, character, and quality. Researchers are operating a threshold-ionization mass spectrometer that can detect H and $Si_x H_n$ radicals at densities of 1 part per million of parent silane gases. The spectrometer also has a threshold sensitivity in the neighborhood of 10^{11} cm^{-3} in the reactor vessel. All electronics, vacuum, and gas-handling apparatus necessary for examining rf and dc discharges and thermal CVD under controlled conditions are available as is a pulsed laser for use in studying surface species by laser blowoff.

Contact: Stephen R. Leone, 303/497-3505 or Alan C. Gallagher, 303/497-3936, Div. 577, NIST, Boulder, CO 80303.

Laser Stabilization

Many sensitive and sophisticated applications of lasers depend on the laser's spectral coherence, frequency stability, and low-intensity noise. NIST scientists have been working on laser intensity stabilization, laser frequency linewidth reduction with active control techniques, and several methods for producing quantitative laser frequency scans. Two new systems have been developed. One, based on optical sideband production by broadband microwave phase modulation of the laser, allows scans over a ±5 GHz range, with inaccuracy below 10 kHz. The other scan technique utilizes a novel interferometer/phase-locked rf system, which maps optical frequency change into corresponding phase change of an rf signal suitable for control, stabilization, and scanning. This system is intrinsically free of errors that accumulate over large scans. By combining a Lambdameter for coarse wavelength identification and a single absorption line used as absolute calibration, NIST scientists can scan a few dozen angstroms with sub-MHz accuracy.

Another NIST system under development works entirely externally to a continuous-wave laser to shift the output laser frequency and reduce the intensity in a controlled manner. The first application of this is a box which will sit in the output beamline of any laser and "eat" both frequency noise and amplitude noise in the intrinsic output of the laser. Institute scientists have demonstrated this function by combining an external electro-optic phase shifter and an acousto-optic frequency shifter that also functions as a fast controlled optical attenuator. Residual noise levels near the values fixed by the fundamental quantum fluctuations have been achieved in laboratory experiments.

Contact: John L. Hall, Div. 577, NIST, Boulder, CO 80303, 303/497-3126.

Study of Atomic Structure of Matter with X Rays

X-ray spectroscopy provides information on electronic structure and on the local atomic structure of atoms in matter. A synchrotron radiation beamline has been constructed by NIST scientists at the National Synchrotron Light

Source, providing the highest flux, intensity, and energy-resolving power of any existing beamline in the x-ray energy range from 500 to 5000 eV. NIST equipment complements the synchrotron radiation instrumentation. X-ray absorption spectroscopy techniques, such as x-ray absorption near-edge structure (XANES) and extended x-ray absorption fine structure (EXAFS), have been used to determine the atomic structure of metals, semiconductors, polymers, catalysts, biological molecules, and other materials of interest to industry. Researchers also use x-ray emission spectroscopy, x-ray photoelectron spectroscopy, and Auger electron spectroscopy to probe the electronic structure of solids, liquids, or gases by using additional experimental capabilities.

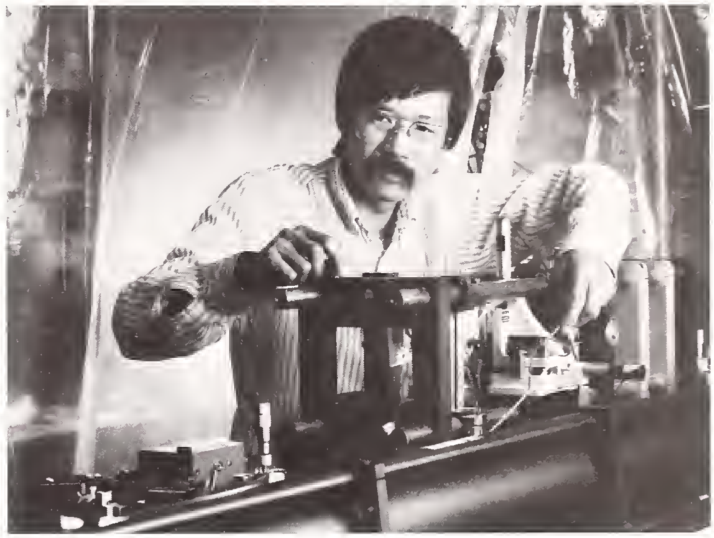
The x-ray standing wave technique uses interference between incident and diffracted x rays to determine the precise location of impurities or imperfections within a crystal or at its interfaces. The technique can be used to investigate the location of dopants and imperfections in semiconductors or optical crystals, growth of overlayers on crystals, and the structure of catalysts supported on crystal substrates. In addition, evanescent x rays, which penetrate only a few nanometers from an interface, can be controlled to study chemical composition in the vicinity of an interface.

NIST scientists recently pioneered a new technique, diffraction of evanescent x rays (DEX), which combines and extends the capabilities of the x-ray standing wave method and experiments based on evanescent x rays. The synchrotron radiation beamline provides an ideal facility for applying these techniques.

Contact: Paul L. Cowan, 301/975-4846 or Richard D. Deslattes, 301/975-4841, A141 Physics Bldg.

Frequency, Time, and Phase Noise Measurement

Advancements in communication and navigation systems require atomic oscillators with increased performance and reliability. NIST has several programs aimed at providing advanced frequency standards with the potential for benefiting commercial atomic standards. NIST scientists currently are working on an optically pumped cesium-beam standard that should significantly surpass the performance of standards based on magnetic state selection and detection. Their studies on ion storage and radiative cooling are exploring the potential for standards operating at accuracy levels of 1 part in 10^{15} and perhaps beyond.



Physicist Wayne Itano studies mercury ions, which are likely to be the basis for new standards of timekeeping.

Aerospace systems often require extreme phase stability, which has led to a need for high-quality phase noise characterization amplifiers, frequency multipliers, oscillators, and other electronic components. NIST has initiated a program to develop methods for measuring phase noise in such components over a broad frequency range (into the millimeter range). The work will involve primarily the two-oscillator technique, but other techniques will be studied.

Requirements for synchronization (time) and syntonization (frequency) of broadly dispersed sets of nodes for communication, navigation, and other electronic systems are increasing significantly. Because of the inherent reliability, simplicity, and low cost of using satellite transfer, NIST is studying several possible approaches for using this technique. The NIST Time Scale and reliable ties to many other international timing centers provide the basis for performance analysis of these time-transfer techniques. In addition, the Institute is equipped with Global Positioning System receivers, Earth communication terminals, and automated systems for statistical analysis of system performance.

Contact: Donald B. Sullivan, Div. 576, NIST, Boulder, CO 80303, 303/497-3772.

Surface Characterization

Surface characterizations are used in a great variety of scientific and technological applications. Two beamlines at the NIST synchrotron ultraviolet radiation facility (SURF-II) have been instrumented for surface characterization. Although the principal characterization techniques utilized are photoelectron spectroscopy and photon-stimulated desorption of positive ions, surfaces also can be characterized by Auger-electron spectroscopy and low-energy electron diffraction. An ancillary chamber is being constructed in which films of different materials can be deposited and transferred to the main chamber for characterization without exposure to the atmosphere. A facility for cooling specimens to cryogenic temperatures is available. Plans call for the installation of an ellipsoidal mirror analyzer, which will be used to measure the energy and angular distributions of photoemitted electrons and the energy, angular, and mass distributions of desorbed ions.

Contact: Richard L. Kurtz, B248 Chemistry Bldg., 301/975-2544.

Ultraviolet and Soft X-ray Radiation Effects

To produce radiation for experimental purposes, NIST has built a synchrotron ultraviolet radiation facility (SURF-II). SURF-II is a 300-MeV electron storage ring that radiates high-intensity synchrotron radiation in the energy range from about 3 nm (400 eV) in the soft x-ray region to wavelengths in the visible region of the spectrum. The radiation is highly collimated, nearly linearly polarized, and of calculable intensity. Six beam lines are available, and a user's program is in operation. SURF-II is well suited for many different types of research, including atomic, molecular, biomolecular, and solid-state physics; surface and materials science; radiation chemistry and radiation effects on matter; ultraviolet and x-ray optical systems; and the calibration, characterization, and development of spectrometers and detectors.

NIST scientists are particularly interested in conducting collaborative research in the use of soft x-ray synchrotron radiation for high-resolution lithography; measurement of the reflection characteristics of novel, high-efficiency, multilayer far-ultraviolet optical devices; and calibration, characterization, and development of spectrometers and detectors. Other available equipment includes a state-of-the-art multipurpose detector calibration facility, a large ultrahigh vacuum spectrometer calibration chamber, and a beamline dedicated to high-resolution radiation research with a 6.65-m vacuum spectrometer with a resolving power of about 300,000.

Contact: Robert D. Madden, A249 Physics Bldg., 301/975-3726 or William R. Ott, B206 Metrology Bldg., 301/975-3709.

Vacuum Ultraviolet Radiometry

As part of its research to understand and measure various forms of radiation, NIST is conducting vacuum ultraviolet studies involving radiation damage, polymerization of organic molecules, and solar simulation. NIST scientists have worked with researchers from industry to develop and test vacuum ultraviolet instrumentation, new spectrometer designs, and detector systems, especially for flight in space. They also have collaborated on special sources, narrow band filters, and lasers. NIST scientists are interested in doing cooperative research in several other areas, including studying hollow cathode lamps, laser plasmas, and spark discharge light sources as secondary standards. State-of-the-art radiometric facilities and advanced optical equipment are available at NIST for these studies.

Contact: J. Mervin Bridges, 301/975-3228 or Jules Z. Klose, 301/975-3230, B66 Physics Bldg.

Submicron Physics

Well-characterized, focused electron beams are used to investigate the properties of surfaces and magnetic materials on a microscopic scale. As part of a broad-based research program at NIST, scientists are exploring the physics of submicron systems using electron microprobes. The program includes studies of electron-surface interactions, surface magnetism, electron interaction theory, and electron spin polarization phenomena. Among the extensive experimental facilities available for this research are sources and detectors of spin polarized electrons, a scanning electron microscope equipped for secondary electron spin polarization analysis, and a scanning tunneling microscope.

Scanning electron microscopy with polarization analysis is a unique measurement capability developed by NIST scientists to allow the high-resolution (~10 nm) imaging of magnetic microstructure independently of surface topography. With this technique, researchers are studying fundamental magnetic phenomena, the properties of high-density magnetic recording media, and small-particle magnetism. NIST researchers are using the scanning tunneling microscope to study surface topography at the atomic level, mechanisms of film growth at the submonolayer level, reconstructions of semiconductor surfaces, and, ultimately, correlation of surface microstructure with macroscopic properties.

Contact: Robert J. Celotta, B210 Metrology Bldg., 301/975-3710.

Characterization of Low-Temperature Plasmas

The properties of low-temperature plasmas play a key role in the processing of materials such as semiconductors. Proper characterization of these plasmas is essential to develop accurate plasma diagnostics and useful plasma models for specific applications. At NIST, plasma discharges are characterized utilizing optical emission spectroscopy, laser-induced fluorescence, laser scattering, and optogalvanic methods. Modeling of the plasma is also an integral part of this characterization. Discharge sources include low-pressure RF plasmas, stabilized arcs, glow discharges, heat pipes with laser resonance ionization, and inductively coupled plasmas. An extensive array of laboratory equipment is available to accomplish this characterization, including several Nd:YAG pumped, high-resolution (<0.1 cm^{-1}) dye lasers; Ar ion-pumped dye and ring dye lasers; a Fizeau wavemeter; a high-throughput (f/4), high-resolution (<0.01 Å) spectrometer with an automated intensified diode array detector; a 80-MHz quadrature He-Ne laser interferometer; UV spectrometers; grazing incidence spectrometers; laboratory computers; and miscellaneous optics. The principal quantities measured are particle density distributions, both spatially and temporally, for electrons, atoms, ions, and molecules. Also included are electric-field distributions, electron and ion temperatures, and nonequilibrium phenomena.

Contact: James R. Roberts, A167 Physics Bldg., 301/975-3225.

XUV Multilayer Characterization

A new capability for fabricating relatively high reflectivity, normal incidence optics for the extreme vacuum ultraviolet (XUV) spectral region has emerged since the beginning of this decade. When a large number of carefully deposited layers of selected materials are placed on a very smooth surface, the reflectivity of the surface can be improved by several orders of magnitude. This new capability has allowed the construction of XUV telescopes revealing images of the sun at selected wavelengths (e.g., 175 Å relevant to Fe^{9+} emission) in unprecedented detail and XUV microscopes with submicrometer resolution for biological studies. A characterization facility, which is available to all researchers on a cooperative basis, is now in operation at NIST to measure reflectivity of these optics between 80 and 600 Å as a function of angle and wavelength. This facility is capable of precise measurements of single thin films and bulk material samples for derivation of optical constants in this region of the spectrum. Plans for the future include a new monochromator-reflectometer system to operate from 30 to 600 Å and an optical test bench to measure the focusing properties of curved optics.

Contact: James R. Roberts, A167 Physics Bldg., 301/975-3225.

Building Technology

Cement and Concrete

NIST researchers are undertaking a computer-oriented research program to develop a fundamental understanding of the relationship between chemistry, microstructure, and service life of concrete and other inorganic building materials. The goal of the program is to be able to predict the behavior of these materials and their service lifetimes. The service life of concrete largely depends on the rate of moisture ingress and of transport of dissolved salts and gases in the pore system of concrete. Models are being developed to consider service conditions, including composition of the environment; the transport rate of reactants by diffusion, convection, and capillary forces; and reaction mechanisms. Researchers are developing mathematical and simulation models to predict the relationships between pore structure and diffusion and permeability of concrete.

Research projects include development and validation of mathematical models of microstructure development in cement pastes as the cement hydrates, the effects of microstructure on permeability and fracture of concrete, and mechanisms of degradation of concrete. Artificial intelligence systems are being developed for optimizing the selection of materials and for diagnosing the causes of material degradation. The research is performed using a variety of techniques, including scanning electron microscopy, computerized image analysis, x-ray diffraction, and thermal analysis.

Contact: James R. Clifton, B348 Building Research Bldg., 301/975-6707.

Structural Engineering

Experimental and analytical research is under way at NIST to develop design criteria for precast concrete frames and masonry structural components subjected to dynamic loads such as winds and earthquakes. The work involves identifying limit states and establishing criteria to ensure structural safety. The researchers use a unique computer-controlled test facility that can impose forces and/or displacements in three directions simultaneously and a 12-million-pound capacity universal testing machine with a lateral load capacity of 1.5 million pounds that can accommodate large-scale structural components 60 feet tall. A high-performance computer graphics laboratory including a VAX computer system and specialized graphics-based finite-element software is utilized for the analytical work.

Contact: H.S. Lew, B168 Building Research Bldg., 301/975-6061.

Lighting

The NIST lighting program focuses on fundamental measurements of interior luminance and illuminance distributions, light fixture output, and the interaction between lighting and HVAC (heating, ventilating, and air-conditioning) systems. A continuing challenge is to develop metrics for lighting quality that evaluate the combined effects of illuminance, luminance, contrast, color rendering, lighting geometry, and configuration.

In the past, researchers have focused on mathematical formulas for predicting the chromatic contribution to brightness, computer programs for predicting energy effects of daylight use, detailed calculation of lighting geometry, and assessments of color appearance under different illuminants. Current research includes a major project on the measurement and modeling of the interaction of lighting and HVAC in a simulated interior office module. This research is expected to result in the development of a detailed computer model for predicting the effects of different types of lighting and HVAC systems. Modifications will be made to the facility in the near future to study the effects of dimming, thermal mass, and external solar conditions.

Contact: Belinda L. Collins, A313 Building Research Bldg., 301/975-6455.

Indoor Air Quality

Measurement and testing procedures, technical data, and comprehensive indoor air-quality models are being developed by NIST researchers as part of a multiyear program to improve indoor air quality in buildings. Experiments are being conducted in several large buildings to develop test methods to evaluate how air moves into and within large commercial buildings. The researchers are developing comprehensive computer models to predict pollutant levels from sources introduced

Materials research engineer Leslie Struble uses a cylinder and piston device to study the causes of concrete failure.

into buildings from outdoor air and those generated inside from sources as combustion equipment and floor and wall coverings.

The first phase of the research is complete, and models exist that can predict indoor contaminant levels as functions of emission, dilution, and intrabuilding air movement. The models currently are being extended to model reactive contaminants. Test procedures also are being developed to evaluate the effectiveness of various filter media for removing gaseous pollutants. A test facility for this purpose has been designed and assembled. Test methods will be developed for commercial gaseous air filters and for those used in residences.

Contact: Richard A. Grot, A313 Building Research Bldg., 301/975-6431.

Organic Building Materials

NIST is conducting basic and applied research to determine the quality and predict the service life of organic building materials, such as protective coatings for steel, adhesives, roofing materials, and plastics. The researchers are investigating degradation mechanisms, improving characterization methods, and designing mathematical models of the degradation processes. They then use research results to derive stochastic models, which have a basis in reliability theory and life-testing analysis, to predict the service life of these materials.

Institute scientists are using computer analysis of infrared thermographic images to study the rates of corrosion and the formation and growth of blisters beneath opaque protective coatings. They employ gel-permeation chromatography, gas chromatography, and spectroscopy to study the mechanisms of photolytic and thermal degradation of poly (methyl methacrylate). Reliability theory and life-testing analysis techniques are used to predict service lives of the materials.

Contact: Larry W. Masters, B348 Building Research Bldg., 301/975-6707.

Refrigeration Machinery

NIST researchers are exploring the use of refrigerant mixtures to improve the efficiency of refrigeration cycles and to replace harmful chlorofluorocarbon (CFC) refrigerants that are damaging the ozone layer of the upper atmosphere. The scientists evaluate a wide variant of refrigeration cycles by using a breadboard heat pump to "plug" and "unplug" circuits and components. The breadboard heat pump will be altered to test new refrigeration cycles based on the results of a theoretical study being conducted to find the optimal combination of mixtures and appropriate refrigeration cycles for the best and most versatile performance.

The "best" of the advanced cycles will be selected, equipment built, and evaluated. A minibreadboard that will use a very small charge will also be built so that rare refrigerants of limited production can be studied.

Contact: David A. Didion, B114 Building Research Bldg., 301/975-5881.

Ceramics

Thermal Insulation

Researchers at NIST are developing basic data and simulation models for heat, air, and moisture transfer through building envelope components. They are developing and validating a theoretical model for moisture transfer, completing research required to develop a low-conductivity Standard Reference Material (SRM), developing a thermal conductivity database for chlorofluorocarbon (CFC) blown thermal insulation products, and refining a dynamic test procedure for building components.

A 1-meter guarded hot plate is used to develop SRM's; to determine thermal conductivity values for various materials, such as CFC blown insulation; and to provide measurement services to manufacturers and researchers. A calibrated hot box is used to measure the steady-state and dynamic performance of full-scale wall systems.

Contact: A. Hunter Fanney, B320 Building Research Bldg., 301/975-5864.

Building Controls

NIST research is fostering the development of more intelligent, integrated, and optimized building mechanical systems. A dynamic building/HVAC control system simulation program is used to study HVAC/control system dynamics and interactions. An expanded building management and controls laboratory is used to assist the building controls industry in the development, evaluation, and testing of communication protocol standards for the open exchange of information.

The application of knowledge-based systems to buildings is a new area of research. Plans call for exploring how real-time models, "tuning" techniques, forecasting, optimal control theory, and a rule-based expert system can be combined to evaluate control system performance, make control strategy decisions that optimize building performance, and perform diagnostics to advise the building operator or manager on building operations, equipment problems, or maintenance requirements. Work has begun for the Department of Energy to develop an HVAC/building emulator/EMCS tester, which will provide a method for evaluating application algorithms.

Contact: George E. Kelly, B114 Building Research Bldg., 301/975-5870.

Ceramic Processing

Sintering of ceramics is a complex process that involves the interaction of many different processing variables. The influence of these processing variables on sintering cannot be determined simply by measuring final density or some other end-point property. Chemical composition of the ceramic powders is known to be of major importance and, under certain conditions, can mask effects of most other processing variables. As part of a ceramics program, NIST scientists are investigating the effect of trace levels of impurities using clean-room processing to produce, compact, and sinter ultrahigh purity ceramics.

Results from this research will enhance investigations of other processing variables, including particle size, shape, agglomeration, compaction method, and atmosphere under controlled composition conditions. The data can be used to design better models for microstructure evolution during sintering. Use of predictive models, in conjunction with other ongoing efforts to produce unique compositions and phases, can lead to new advanced ceramic materials with unique microstructure and properties.

Contact: Edwin R. Fuller, Jr., A256 Materials Bldg., 301/975-5795.

The NIST ultra-clean ceramic processing laboratory is specially designed for the production and processing of advanced ceramic powders and samples with controlled levels of impurities and dopants.

Tribology of Ceramics

Researchers in the NIST ceramics tribology program are investigating the fundamental mechanisms of friction and wear of advanced materials and lubricants and are developing test methods for evaluating the performance of these materials. The program's primary focus is on the characterization of the interfacial phenomena that occur when two solid surfaces interact. Research activities include analysis of chemical reactions and formation of tribochemical films, physical and mechanical behavior of surface films, and deformation and fracture processes leading to wear and failure. Tribology laboratories consist of state-of-the-art tribometers, such as high temperature (1000 °C) wear testers, and analytical instruments, such as time-resolved micro-Raman laser systems, which can be used for cooperative research with industry and other federal agencies. NIST researchers are compiling wear data in the form of "wear maps" and are studying the mechanisms of wear of structural ceramics at elevated temperatures, self-lubricating metal-matrix and ceramic-matrix composites, and wear resistant coatings.

Contact: Said Jahanmir, A215 Metrology Bldg., 301/975-3671.

Electro-optic Crystals

Imperfections in highly perfect crystals typically limit their performance in high-technology applications such as optical communications and optical signal processing. In particular, limitations in the perfection of electro-optic and photorefractive materials, such as lithium niobate and bismuth silicon oxide, have inhibited severely the development of optical switches and modulators. NIST researchers are investigating crystal perfection at a unique, monochromatic x-ray topography facility at the NIST/Naval Research Laboratory beamlines on the high-energy ring at Brookhaven National Laboratory's National Synchrotron Light Source. The data collected from current studies, conducted jointly with growers of high-quality crystal, are expected to improve substantially the quality, and hence the performance, of these crystals.

Contact: Bruce W. Steiner, A329 Materials Bldg., 301/975-5977.

Mechanical Properties of Ceramics

Several long-term programs are being conducted at NIST on the fracture, creep, and creep rupture of monolithic and composite ceramics. Researchers, for example, are examining the effect of very near surface forces on the fracture properties of monolithic ceramics. These forces have been measured for mica, sapphire, and fused silica surfaces, using a crossed cylinders apparatus.

A second program uses an indentation strength procedure to determine the R-curve behavior of monolithic alumina ceramics and to relate the R-curve to the specific microstructure of the material. In-situ microscopic observations of the crack growth demonstrate the presence of grain bridging and frictional sliding in the crack wake as a significant source of material toughening.

The program in composites is aimed at determining the effects of the fiber/matrix interface on fracture behavior of these materials. An instrumented microindenter is available to measure the fiber/matrix interface strengths. Researchers also are investigating the stresses developed in composites during conventional sintering processes to determine methods of reducing these stresses through the use of fiber coatings—thus minimizing or eliminating cracking of the matrix as densification proceeds.

High-temperature deformation and fracture behavior of ceramics are other areas of research. Creep and creep rupture of several varieties of siliconized SiC have been investigated and their behavior related to differences in microstructure, particularly grain size. Research continues on whisker-reinforced Si_3N_4 and Al_2O_3, SiC, and other high-temperature materials. Facilities exist for performing creep measurements in tension, compression, and flexure at temperatures up to 1800 °C. The tensile creep apparatus is almost completely automated, and measurements are made using a laser imaging technique. Displacement measurements are accurate to ±1 μm at 1500 °C.

Contact: David C. Cranmer, A361 Materials Bldg., 301/975-5753.

Ceramic Powder Characterization

Improved characterization of particle size, shape, and crystal chemistry of ceramic powders is important to the development and production of high-quality ceramics for advanced technological applications. To obtain precise and reproducible measurements of these characteristics, NIST scientists are utilizing a variety of instrumental methods, including scanning electron microscopy with image analysis. Theoretical investigations and statistical analyses of data are then used to compare the results of the measurement methods.

Improved understanding of the changes which occur in materials at high temperatures is necessary to process and use advanced materials. High-temperature x-ray diffraction provides a means for NIST scientists to record these changes as they occur. Current studies focus on formation of high T_c ceramic superconductors, reactions in ceramic composite materials, sintering of ceramics, and high-temperature phases in superalloys.

A scanning electron microscope (SEM), equipped with an image analysis system and backscatter electron imaging, is used to obtain a precise understanding of the relationship between microstructure and bulk physical and chemical properties of powders and ceramics. A special sample holder can be installed in the large SEM sample chamber so a sample may be observed while a crack is being driven through it.

To improve measurement procedures, NIST researchers are studying the sample preparation factors that influence particle size measurements. Measurements of particle size distribution by sedigraph and centrifugal photosedimentation and of specific surface are used in conjunction with quantitative SEM/image analysis to document fully the geometric characteristics of a powder. The properties of powder suspensions and the effect of the suspending liquid on the surface chemistry of the powder are studied also. Elemental characterization of the treated powder is characterized by various spectroscopic methods. Suspension properties are characterized by measurements of pH, surface charge, ionic activity, acoustophoresis, zeta potential, and viscoelastic properties. NIST scientists also are studying the application of colloidal processing methods to the formation of monolithic and composite ceramics.

Contact: James P. Cline, 301/975-5793, James F. Kelly, 301/975-5794, or Subhaschandra Malghan, 301/975-6101, A256 Materials Bldg.

Ceramic Phase Equilibria

Ceramic phase equilibria studies at NIST involve complementary research activities in experimental theoretical, data-evaluation, and compilation aspects of ceramic phase equilibria. The data-evaluation and compilation work is carried out under the joint American Ceramic Society (ACerS)/NIST program to provide industry and others with a comprehensive database of up-to-date, critically evaluated phase diagram information. Ceramic phase diagrams are being determined for systems of technical importance, such as high-transition-temperature ceramic superconductors.

Contact: Stephen Freiman, A329 Materials Bldg., 301/975-5761.

Ceramic Chemistry

NIST scientists are investigating low-temperature synthetic approaches to both oxide and nonoxide ceramic powders and coatings. They are using novel chemistry and techniques to solve the problems of generating homogeneous, multicomponent materials with predictable and optimal properties. The researchers are studying the following materials: high T_c ceramic superconductors; ultrafine ceramic powders with high-electrical conductivity; ceramic coatings with selected optical, electronic, or structural properties; ultrafine magnetic composites; ceramic whiskers-ceramic matrix composites; and ultrafine, pure oxide powders. Depending upon requirements of the study and the powder, synthesis is carried out either in small bulk reactors or in a flow reactor.

The researchers are examining the relationship of process conditions to surface chemistry of the powder, particle size and shape, the phases formed during thermal treatment of the powder, and properties of the powder or sintered ceramic, such as electrical conductivity. Coupled with the powder synthesis is the development of characterization methods, including micro-Raman, Fourier transform infrared spectroscopy, and nuclear magnetic resonance spectroscopy.

Contact: Joseph R. Ritter, 301/975-6106 or Pu Sen Wang, 301/975-6104, A256 Materials Bldg.

Chemical Technology

Center for Advanced Research in Biotechnology

The Center for Advanced Research in Biotechnology (CARB), a joint research venture between NIST and the University of Maryland, studies protein structure/function relationships. Scientists at CARB are focusing on the measurement of protein structure by x-ray crystallography and nuclear magnetic resonance spectroscopy, and the manipulation of structure by molecular biological techniques including site-directed mutagenesis. Protein modeling, molecular dynamics, and computational chemistry are used to understand protein structure and to predict the effects of specific structural modifications on the properties of proteins and enzymes. A variety of physical chemistry methods are used to measure and analyze structural changes, activities, and thermodynamic behavior of proteins under investigation. CARB maintains state-of-the-art facilities for crystallography, NMR spectroscopy, molecular biology, and physical biochemistry. Its computer facilities include a mini-supercomputer, several high-resolution graphics workstations, and access to the NIST Cyber 205 supercomputer.

Contact: Walter J. Stevens, 9600 Gudelsky Dr., Rockville, MD 20850, 301/251-2272.

Chemical and Biochemical Thermodynamics

NIST researchers have developed precision oxygen combustion calorimeters to measure the enthalpy of combustion, from which enthalpy of formation can be derived, for samples varying in mass from 10 milligrams to 2.5 kilograms. These instruments are used to characterize thermodynamic properties for species of interest to biochemistry, organic chemistry (including strained species), phosphorous chemistry, and heterogeneous fuel technologies. The measurements also serve as the basis for Standard Reference Materials and Standard Reference Data for a variety of technologies, including energy.

In the area of biothermodynamics, NIST researchers have developed accurate and precise microcalorimeters to measure the heat released in enzyme-catalyzed biochemical reactions of interest to technology. When coupled with equilibrium measurements, these measurements enable the reliable modeling of the thermodynamics of these processes. These data are used to predict reliably the efficiency of biochemical processes outside the normal measurement ranges for temperature, pH, and ionic strength.

Contact: Stanley Abramowitz, B348 Chemistry Bldg., 301/975-2587.

Thermodynamic Data Evaluation

NIST maintains several data centers that evaluate thermodynamic data in inorganic, organic, and aqueous chemistry. Researchers in the data centers examine existing data, extrapolate these data to temperatures outside the range of measurement, create algorithms for data evaluation and manipulation, and produce reliable estimation schemes for predicting the properties of species for which measurements are not available. Current interests include the technological problems of combustion, nuclear waste disposal, and atmospheric ozone depletion; the prediction of the formation properties of organic species in the gaseous, liquid, solid, and aqueous phases; and the production of databases of the ubiquitous biochemical species of interest to biotechnology. The data center researchers are active in national standards-setting organizations such as ASTM, have bilateral collaborative research projects with research organizations in several countries, and are active in international research organizations such as CODATA and IUPAC.

Contact: Stanley Abramowitz, B348 Chemistry Bldg., 301/975-2587.

Chemical Kinetics

The chemical kinetics program at NIST provides reliable chemical kinetics data, measurement methods, and theoretical models. Applications of this research include combustion, new chemical technologies, the chemistry of the upper atmosphere and other planetary atmospheres, effects of ionizing radiation on materials, solar energy conversion, biotechnology, flue-gas cleanup chemistry, acid rain, toxic waste incineration, coal conversion, and analytical applications of kinetics. Among the experimental projects under way at NIST are pulse radiolysis of aqueous solutions, and kinetic mass spectrometric studies (Fourier transform ion cyclotron resonance, high-pressure mass spectrometry, tandem mass spectrometry) of the kinetics and thermochemistry of ion/molecule reactions and ion/molecule clustering processes.

Researchers also are studying free-radical kinetics using heated single-pulse shock tubes, flash photolysis kinetic absorption spectroscopy and a flash photolysis resonance fluorescence technique, vacuum ultraviolet laser photolysis with kinetic absorption detection, and high-temperature reactors. Resonance enhanced multiphoton ionization (REMPI) spectroscopy is used to provide new, previously unobtainable data about the electronic structures of a wide variety of free radicals. REMPI procedures also lead to very sensitive and selective schemes for the optical detection of the radicals. An important focus of the kinetics program is the production of databases of evaluated chemical kinetic data, as well as the design of databases and relevant software.

Contact: Sharon G. Lias, A260 Chemistry Bldg., 301/975-2562.

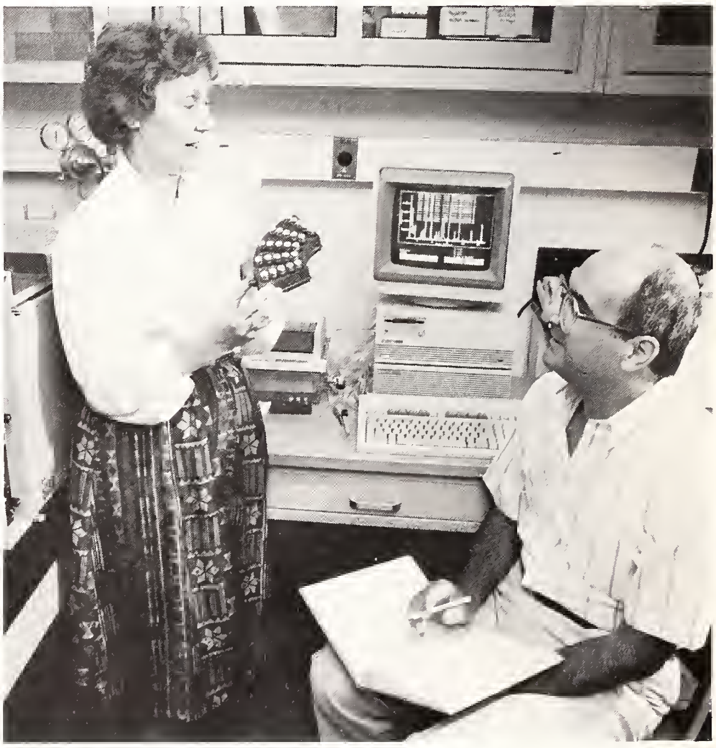
Separations

Separation and purification are critical steps in the manufacture of chemical products using existing and emerging process technologies, such as biotechnology. Separation processes affect both the economies of production and the fundamental ability to produce a product of desired form or purity. NIST is creating an engineering science base in two broad areas—membrane-based separations and bioseparations.

In the membrane area, NIST scientists are studying gas separations, biomolecule transport and adsorption, and reactive membranes; in the area of gas separations, researchers are investigating novel facilitated transport membranes for use in acid gas removal and air separations. Reactive membrane systems are being studied for trace component removal and for gas cleanup/recycle applications. In an interdisciplinary project, researchers are examining the adsorption of biological macromolecules to ultrafiltration membranes, with the objective of developing better predictive models for fouling, flux decline, and chromatographic applications. Other study areas include pervaporation membranes for close boiling mixtures and composite and polysaccharide membranes for small biomolecule separations.

To assist the biotechnology industry, NIST scientists are developing the fundamental transport data, experimental methods, and models for a number of aqueous two-phase partitioning systems. These liquid-liquid extraction processes are useful for inexpensively and selectively separating proteins and other biomolecules from complex mixtures. Fundamental studies of electrophoresis, novel crystallization technologies, and chromatography are also being conducted. State-of-the-art analytical techniques are used to characterize the processes under study. The insights gained from the separations program at NIST have been the basis of applied research in novel bioreactor designs for the production of stereospecific chemicals.

Contact: Subhas K. Sikdar, 303/497-5232, Paul Todd, 303/497-5563, or John Pellegrino, 303/497-3416, Div. 583, NIST, Boulder, CO 80303.



Research chemists Ewa Gajewski (left) and Miral Dizdaroglu determine the chemical structure of a major type of DNA damage caused by oxygen-derived free radicals.

Properties of Fluids

Thermophysical properties data are essential for the design and operation of many chemical processes such as supercritical extraction. To obtain these data, NIST scientists are using three new phase equilibria apparatus for studies at elevated temperatures. One apparatus is used to perform VLE measurements on carbon dioxide-hydrocarbon systems and refrigerant-hydrocarbon systems, the second is a dew/bubble point apparatus extending to 800 K, and the third employs a palladium-silver membrane to measure the fugacity of hydrogen-containing mixtures. Five exceptional instruments are available for making PVT, PVT_x, and heat capacity measurements on pure fluids and fluid mixtures: an isochoric PVT apparatus, a Burnett apparatus, a combined Burnett/isochoric PVT apparatus, a magnetic suspension densimeter for PVT and PVT_x measurements, and an instrument to measure constant volume heat capacity. Facilities also exist to determine properties along the two-phase coexistence line of pure fluids and mixtures and to make sound speed measurements. A well-equipped analytical laboratory and specialized apparatus enable NIST researchers to devise techniques for characterizing fluids and fluid mixtures when the temperatures, pressures, and times involved can result in reactions during the measurement process.

Contact: William M. Haynes, Div. 584, Boulder, CO 80303, 303/497-3247 or Michael R. Moldover, A103 Physics Bldg., 301/975-2459.

Thermophysical and Supercritical Properties of Mixtures

Chemical process technology requires an accurate knowledge of various thermophysical properties of pure, polyfunctional chemicals and their mixtures. Research is being conducted at NIST on the most important of these properties—equilibrium phase composition, density, and enthalpy. NIST researchers are developing predictive methods for the properties of chemically dissimilar compounds, especially complex mixtures and aqueous solutions. Another project, a combined experimental and theoretical study, is aimed at developing accurate predictive models for the thermodynamic and transport properties of near critical and supercritical mixtures. This work includes PVT_x and VLE measurements on mixtures containing carbon dioxide, halogenated hydrocarbons, and similar supercritical solvents. Other experimental work involves using supercritical chromatography to measure diffusion coefficients in supercritical mixtures and theoretical studies to focus on the application of extended corresponding states to supercritical systems.

Contact: James F. Ely, 303/497-5467 or Thomas J. Bruno, 303/497-5158, Div. 584, NIST, Boulder, CO 80303; J.M.H.L. Sengers, A121 Physics Bldg., 301/975-2463.

Properties of Interfaces

A wide array of experimental and theoretical tools are being applied to obtain practical and fundamental understanding of the structure, properties, and effects of interfaces between fluid phases. NIST scientists are investigating a number of problems in this area ranging from the conceptually simple (e.g., measuring and/or calculating the interfacial tension between a liquid and its vapor) to the more complicated (e.g., determining the phase behavior of surfactant mixtures at water-air interfaces, the thicknesses of adsorbed liquid layers at solid-gas interfaces, the stability of foams, and the evolution of mists). NIST facilities include an automated ellipsometer and an automated film balance, quasielastic light scattering for studying the evolution of mists, an apparatus for measuring foam stability, and simple setups for measuring interfacial tension. Computing facilities include a CDC 855, a Cyber 205 supercomputer, software, and experience in simulation of fluids.

Research projects are planned in several areas. One project will involve applying quasielastic light scattering to the measurement of interfacial tension of liquid-vapor mixtures at high pressure and the measurement of the dynamics of wetting layers. Another project will focus on measuring the permeability, surface viscosity, and surface-diffusion coefficients of surfactant layers. The researchers will test NIST theories developed for the large increase of the surface tension of a liquid-vapor interface when it forms in a confined geometry (such as in a pore within a pellet) and for the large effects of ions on the thicknesses of adsorbed layers. They will also study the evolution of the drop-size distribution of simple, but nontrivial, mists comprised of two hydrocarbons suspended in their own vapor.

Contact: Michael R. Moldover, A103 Physics Bldg., 301/975-2459.

Properties of Atmospherically Safe Refrigerants

Chlorofluorocarbons (CFC's) have been used widely for the past 50 years as refrigerants; as foam in building insulation, furniture, car seats; and in many other applications. Recent evidence has shown, however, that chlorofluorocarbons (CFC's) are breaking down the ozone layer which protects the Earth from harmful levels of ultraviolet radiation. Alternative chemicals must be found to replace the existing fluids within the next decade. For this to be achieved, an accurate knowledge of their thermophysical properties is required. NIST has a research program designed to provide these data to industry, ultimately in the form of interactive computer codes. The research includes extensive experimental measurements on pure fluids and mixtures, including PVT, PVT_x, vapor pressure, saturation density, heat capacity, thermal conductivity, viscosity, sound speed, and surface tension. The program also includes substantial effort in modeling fluid properties and in developing equations of state.

Contact: Neil A. Olien, Div. 580, NIST, Boulder, CO 80303, 303/497-5108.

Radio Frequency Wave Diagnostic of Disperse Systems

The successful processing of paper pulp, flour, coal slurries, and sludge depends on accurate measurements of the percent of solids suspended in water in a pipeline. To help improve these measurements, NIST is studying the propagation of radio waves inside a conducting pipe filled with complex materials. One result of this research has been the successful measurement of the solid slurry, which was accomplished by measuring the wavelength and attenuation of radio waves in a pipeline with a 32-element antenna array placed along the axial direction. From the known frequency and wavelength, the speed of the radio wave, and hence the dielectric constant, can be deduced. By then applying a mixing rule and the dielectric properties of the individual components, researchers can determine the solids fraction in a slurry. NIST is extending the project to incorporate systems with axially varying dielectric constants, adsorption columns and settling suspensions, for example. Other measurements, such as polarization rotation in a swirling slurry flow and Doppler shifts due to fluid flow, are being planned.

Contact: Adolfas K. Gaigalas, 109 Fluid Mechanics Bldg., 301/975-5941.

Flow Measurement Research and Standards

The accelerating costs of scarce fluid resources—particularly petrochemical fluids—are producing increased concerns about the performance levels of flow meters. Improved flow measurement traceability needs to be established and maintained so that realistic, quantified data are generated on a continuing basis to assure practical fluid measurements at satisfactory, specified levels of performance. To achieve the desired flow measurement traceability, NIST is designing transfer standards to link the performance of calibration facilities to appropriate national reference standards.

Because of the importance of these measurements, transfer standards need to be designed so that high levels of confidence can be placed in them and their performance. The new transfer standards will be rigorously evaluated against NIST fluid flow calibration standards. As part of evaluation, the appropriate range of calibrations will be done on the developed standards so that performance levels can be assured at specified levels. Current fluid metering research programs use laser Doppler velocimetry (LDV) techniques to focus on the pipeflows produced by conventional pipeline elements and by standard flow conditioning elements. New experimental programs are feasible using LDV or other anemometry or flow visualization techniques to study other flows. NIST also has computational capabilities to model numerically a number of closed conduit flow fields.

Contact: George E. Mattingly, 103 Fluid Mechanics Bldg., 301/975-5939.

Fluidized-Bed Reactors

The understanding of transport and kinetic processes in fluidized beds at elevated temperatures is of great importance in many areas of chemical engineering, including pyrolysis and combustion of solid and liquid fuels, catalytic reactions, and destruction of hazardous wastes. NIST maintains a fluidized-bed facility designed and instrumented to address research problems in these technical areas. Past projects include time-resolved optical temperature measurements of single particles inside the bed, as well as optical studies of mixing of solid particles at elevated temperatures.

Currently, the facility is used for studies of pyrolysis and combustion of chlorinated hydrocarbons representative of hazardous-waste constituents. Researchers are investigating the effects of temperature, residence time, and chemical composition of bed particles on destruction efficiency of the model compounds and the formation of intermediate products of incomplete combustion. The analytical instruments used include on-line gas monitors, gas chromatography with mass-spectrometric detection, and FTIR spectroscopy.

Contact: Andrej Macek, B312 Physics Bldg., 301/975-2610.

Chemical Sensor Research

To understand performance of thin-film and chemical sensors, NIST scientists are conducting research aimed at improving their accuracy, stability, selectivity, and response, as well as developing ideas for new measurement techniques. Activities incorporate adhesion, oxidation, interlaminar diffusion, surface adsorption and desorption, and phase morphology to investigate mechanisms of chemical sensing. The scientists use analytical methods to relate the structure and composition of sensing devices to fabricating parameters and performance. Research areas include thin-film thermocouples, thin-film resistance devices, moisture sensors, pH sensors, and gas detectors. Fabrication facilities

Mechanical engineers George Mattingly (right) and T.T. Yeh (center), with technician Boyd Shomaker, study flow-measuring devices using laser Doppler velocimetry at the NIST fluid metering research facility.

available are rf and dc sputtering for both alloy and reactive film deposition and gas reactors. The feasibility of thin-film systems as chemical sensors is being determined as the scientists investigate the electronic properties of films and single crystals for dielectric strength, surface conductance, and capacitance. For surface-sensitive techniques, they are employing x-ray and uv photoemission, thermal desorption spectroscopy, SIMS, and in-situ electrical measurements to characterize appropriate chemisorptive and molecular film systems.

Contact: Kenneth G. Kreider, B312 Physics Bldg., 301/975-2619 or Stephen Semancik, B346 Physics Bldg., 301/975-2606.

Optical Sensing in Bioreactors

Industries now recognize the potential benefit of applying recent advances in molecular biology in a diversity of sectors, such as the production of new drugs, food additives, and chemicals and conversion of biomass. However, implementation of bioprocesses requires a closely controlled environment, normally realizable only in batch processes. This is primarily due to the complex kinetics of most bioreactions, separate periods of growth and product formation, biocatalyst degeneration, contaminant risks, and mechanical difficulties of handling rheologically complex materials. For bioprocesses to be implemented in the future, new on-line measurement techniques must be developed as well as nonintrusive measurement methods to avoid the difficulties associated with sampling contamination and long response time.

To help solve some of these problems, NIST scientists are developing optical techniques for making nonintrusive, rapid, and selective measurements. Using fiber optics, they are able to develop probes which are sterilizable, can provide measurements with good spatial resolution, and can be multiplexed to provide multipoint monitoring capability. Researchers are employing fluorescence techniques to determine characteristics of amino acids, dipeptides, polypeptides, and esters while Raman and resonance Raman scattering will be used to provide more species selectivity. Fluorescence techniques are also expected to provide a powerful tool for cell activity and intracellular kinetics measurements.

Contact: Hratch G. Semerjian, B312 Physics Bldg., 301/975-2609.

Electrical Measurements in Bioreactors

Biological cells are known to be electrically active as demonstrated by the membrane potential present in all living cells. A NIST program is concerned with developing measurement techniques for observing electrical activity of cell suspensions to provide fundamental data for sensor development in bioreactors. Both linear and nonlinear electrical responses are under investigation. The nonlinear properties are especially interesting since they are expected to originate from the cell membrane. Theoretical investigations are in progress to relate the observed electrical behavior to the activity of membrane transport proteins. The researchers are working to achieve a better understanding of the coupling of applied electric fields to membrane proteins, which can lead to practical schemes to influence the activity of cells. Research areas include electrical impedance measurements, study of microwave propagation in cell suspensions, electrostimulation of membrane processes, and observation of electrophoretic mobility with dynamic light scattering. Additional work is planned to measure the modulation of fluorescence from membrane proteins by applied electric fields.

Contact: Adolfas K. Gaigalas, 109 Fluid Mechanics Bldg., 301/975-5941 or R. Dean Astumian, 111 Fluid Mechanics Bldg., 301/975-5951.

Particulate and Droplet Diagnostic in Spray Flames

To minimize the cost of high-priced fuel, U.S. industry needs to obtain maximum energy output from fuel combustion. NIST researchers are tackling this problem by attempting to improve combustion efficiency. The researchers are studying the dynamics of spray flames to investigate droplet vaporization, pyrolysis, combustion, and particulate formation processes and to delineate the effect of chemical and physical properties of fuels on the above processes. The research results will provide an experimental database, with well-defined boundary conditions, for developing and validating spray combustion models.

The experiments are being carried out in a spray combustion facility, with a moveable-vane swirl burner, which simulates operating conditions found in practical combustion systems. A combination of nonintrusive probing techniques is used to obtain comprehensive data on spray combustion characteristics, including soot particle and droplet size, number density and volume fraction, gas composition, and velocity and temperature fields.

Currently NIST scientists are focusing their efforts on laser scattering and laser Doppler velocimetry measurements in order to determine the correlation between droplet size and velocity distributions, respectively, in both low-temperature and burning sprays.

Contact: Hratch G. Semerjian, B312 Physics Bldg., 301/975-2609.

Pressure Standards

Achieving better understanding and control of the pressure measurement process will lead to better quality control in the manufacture of new materials and better design and performance of transducers for thousands of applications in modern technology. The measurement of pressure from subatmospheric to 100,000 psi and above with uncertainties of tens to hundreds of parts per million is essential in modern technology. The most fundamental instrument at these high pressures is the deadweight piston gauge. In the piston gauge a force generated in a working fluid acts against the surfaces of a piston and against the walls of a cylinder that confines the piston. At high pressures, the materials undergo significant distortion, which leads to limitations and uncertainties in the area on which fluid is acting. The fluid interacts with the side of the piston creating upward forces that are difficult to interpret. NIST scientists are using various tools—finite element analysis to characterize distortion, better hydrodynamic measurement and modeling of the annular region through which the fluid flows, and improved piston gage designs—to understand these effects.

Contact: Charles D. Ehrlich, A45 Metrology Bldg., 301/975-4834.

Temperature Sensor Research

Improved industrial processes and sophisticated scientific research require temperature sensors that cover wider temperature ranges with better accuracy and precision than previously required. For example, the degradation of thermocouples exposed to high temperatures for extended periods of time represents a serious impediment to temperature measurements in jet engines, furnaces, and so forth. NIST has several projects under way to test and improve the performance of currently available sensors, including thermocouples, resistance thermometers of various types, and optical fiber thermometers. The temperature range covered by these projects extends from about 0.2 K to 2100 °C. NIST has excellent temperature calibration facilities, an automated laboratory equipped to evaluate thermocouples at high temperatures, several laboratories equipped for work on resistance thermometers, and a laboratory to evaluate optical fiber thermometers. NIST scientists are planning a series of new materials, new principles, and new techniques to provide highly precise and accurate temperature measurements.

Contact: A.O. McCoubrey, B128 Physics Bldg., 301/975-4802.

Dynamic Pressure and Temperature Research

U.S. industry increasingly relies on real-time monitoring of process parameters, particularly temperature and pressure, to produce efficiently a desired end-product, to warrant safe operation, and to assure equity in commerce. This trend is pervasive in the chemical and materials processing industries, as well as in energy and raw materials production and transfer. NIST currently has a research program and is developing a test facility to provide a reliable basis for the evaluation and calibration of transducer dynamical response functions. The research seeks to develop a primary standard for dynamic temperature and pressure based on the fundamental properties of the molecular constituents of a dynamical system. Information about the molecules is accessed via laser-optical diagnostic techniques, and measurement times of the order of 10 nanoseconds at accuracy levels of 5 percent appear feasible. Through the

Computer Systems

use of these measurement techniques, an accurately characterized dynamical source will be developed. This reference source and its associated measurement system will provide industry with a means for assuring the accuracy of transducers used to measure time varying temperature and pressure.

Contact: Gregory J. Rosasco, B118 Physics Bldg., 301/975-4813.

Vacuum and Leak Standards

Many industries depend on accurate vacuum (pressure) and leak measurements for research and development and for process and quality control. NIST develops and maintains pressure and vacuum standards from above atmospheric pressure to ultrahigh vacuum; leak or flow standards are also operated from 10^{-3} to below 10^{-9} std cc/s. Facilities for this research include five ultrahigh vacuum systems; two low-range flowmeters; high-accuracy mercury manometers; pressure and vacuum control systems; and a variety of vacuum, electronic, data acquisition, and data analysis equipment.

These facilities and measurement capabilities are used by NIST researchers to develop improved measurement techniques and equipment and to investigate the performance of vacuum and pressure equipment, specifically mechanical pressure gauges, momentum transfer gauges, ionization gauges, standard leaks, and residual gas analyzers. In addition, NIST plans to use this measurement capability to investigate properties of materials and physical phenomena of fundamental interest. Among the planned projects is the development of reference standards for the transition regime between low pressures measured by mechanical or electromechanical gauges and pressures measured by vacuum technology devices. The development of accurate methods to measure and characterize ultrahigh vacuum systems is also under investigation.

Contact: Charles R. Tilford, A51 Metrology Bldg., 301/975-4828.

Computer Systems Security

Computer systems are critical elements of today's business and scientific environments. However, as sensitive and critical information is processed and stored on computer systems that are often interconnected by local area networks, there is an increasing need for methods to protect that information from unauthorized access or modification. But selection of information security measures should be based on a cost analysis of such measures and the resulting reduction in losses. NIST researchers are investigating various technologies that can be employed to achieve additional control and security of information on computer systems. Their research involves the identification, analysis, development, and application of these technologies.

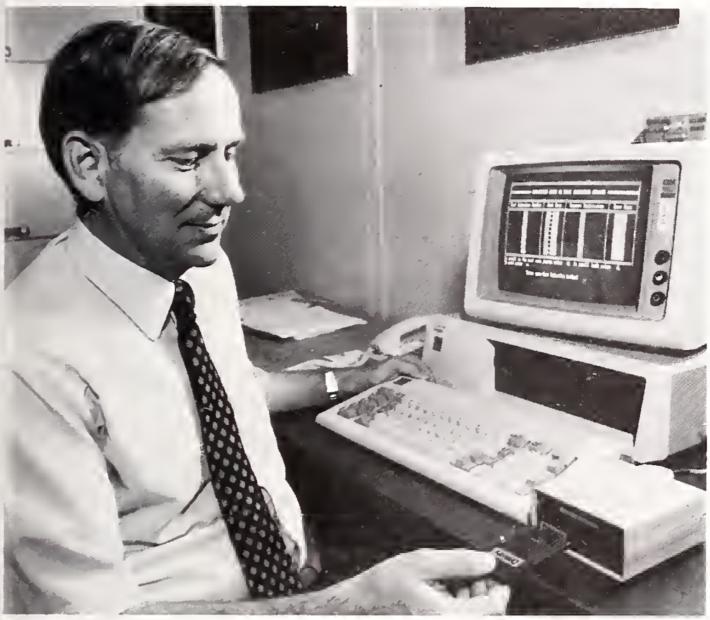
Although it is desirable to have security mechanisms as an integral part of computer systems and networks, this is not always possible or economical because such mechanisms are often not part of the original system design. NIST researchers also are examining the technology available to enhance the security of existing systems. This research involves identifying, analyzing, and comparing security mechanisms used in isolation or combination.

Contact: Stuart Katzke, A216 Technology Bldg., 301/975-2929.

Integrated OSI, ISDN, and Security Program

NIST has initiated a program to bring together government organizations and contractors interested in interoperability and security in the Open Systems Interconnection (OSI) computer network architecture and the Integrated Services Digital Network (ISDN) communications architecture. Researchers in the laboratory-based program develop prototype systems to demonstrate the interoperability of proposed standards for OSI and ISDN using a selected set of security services. These standards are expected to be implemented in commercial applications with a broad market.

The technical objectives of the program are: (1) to develop demonstration prototypes of applications and equipment, including hardware and software, that provide one or more levels of security in an OSI and/or ISDN environment;



NIST researchers are working with the Defense Advanced Research Projects Agency and a private company to develop a prototype system using a "smart" token that will make it tougher for hackers to gain access to a computer network.

(2) to develop specifications for data formats, protocols, interfaces, and support systems for security in an OSI/ISDN environment that can be used as a basis for Federal Information Processing Standards; and (3) to provide a laboratory in which users, developers, and vendors jointly can define, develop, and test systems that will provide a range of telecommunications, network management, and security services in a distributed information processing environment.

Contact: Stuart Katzke, A216 Technology Bldg., 301/975-2929.

Database Testing

To implement the management of information resources, NIST researchers are developing test methods and techniques to evaluate implementations of network database language (NDL), structured query language (SQL), information resource dictionary system (IRDS), Abstract Syntax Notation 1 (ASN.1), and data descriptive file (DDF) for conformance to federal, national, and international standards. The researchers are attempting to derive a general methodology for designing conformance tests, to use this methodology to generate test suites, and to evaluate the test suites for effectiveness. A prototype implementation of the IRDS specifications, which may be suitable for such tasks as modeling the structure of a standard and for recording the parts of a standard specifically tested, will be used in this project.

Contact: Alan Goldfine, A266 Technology Bldg., 301/975-3252.

Public Key Cryptographic Protocols

NIST researchers are helping to protect data communicated through computer networks by developing protocols for secure key distribution and secure data transmission using public key algorithms. The protocols are intended to protect keys from initial generation to final distribution to all authorized parties. In designing the protocols, researchers are giving special attention to preventing substitution of the keys by unauthorized parties. The protocols will transmit keys and data within a large computer network with automated communications capabilities and will be consistent with those used in the Open Systems Interconnection Reference Model. Project results will be published in a NIST publication on public key cryptographic protocols.

Contact: Stuart Katzke, A216 Technology Bldg., 301/975-2929.

Geographic Information Systems

Geographic information systems (GIS) technology allows users to collect, manage, and analyze large volumes of spatially referenced and associated data. New research directions are emerging from the interdisciplinary uses of GIS. NIST researchers are exploring future GIS technology through studies into integrating computer graphics standards, database management standards, expert systems technology, and optical disk technology to support GIS applications. Their research is focused on providing GIS compatibility through standards and conformance testing for future GIS standards such as the

Digital Cartographic Data Standard. Because the activities of many governmental and private organizations are land and/or locationally related, GIS technology will be important in integrating existing spatial data for these organizations.

Contact: Henry Tom, A266 Technology Bldg., 301/975-3271.

Computer Graphics Testing

The development of several graphics standards and work on related conformance testing and measurement techniques for graphics software are under way at NIST. Specifically, NIST researchers are testing implementations of the graphical kernel system (GKS), the computer graphics metafile (CGM), GKS for three dimensions, and the programmers hierarchical interactive graphics standard (PHIGS) for conformance to existing and emerging federal, national, and international standards. Researchers are attempting to derive a general methodology for designing conformance tests, to use this methodology to generate test suites, and to evaluate the test suites for effectiveness. The computer graphics laboratory, which contains various computer graphics hardware and software systems designed to support standard specifications, is used in these efforts. An existing test suite for GKS is available with FORTRAN interface. Priority is being given to testing methodologies and test suites for PHIGS, CGM, and the conversion of FORTRAN tests for all computer graphics standards to other languages (C, Pascal, and Ada).

Contact: Mark W. Skall, A266 Technology Bldg., 301/975-3265.

Automated Protocol Methods

NIST researchers are designing tools for editing, compiling, and interpreting computer communications protocol specifications. The goal of the research is to advance the state of the art in using such tools to realize automatically executable implementation of the protocols. As part of this project, NIST researchers are developing a syntax-directed editor for Estelle and, using the same grammar, devising a portable compiler for Estelle and the supporting runtime libraries.

Contact: Kevin Mills, B217 Technology Bldg., 301/975-3618.

Network Security Architecture

To protect computer systems and networks, NIST is developing a comprehensive security architecture consistent with the Open Systems Interconnection (OSI) Reference Model. Cryptographic functions are being implemented in certain OSI layers to provide data secrecy, data integrity, and peer entity authentication. The research will combine the security standards for individual OSI layers into a unified security framework. As part of this project, NIST researchers will define a common interface for cryptographic algorithms and develop a key management methodology capable of providing keys to the cryptographic functions of any layer.

Contact: Stuart Katzke, A216 Technology Bldg., 301/975-2929.

Network Management

NIST researchers are working with industry to establish a set of standards to exchange network management information between heterogenous management systems. Their goal is to establish a standard enabling integrated, interoperable, automated management of multivendor computer systems, routers, bridges, switches, multiplexors, modems, and provider services. The researchers are defining protocols to exchange management information; identifying, collecting, and specifying the format of managed objects; defining protocols to support management functions in the areas of fault, configuration, performance, security, and accounting; and implementing prototype management systems reflecting the protocols and specifications. Other research areas of interest include network management user displays, network management applications software development, and application of expert systems to network management.

Contact: Kevin L. Mills, B217 Technology Bldg., 301/975-3618.

Directory Services and Dynamic Routing

In cooperation with industry, NIST is pursuing development of commercial off-the-shelf products implementing standard distributed directory services and dynamic routing. The distributed directory services require research work in several areas, including access control, replication of information, extension of directory schemas, and distributed update. Proposed solutions to these directory problems are implemented and tested in a NIST prototype directory implementation conforming to the international directory standard (X.500).

The NIST dynamic routing research is focused on exchange of routing information between routing systems in autonomous domains. NIST researchers propose and analyze a variety of mechanisms to accommodate such exchanges, and they investigate proposed algorithms through simulation models. The aim of this research is development of an international standard for exchange of routing information between autonomous domains.

Contact: Kevin L. Mills, B217 Technology Bldg., 301/975-3618.

Performance of Modern-Architecture Computers

NIST researchers in the area of computer-systems performance are promoting the effective evaluation and efficient use of advanced computers by the federal government. Their areas of interest include: characterization of new computer architectures to identify improved ADP technology for applications; exploration of economical programming methods that standardize across classes of architecture; and design of coherent evaluations that economically and reliably characterize the machines. Two dedicated, instrumented multiprocessors serve as special project resources. One has 16 nodes loosely coupled as a hypercube, and the other has 16 processors in a shared-memory configuration.

Contact: Robert Carpenter, B364 Materials Bldg., 301/975-5677.

Optical Disk

As industrial standards for optical disk media evolve, test methods will be needed for conformance testing of the media. NIST researchers are setting up a laboratory to develop and demonstrate data/media interchange tests and to verify conformance to established or planned national and international standards for rewritable and write once, read many (WORM) type optical disks. The program will be coordinated with voluntary standards committees and interested federal agencies.

Contact: Dana S. Grubb, A61 Technology Bldg., 301/975-2915.

Distributed Systems

NIST researchers are developing standards and guidelines for implementation and use of distributed computer systems. Their current activities include: participation in the development of a voluntary industry standard for distributed transaction processing, development of a software backplane (a standard platform for the development of distributed applications), research in distributed information retrieval systems, and formal description of distributed systems. The distributed systems laboratory is maintained to support prototype development of research activities.

Contact: Wayne H. McCoy, A216 Technology Bldg., 301/975-2984.

Automatic Speech Recognition

Recent advances in automatic speech recognition technology have resulted in improved abilities to recognize correctly continuous speech with lexicon sizes of at least 1,000 words. Speech databases are typically large in size (gigabytes) and too costly for any one organization to develop. To improve the technology, the research community relies heavily on shared use of the databases and standard test methodologies. With support from DARPA and other agencies, NIST has collected speech database material and, using CD-ROM technology, distributed this material to more than 100 research organizations. Researchers at NIST also have developed CD-ROM format speech databases that are used for speech recognition research in large vocabulary speech (5,000-word office correspondence), word spotting, speaker identification/verification, and goal-directed

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spontaneous speech. Among the research facilities are a VAX 11/780, a Sun workstation, and speech processing peripherals and software tools. Areas of interest include characterization of the speech database materials (e.g., acoustic-phonetic locators and classifiers), artificial neural nets, performance measurement, and natural languages.

Contact: David S. Pallett, A216 Technology Bldg., 301/975-2935.

Image Recognition

Image-recognition research at NIST focuses on developing methods for evaluation of image quality, compression efficiency, and image systems used in optical-character recognition. These methods of evaluation are designed to include highly parallel computers and special-purpose chips as well as conventional computer architectures. The methods being developed are used for automated fingerprint recognition, automation of data entry from images of forms, and measurement of recognition systems on realistic applications. A general model of the recognition process in parallel computers is being implemented to provide better methods to analyze the performance of SIMD (single instruction multiple data) computers for image compression, image quality evaluation, and recognition accuracy.

Contact: Charles L. Wilson, A216 Technology Bldg., 301/975-2080.

Integrated Services Digital Networks

In cooperation with industrial and other users, NIST advances the development of standards for Integrated Services Digital Networks (ISDN) which combine voice, data, text, and image communications over a single network connection. Research in this area focuses on the measurement capabilities and testbed facilities required to develop conformance tests and performance metrics for emerging ISDN standards. Activities include support for standards writing, development of the technical foundation for implementation agreements on protocol options, and testing ISDN implementations for interoperability.

Contact: George Kraft, B364 Materials Bldg., 301/975-3389.

Antenna Measurements

Researchers in the NIST antenna metrology program are developing reliable techniques and standards for measuring key performance parameters of antennas and components used with satellites, earth terminals, radars, and communications systems. Scientists now are using near-field scanning to characterize microwave and millimeter-wave antennas. Their current goals are to improve software and error analysis for the spherical near-field technique and to apply all the near-field techniques to higher frequencies. Other research areas include spacecraft and phased-array antenna measurements and antenna systems measurements using celestial radio sources.

Contact: Allen C. Newell, Div. 723.05, NIST, Boulder, CO 80303, 303/497-3743.

Dielectric Properties of Materials

Inadequate knowledge of the electromagnetic properties of materials inhibits development of new technologies, drives up the cost of systems and components, and may prevent achievement of optimal performance levels. A relatively new NIST program in materials is aimed at developing primary standards and accurate techniques for measuring the dielectric properties of materials used in electromagnetic applications. Scientists at NIST have developed new precision measurement techniques for complex permittivity based on improved theory and new cavity and transmission line sample holders. The researchers currently are performing the necessary error analyses and, in the future, plan to cover a variety of important materials and temperature ranges over the frequency range of approximately 10 MHz to 100 GHz. Reliable nondestructive methods are needed to measure complex permittivity and the reflectivity of large sheets of material or structures.

Contact: William A. Kissick, Div. 723.02, NIST, Boulder, CO 80303, 303/497-3339.

Electromagnetic Interference and Compatibility

NIST researchers are engaged in a wide range of projects aimed at quantifying electromagnetic interference (EMI) and electromagnetic compatibility (EMC). One thrust of the NIST work is to develop measurement techniques and methodologies for measuring emission of unintentional radiation from electronic devices. Another aspect under active investigation is the susceptibility of electronic equipment to such radiation. The researchers are identifying and defining quantities that characterize the susceptibility of a device and then developing methods to measure those quantities. Successful completion of this research should result in the development of standards and measurement techniques for EMI and EMC, which are meaningful, technically practical, and reliable. These techniques could then be incorporated into voluntary standards by both U.S. and international standard organizations.

Contact: Motohisa Kanda, Div. 723.03, NIST, Boulder, CO 80303, 303/497-5320.

Advanced Microwave/ Millimeter Wave Metrology

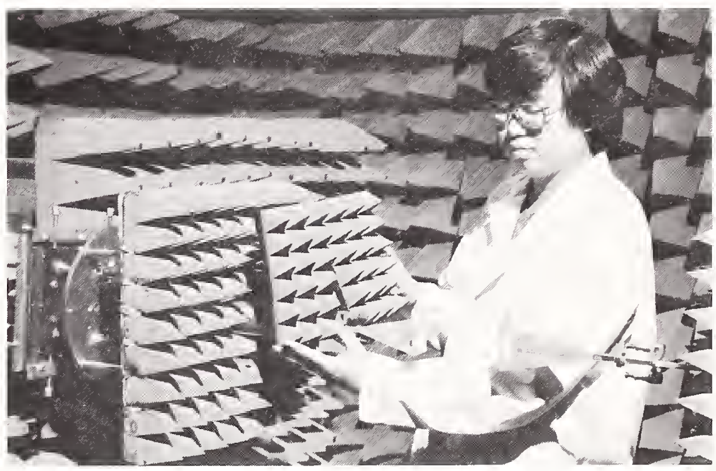
The rapidly developing and expanding microwave technology requires research in advanced microwave measurements and standards. The microwave industry and the Department of Defense depend on NIST for calibrations of transfer standards to provide the measurement traceability required for quality assurance and performance evaluations. NIST researchers have developed new, highly accurate six-port techniques for automated measurements of microwave power, attenuation, impedance, scattering parameters, and noise. They currently are developing greatly improved power and impedance standards and extending measurement services to cover millimeter waves and miniature coaxial connectors. Collaborative work is particularly desirable in microwave and millimeter wave circuit theory as applied to both traditional and advanced circuits and systems such as MIMIC devices. Applications include development of advanced automated network analyzers using six-ports.

Contact: David Russell, Div. 723.01, NIST, Boulder, CO 80303, 303/497-3148.

Magnetics

To provide a sound basis for measurement techniques, NIST researchers are developing a basic understanding of the magnetic properties of materials and structures. Specifically, they are studying precision cryogenic vibrating sample magnetometers, systems based on superconducting quantum interference devices (SQUID's), and laser-based magneto-optical systems. The primary emphasis of the program is on computer-related magnetics, but work is also under way on the basic physics of magnetic materials, such as spin glasses, and on the measurement of very low-level magnetic effects. In a related program in eddy current nondestructive evaluation (NDE), researchers are developing methods for mapping the very small ac magnetic fields associated with eddy current test probes.

Contact: Fred R. Fickett, Div. 724.05, NIST, Boulder, CO 80303, 303/497-3785.



Douglas T. Tamura, an electronics technician, aligns antennas being calibrated on the extrapolation range, which is part of the near-field antenna measurement facility.

Superconductor Measurements

Recent advances in superconductivity have resulted in a critical need for measurement technology to characterize the different types of superconductors, which now range from very fine filament alloy conductors used in the Superconducting Super Collider cables to a variety of high-temperature ceramic superconductors. Active research programs at NIST involve measurement techniques for critical current, critical magnetic field, ac losses, magnetic hysteresis, and electron tunneling. In addition, specialized experimental work is being done to determine the effect of strain on the superconducting properties of low-temperature commercial conductors and the high-temperature materials.

In a recent collaboration with industry, the resistance of contacts between normal metals and high-temperature superconductors was decreased by eight orders of magnitude, allowing accurate measurements of the magnetic-field dependence of the critical current. A standard for measuring critical current in low-temperature superconductors has been published through ASTM, and a Standard Reference Material (SRM) has been produced for use in calibrating critical current measurement apparatus. A new Reference Material for large currents is under development.

Contact: Fred Fickett, Div. 724.05, NIST, Boulder, CO 80303, 303/497-3785.

Raman Scattering

Some of the world's most advanced measurement facilities for the rapid advancement of electrical and electronic technology are available at NIST. One example is the Raman spectroscopy facility, which is used for light-scattering studies of liquids, solids, and gases. Specific research conducted at the facility includes chemical and structural analysis of thin films and ion-implanted layers, investigations of impurities and other defects in semiconductors, studies of the structural and electrical properties of semiconductor superlattices and quantum wells, and development of new quantitative spectroscopic methods.

Equipment is available for studies of the pressure and temperature dependence of Raman spectra in the range 4 to 600 K and up to approximately 100 kbar using a diamond-anvil pressure cell. The laboratory is equipped with variable wavelength lasers, multiple-grating monochromators, and automated digital data acquisition and processing.

Contact: Michael I. Bell, A305 Technology Bldg., 301/975-2044.

Compound Semiconductor Studies

Research to improve the metrology used to characterize compound semiconductors, including alloys and artificially structured materials, is under way at NIST. Scientists are studying the electrical, optical, and physical properties of materials, such as gallium arsenide and mercury cadmium telluride, to better understand and characterize presently available device material. A number of measurement techniques are used in this work, including ellipsometry, optical absorption, photoluminescence, infrared and Raman spectroscopy, Hall effect and resistivity measurements, capacitance-voltage profiling, deep-level transient spectroscopy, photoconductivity and photocapacitance, infrared imaging, and x-ray topography absorption and rocking curve analysis using synchrotron radiation.

Contact: Michael I. Bell, 301/975-2044 or David G. Seiler, 301/975-2074, A305 Technology Bldg.

Synchrotron Radiation

Studies of structural properties of matter have always relied on the use of x-ray techniques. Accordingly, NIST has constructed several x-ray beam lines at the National Synchrotron Light Source, Brookhaven National Laboratory. One of these beams provides collimated, intense energy-tunable x rays between 5 and 30 keV, which are 4 to 6 orders of magnitude brighter than x rays from conventional laboratory sources. The facility supports x-ray absorption and x-ray fluorescence measurements; x-ray scattering, diffraction, and standing wave capabilities are being added. Researchers are investigating semiconductor structures, including ohmic and Schottky metallizations, AlGaAs/GaAs interfaces, buried implanted layers, and heavily doped layers. A number of collaborative projects are under way with industrial and university research groups and with other government laboratories.

Contact: Charles E. Bouldin, 301/975-2046 or Michael I. Bell 301/975-2044, A305 Technology Bldg.

Silicon Characterization

NIST conducts research in semiconductor materials, processes, devices, and integrated circuits to provide the necessary basis for understanding measurement-related requirements in semiconductor technology. As part of this program, NIST scientists are employing electrical, optical, and x-ray methods to study the resistivity, dopant distribution, and concentration of electrically inactive impurities, such as carbon and oxygen, in silicon. They are developing new or improved techniques by two- and three-dimensional mapping of these properties, refining the quantitative aspects of existing methods, and developing nondestructive methods. Measurement techniques include four-probe, spreading resistance, and capacitance-voltage; Fourier transform infrared spectroscopy; deep-level transient spectroscopy; x-ray topography; and synchrotron radiation studies.

Contact: Michael I. Bell, A305 Technology Bldg., 301/975-2044 or Jeremiah R. Lowney, B310 Technology Bldg., 301/975-2048.

Semiconductor Processing

Theoretical and experimental research on semiconductor materials and process physics at NIST is focused on improving understanding of integrated circuit fabrication technology and increasing capability to characterize materials and processes. Utilizing processing equipment and techniques appropriate to VLSI chip fabrication, NIST scientists are conducting experimental studies on issues related to state-of-the-art semiconductor processing in a well-equipped clean-room semiconductor processing laboratory. Researchers are studying ion-implantation damage, oxidation growth and interface trap formation, materials effects caused by ion etching, thin-film properties, and plasma and ion-beam chemistry. Other areas of interest include submicron (submicrometer) photolithography, reactive ion etching, development of Standard Reference Materials for use in the semiconductor industry, and chemical and vapor deposition.

Contact: Donald Novotny, 301/975-2699 or James Comas, 301/975-2061, A357 Technology Bldg.

Advanced Integrated Circuit Test Structure Metrology

Integrated circuit test structures and test methods developed by NIST are widely used by the semiconductor industry and other government agencies. These devices can be used to characterize integrated circuit (IC) manufacturing processes, to evaluate the effectiveness of semiconductor processing equipment, to obtain crucial parameters for process or circuit simulators, and for product acceptance. NIST work involves test structure design, modeling, data acquisition, and data analysis. Institute engineers are investigating artificial intelligence techniques for the rapid diagnosis of IC manufacturing processes and for establishing methods to determine the reliability of thin films used in state-of-the-art microcircuits.

Contact: Loren W. Linholm, B360 Technology Bldg., 301/975-2052.

Semiconductor Devices

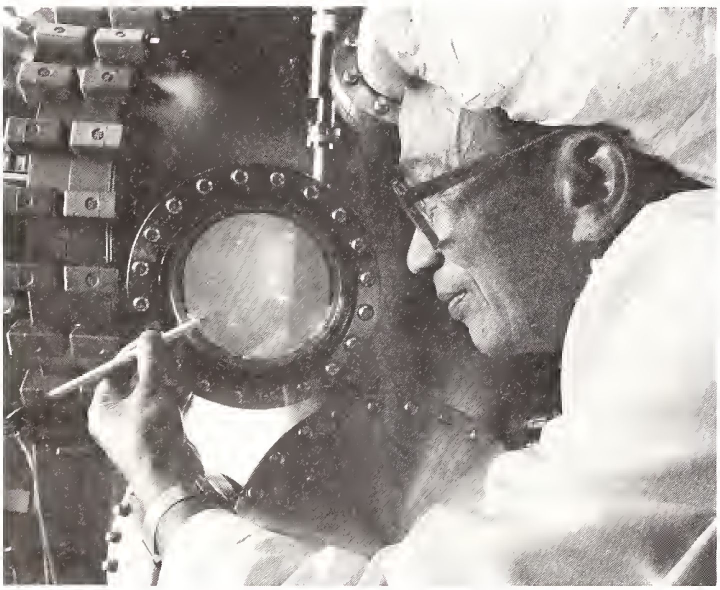
To develop physically sound techniques for characterizing, analyzing, and predicting the operation and performance of semiconductor devices, NIST researchers are designing and improving measurement methods to determine critical device parameters for both VLSI-scale and power devices. Research in device modeling includes two-dimensional silicon MOSFET and GaAs MESFET model development and investigations into the validity of the physical assumptions typically employed in silicon bipolar and GaAs device models. Theoretical research is carried out on the transport of ions and electrons in semiconductors for improved process modeling, and experimental research on the nature and characterization of electronic states in oxides and at oxide/semiconductor interfaces is under way. NIST scientists are developing methods for physical and electrical measurements of device and material parameters which are critical for verifying the accuracy and validity of device models. In addition, they are researching the electrical and thermal properties of power semiconductor devices.

Contact: Herbert S. Bennett, B310 Technology Bldg., 301/975-2053.

Molecular Beam Epitaxy

The controlled growth capabilities of molecular beam epitaxy (MBE) have resulted in the fabrication of structures that represent a new class of semiconductors with properties which do not exist in bulk materials. The MBE program at NIST includes the growth and characterization of GaAs and AlGaAs layers, as well as the growth of heterostructures for superlattice and quantum confinement studies. Scientists examine fundamental properties of the MBE layers using photoluminescence, deep-level-transient spectroscopy, Hall effect, secondary-ion-mass spectroscopy, and in-situ reflection electron diffraction (RED). Studies are under way to correlate RED oscillation intensity measurements with material quality and growth parameters.The MBE program is an interactive effort, and cooperative research opportunities exist in a variety of materials characterization and device-related areas.

Contact: James Comas, 301/975-2061, Wen Tseng, 301/975-5291, or Joseph Pellegrino, 301/975-2123, A357 Technology Bldg.



Wen Tseng, materials research engineer, observes an in-situ reflection electron diffraction pattern during the growth of gallium arsenide.

Solid-State DC Voltage Standards

Precision voltage standards based on solid-state references are finding increasing use in dc voltage metrology, particularly in the design and support of high-accuracy digital voltmeters and automated test equipment. To improve the quality of these standards, NIST scientists are carrying out a research program on Zener diodes and similar devices. They are investigating device properties such as temperature coefficient, short-term noise, long-term stability, and performance under temperature shock and power interruption. The aim of these investigations is to identify devices suitable for a rugged 10-V transportable standard capable of providing sub-part-per-million (ppm) accuracy when used as a transport standard between laboratories. The effects of temperature extremes, physical shock, and shipping delays on diode output are of special interest.

NIST also is producing a stable 1.018-V output derived from a solid-state reference. Researchers are focusing on the design and manufacture of low-noise, stable resistors that are immune to temperature shock and power interruption. Facilities are available to test Zener diodes with 0.1-ppm resolution and to manufacture both bulk metal foil and wire-wound resistors. Scientists are able to study in detail the dependence of device performance on fabrication parameters as a result of high-accuracy measurements referenced to national standards and through collaborative efforts on the fabrication of Zener devices.

Contact: Bruce F. Field, B258 Metrology Bldg., 301/975-4230 or Alan F. Clark, B258 Metrology Bldg., 301/975-2139.

Advanced AC Voltage and Current Measurements

Thermal voltage and current converters offer the most accurate and broadband method for measuring ac voltage and current for applications in communications, power generation, aerospace, and defense. Thermal transfer standards are calibrated by NIST in terms of reference converters which have themselves been characterized by reference to the NIST primary standards—special multijunction thermal converters whose performance is known. These primary and working standards in common use throughout the metrology community employ thermal converters fabricated from wire elements. Researchers at NIST are studying new methods for the manufacture of film thermal converter structures made by the use of photolithography on silicon substrates. The application of this new technology may result in improved performance and reduction in the cost of thermal converters.

Contact: Joseph R. Kinard, 301/975-4250 or Norman B. Belecki, 301/975-4223, B146 Metrology Bldg.

Waveform Recorder Standards

As part of a program aimed at meeting the metrological needs involved in improving signal acquisition and processing systems, NIST researchers are developing theory, methods, and standards for waveform metrology of conducted signals. The scientists are conducting the theoretical and experimental research necessary to develop standards for determining the performance of waveform recorders operating nominally below 10 MHz and will develop techniques for synthesis of precision waveforms and for characterization of those waveforms. Theoretical studies will be conducted on Fourier analysis, deconvolution techniques, and time-domain analysis. Program plans include experimental work in precision pulse generation, static and dynamic testing, and assembly and interpretive level programming for hardware control.

Contact: Barry A. Bell, B162 Metrology Bldg., 301/975-2402.

Electro-optical Metrology

Researchers at NIST are developing electro-optical methods to measure electrical quantities and phenomena as part of a program to develop theory, methods, and physical standards for measuring electrical quantities in advanced high-voltage/high-power systems. Theoretical studies are focused on the use of finite-element code for electric-field computation and computer-aided data acquisition and analysis. Experimental research includes high-voltage ac, dc, and impulse measurements; high-speed camera techniques; optical multichannel analyzers; and lasers and detectors.

Contact: William E. Anderson, B344 Metrology Bldg., 301/975-2403.

AC Voltage Standards

NIST is conducting both theoretical and experimental research on the synthesis of precision ac waveforms for use in ac voltage standards operating nominally below 10 MHz. The theoretical work includes Walsh functions and Fourier analysis, time-domain analysis, and precision RMS-to-dc conversion techniques. Experimental work involves high-speed, high-accuracy digital-to-analog conversion; precision, high-speed switching; assembly and interpretive level programming for hardware control; and wideband, fast-settling amplifiers.

Contact: Barry A. Bell, B162 Metrology Bldg., 301/975-2402.

Testing Electronic Systems

New strategies are needed to evaluate the performance of complex electronic circuits using the fewest possible tests. A new program is under way at NIST which includes theoretical studies of modeling for nonlinear systems, optimization techniques using matrices, statistical and random processes, and artificial intelligence. In addition, experimental work will address test strategies for component and instrument testing; fault diagnosis, function testing, and calibration; and computer analysis using both desktop computers and supercomputers.

Contact: Barry A. Bell, B162 Metrology Bldg., 301/975-2402.

Gaseous Dielectrics

Scientists at NIST are developing measurement methods to characterize gaseous dielectrics for high-voltage power systems. Theoretical work is expected to address Boltzmann equilibrium statistics, chemical kinetics code, and computer-aided data acquisition and analysis. Experimental work will focus on high-voltage ac and dc tests, gas chromatograph and mass spectrometer techniques for chemical characterization, and partial discharge measurements. Much of NIST's work in advanced power metrology is performed in newly completed high-voltage and high-current laboratories. These facilities can generate voltage pulses with peak amplitudes up to 600,000 volts and current pulses with peak amplitudes up to 100,000 amperes.

Contact: William E. Anderson, B344 Metrology Bldg., 301/975-2403.

Fire Research

Flammability and Toxicity Measurement

Institute researchers are creating ways to measure and characterize the combustibility of furnishings and building materials and the extent to which combustion products affect living organisms. NIST research typically focuses on assessing the appropriate applications of the NIST toxicity screening test, evaluating the extent to which a limited number of gases determine the lethality of combustion products, and developing a methodology for predicting soot and gas production in full-scale fires from bench-scale methods. In addition, Institute researchers are generating a detailed model for the burning of upholstered furniture and aiding the use of the cone calorimeter in engineering and code applications.

Contact: Vytenis Babrauskas, A363 Polymer Bldg., 301/975-6679.

Fire Simulation

This project in fire research is designed to provide the expedient transfer of scientifically based technology from NIST to the professional user community and to create a link between NIST computer-based activity and others doing similar or complementary work. Over the past decade, NIST researchers have developed many computer models of various aspects of fire. Researchers develop engineering systems for design application as well as expert systems, collect supporting data and programs, and operate a working and training laboratory dedicated to computer modeling and other fire-safety computations.

Contact: Harold E. Nelson, A247 Polymer Bldg., 301/975-6869.

Hazard Analysis

The United States has one of the worst fire records in the industrialized world. NIST researchers are helping to reduce the losses and the cost of fire protection by providing scientific and engineering bases needed by manufacturers and the fire protection community. One project involves the development of predictive, analytical methods which permit the quantitative assessment of hazard and risk from fires. Researchers base these methods on numerical modeling but also include hand-calculation methods for estimating hazards and production of design curves/tables to be used by architects and engineers. To ensure widespread use, the necessary data must be readily available, and data input and presentation must be in terms readily understandable by the average professional. Thus, the projects include a strong emphasis on state-of-the-art computer graphics and computer-aided design techniques.

Contact: Richard W. Bukowski, B356 Polymer Bldg., 301/975-6850.

Fire Growth and Extinction

Predicting fire growth requires a fundamental understanding of elemental fire processes. The Institute is helping to improve this understanding by developing predictive methods to describe the processes of fire growth and the elemental processes of fire growth and extinction as related to gaseous, liquid, and solid fuel combustion and the performance of fire safety systems. Researchers are exploring fire growth within a single compartment, the spread of fire to adjoining spaces in multicompartment structures, and the action of fire suppressants. In addition, they are examining the overall dynamics of the fire scenario and related elemental processes, such as ignition, flame spread, pyrolysis, extinction, and fire-related transport processes. For these studies, they utilize mathematical techniques, experimental studies, correlations, and similitude methods to develop predictions.

Contact: James G. Quintiere, B250 Polymer Bldg., 301/975-6863.

Polymer Combustion Research

NIST is conducting research to develop a scientific base for the gasification and combustion of natural and synthetic polymers, particularly for the more applied fire research activities. For example, NIST scientists are working on the kinetics and heats of combustion for wood, theoretical modeling of thermal degradation of polymers, smoldering research, and detailed degradation mechanisms of polymers.

Contact: Takashi Kashiwagi, B258 Polymer Bldg., 301/975-6693.

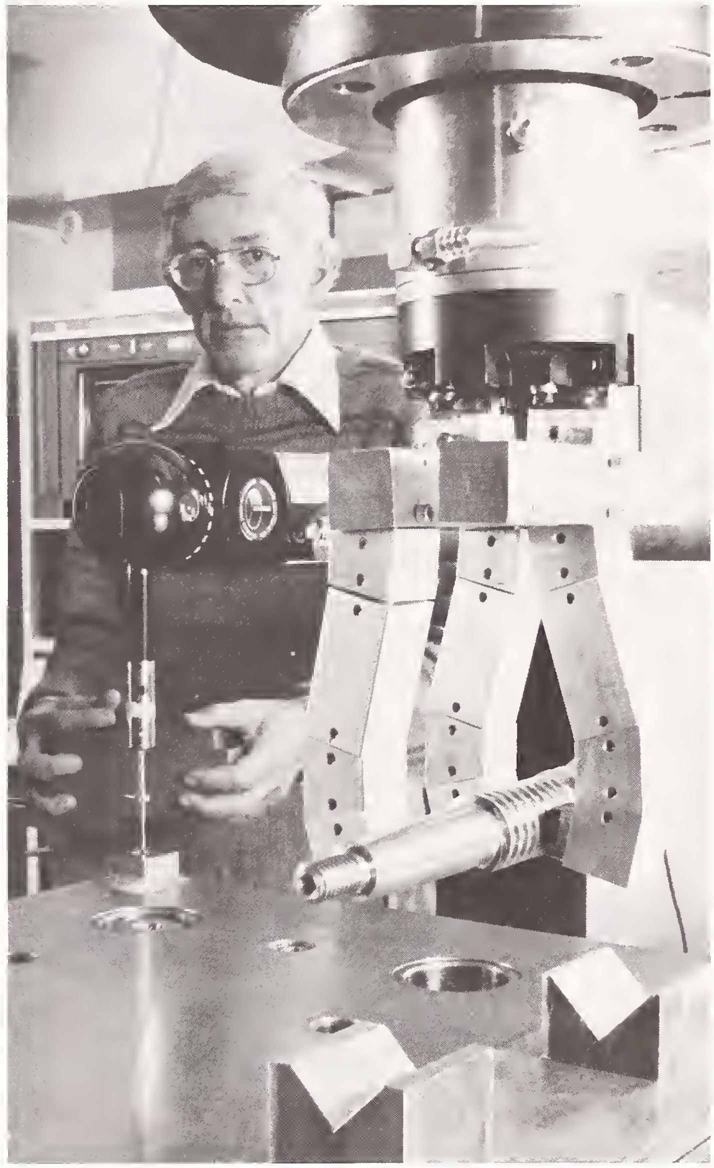
Manufacturing Engineering

Automated Manufacturing Systems Hardware

Automated manufacturing systems include flexible, small-batch manufacturing systems, and machine tools into which intelligent sensors and controls of the production processes, as well as the machining itself, have been embedded. To support such developments by industry, NIST scientists are investigating generic control systems, full-task programming, data organization, sensor organization, system initialization, and the object-data analogy. In the area of process monitoring, researchers are developing techniques for dimensional and surface condition monitoring during the machining process.

NIST efforts in real-time error correction of machine tools are centered on extending microprocessor-based techniques for real-time correction of the kinematic (as well as static) machine errors and tool wear for conventional machining as well as diamond turning. The researchers are studying transient waves in solids by investigating the origin, propagation, measurement, and direct- and inverse-prediction of micromechanical waves in acoustic emission and ultrasonics. Transducer field studies are focused on the fields produced in solids by electromechanical transducers by modeling and measuring the fields point-by-point within the solids.

Contact: Donald S. Blomquist, B108 Sound Bldg., 301/975-6600.



Metrologist Ralph Veale monitors the performance of a robot at the inspection workstation in the NIST Automated Manufacturing Research Facility.

Precision Engineering and Nanotechnology

Precision engineering forms the foundation for established devices such as modern coordinate measuring machines (CMM's) as well as for the emerging "nanotechnology" of nanostructures—the fabrication of devices with physical features of the order of 1 nanometer (one-billionth of a meter or 40-billionths of an inch) in size. Nanotechnology holds the promise of many new industrial products including, for example, mechanical pumps small enough to be implanted into arteries, surgically altered DNA molecules, and electronic devices hundreds of times smaller than those available today. Using an array of state-of-the-art coordinate measuring machines and advanced electron-probe instruments, NIST precision engineering researchers are developing the capabilities to precisely observe, locate, fabricate, and measure the nanometer-sized features of such devices.

Contact: Dennis A. Swyt, A109 Metrology Bldg., 301/975-3463.

Materials Reliability

Automated Manufacturing Systems Software

For industries creating and using computer-controlled manufacturing systems, software systems are the critical element. NIST provides research for software in automated manufacturing systems in several areas. In automated process planning, researchers are investigating data structures for automated process planning, distributed system architectures, machinable-feature identification, and expert systems/machine-learning for manufacturing systems. Researchers also are studying architectures, algorithms, and techniques for real-time adaptive control, scheduling, and optimization of cell- and workstation-level operations for FMS cell and workstation control systems. In addition, for manufacturing systems architectures, they are devising functional models of manufacturing organizations to standard system architectures.

Contact: Howard M. Bloom, A127 Metrology Bldg., 301/975-3508.

Robot Systems

NIST conducts research in intelligent-machine systems for manufacturing, construction, space satellite servicing, and intelligent vehicle applications. NIST researchers are investigating standard architectures for real-time intelligent control, which involves hierarchical task decomposition, world modeling, and sensory processing. The research includes real-time planning; the representation of space, time, objects, and events; and the analysis of data from a variety of sensors, such as TV cameras, sonar, and tactile arrays. Researchers are also studying programming methods and operator interfaces for intelligent vehicles and telerobots. Methods are being developed for measuring the performance of intelligent machine systems, including software performance. Research in advanced structures for robot systems includes robot cranes and inflatable structures.

Contact: James S. Albus, B124 Metrology Bldg., 301/975-3418.

Composite Mechanics

NIST researchers are exploring ways to achieve the great potential of composite materials for structural applications. Using acoustical and optical techniques, the researchers are investigating the mechanisms of fracture in laminated plates. In support of the nondestructive evaluation program, researchers are using finite-element and finite-difference methods to simulate and model acoustic-wave propagation. Another project involves refining theoretical models and computer programs to predict near- and far-field singularities of the various damage types in laminated structures. NIST scientists also are monitoring damage initiation in situ by embedding optical fiber sensors in composite structures. All projects emphasize evaluation of the potential structural performance of new advanced composite materials.

Contact: Ronald D. Kriz, Div. 430, NIST, Boulder, CO 80303, 303/497-3547.

Nondestructive Evaluation (NDE)

NIST scientists are developing acoustic and electromagnetic sensors for material characterization, including electromagnetic-acoustic transducers (EMAT's), arrays of piezoelectric polymers, and eddy current and capacitive probes.

EMAT's are used for noncontacting applications, where it is not possible to have an intervening material couple sound from transducer to specimen. For example, an EMAT embedded in a rail is used to inspect railroad wheels for cracks in a roll-by mode. Researchers are investigating the possible use of EMAT's at the input to an automated press shop, where automobile body parts are formed. Formability measurements could be made on moving sheet, and materials with improper formability would be rejected from the production line.

Acoustic arrays are useful in medical imaging, where their unique advantages allow suppression of artifacts to give better image quality. Research is being conducted by NIST to use these techniques to characterize composites. Various types of arrays are being constructed and interfaced with signal processing devices.

NIST scientists have developed eddy current probes and techniques for detecting and sizing small defects that could prove to be critical in aircraft and other structures. Capacitive probes are being investigated as a noncontacting means to monitor sintering of ceramics, with possible use as a process control in the production of superconductors. Another application under study is noninvasive cure monitoring of composites.

Contact: Alfred V. Clark, Div. 430, NIST, Boulder, CO 80303, 303/497-3159.

Thermo-mechanical Processing

Metals producers and manufacturers rely heavily on pilot-scale or production facilities for the development of new alloys or new manufacturing schedules. This is not only expensive but can also yield unreliable results. These processing problems can be alleviated by using a more economical, versatile, and reproducible laboratory facility. Controlled thermomechanical processing (TMP) offers the opportunity to produce superior steels at lower cost due to the elimination of post-heat treatment—an energy-intensive process.

NIST scientists and engineers have designed and built a computerized, laboratory-scale, hot-deformation apparatus that can simulate manufacturing processes, such as forging and plate rolling, and measure important properties incurred during processing. The apparatus can be used to study static and dynamic recrystallization, high-temperature deformation resistance in terms of true stress-strain curve at high strain rates, and phase transformation characteristics. The apparatus is used to characterize directly cooled forging steel during simulated forging operations in an attempt to develop optimized steels and forging procedures.

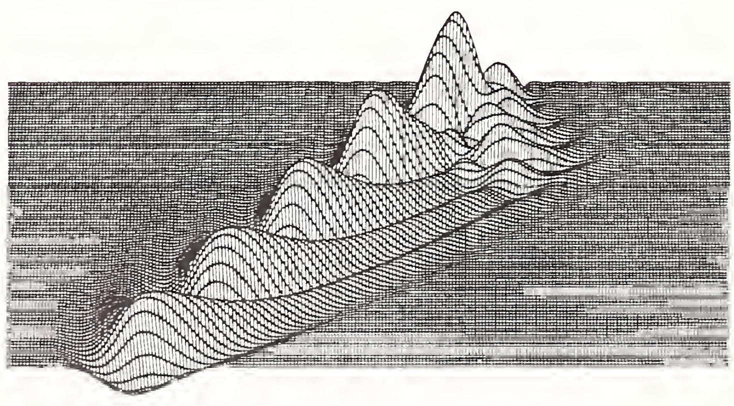
Contact: Yi-Wen Cheng, Div. 430, NIST, Boulder, CO 80303, 303/497-5545.

Fracture Mechanics

Research in fracture mechanics helps to determine the performance and safety requirements of structural materials. NIST's most advanced measurement techniques are aimed at two complementary quantities: fracture-driving force and fracture resistance. Fracture-driving force is analogous to stress but is much more complicated. By measuring stresses and strains in the material surrounding a crack, fracture-driving force at the crack tip can be calculated mathematically. A previous NIST technique used 36 strain gauges but now a new grid method has been developed in which a fine grid is bonded to the specimen. A photographic image of the deformed grid is read using an automated laser diffractometry system. All in-plane strain components are measured with a precision of 50 microstrain and a spatial resolution of 1 mm.

Fracture resistance is studied by examining fracture surfaces with a scanning electron microscope to find the microscopic origins of brittle fracture or the nuclei of the voids that join to form ductile fracture surfaces. A quantitative metallography facility makes it possible to measure accurately the density and characteristics of inclusions fundamental to the fracture process.

Contact: David T. Read, Div. 430, NIST, Boulder, CO 80303, 303/497-3853.



This computer-generated diagram shows a stress wave moving along the fiber orientation in a unidirectional graphite-epoxy composite. Each of the humps represents a period of the wave and the ripples coming off these periods.

Metallurgy

Cryogenic Materials

Comprehensive low-temperature facilities are available to conduct both characterization testing and fundamental studies on the mechanical and physical properties of high-strength structural alloys, high-conductivity metals and superconductors, metal and polymer-based composites, and polymer foams. Properties studied include tensile strength, compression, fatigue, creep, fracture toughness, stress relaxation, elasticity (ultrasonic), and thermal expansion. Strain sensitivities of 10^{-7} at liquid helium temperature (4 K) are now possible, permitting precise low-temperature microstrain measurements. Researchers are assembling equipment to permit load capacities of 5 MN for testing at 4.2 K.

Contact: Richard P. Reed, Div. 430, NIST, Boulder, CO 80303, 303/497-3870.

Joining Research

The integrity of welded joints is a primary concern in the design and fabrication of engineering structures. Researchers at NIST are investigating ways to improve the fracture resistance of weldments and are assessing weld quality by nondestructive evaluation (NDE) techniques. Specific goals of the research are to improve fracture toughness in the heat-affected zone of steel weldments and in the weld metal of materials for low-temperature service and to improve the soundness of welds through increased understanding of the metal transfer process in arc welding. In addition, the researchers are applying fine-resolution NDE techniques to evaluate solder joints in printed circuit boards for the electronics industry. NIST scientists have developed techniques to reduce porosity in aluminum weldments, to reduce spatter in gas metal arc welding of steels, and to predict accurately the Ferrite Number in stainless steel welds.

The NIST welding and NDE laboratories house equipment for shielded metal arc, gas metal arc, and gas tungsten arc welding; radiographic and penetrant techniques for nondestructive evaluation of weldments; and a precision power supply, high-speed photography, and laser shadow techniques for metal-transfer studies.

Contact: Thomas A. Siewert, Div. 430, NIST, Boulder, CO 80303, 303/497-3523.

Corrosion Data Program

Corrosion is a major limiting factor in the service life and cost of many products, plants, and equipment. The costs of metallic corrosion to the U.S. economy are estimated to be $200 billion in 1988 dollars, $30 billion of which could be saved by using existing technology. The National Association of Corrosion Engineers (NACE) and NIST have joined together in a collaborative NACE/NIST Corrosion Data Program to reduce the enormous costs of corrosion. The focus of this program is to establish an evaluated corrosion database that can be accessed easily by computer using intelligent interfaces to obtain data in a number of graphical, tabular, or textual formats. The researchers are developing evaluation methodologies and a prototype database for areas covering thermodynamic and kinetic corrosion data. NIST scientists are emphasizing interactions with industry both to help set priorities for data projects and as a source of corrosion data for the database.

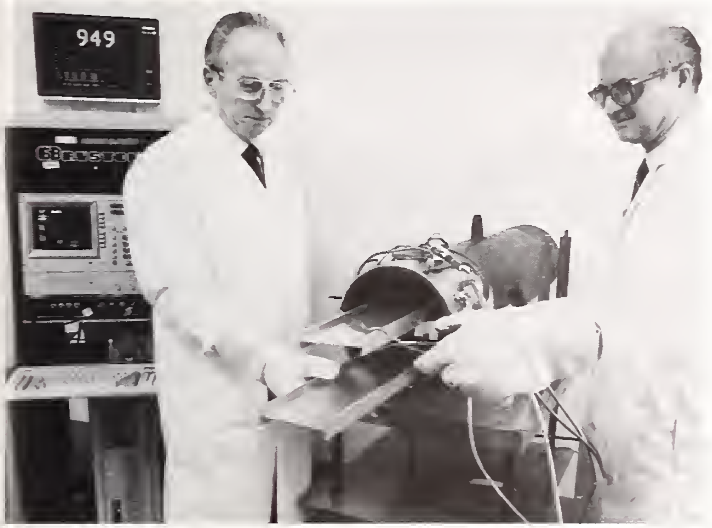
Contact: David B. Anderson, A109 Materials Bldg., 301/975-6026.

Corrosion Measurements

Corrosion has been recognized as a major cause of degradation of all kinds of metallic structures, with financial costs well in the billions-of-dollar range. Since corrosive reactions are of electrochemical nature, electrochemical measurements can give important information about the chemical processes causing the corrosion and the rate of corrosion as well as its forms, whether uniform or localized. Researchers at NIST are determining current and potential and their variations with time, measuring the frequency spectrum of the ac impedance of corroding electrodes, and detecting and analyzing random fluctuations of electrical parameters.

Electrochemical methods for measuring corrosion rates offer the possibility of tracking the process in a nondestructive way and assessing the effect of various environmental variables. Other electrochemical techniques can shed light on the kinetics of the corrosion reactions and on the critical factors which may contribute either to catastrophic failures or corrosion prevention.

Contact: Ugo Bertocci, B242 Materials Bldg., 301/975-6017.



Arnold Kahn (left), a NIST physicist, and Michael Mester, a research associate from the Aluminum Association, have developed a process control sensor, designed to be used in the production of extruded aluminum products.

Process Control Sensors

Special facilities at NIST enable researchers to develop advanced measurement methods and standards in support of emerging sensors and their application to process modeling and control for intelligent processing of materials. Measurement methods available include ultrasound, eddy currents, and acoustic emission. In particular, noncontact ultrasonic facilities have been designed featuring high-intensity pulsed lasers and electromagnetic acoustic transducers. Coupled with state-of-the-art materials-processing equipment and expertise, these facilities offer a unique opportunity to ascertain feasibility and develop prototype specifications for a wide spectrum of sensor needs, including the measurement of internal temperature, phase transformations, surface-modified layers, porosity, grain size, and inclusion/segregate distributions.

Contact: H. Thomas Yolken, A165 Materials Bldg., 301/975-6140.

Rapid Solidification

The rapid solidification of alloys can produce new types of materials, unobtainable by conventional means. Because of their special properties, rapidly solidified alloys are being investigated widely and are beginning to be introduced into commercial devices. Equipment is available at NIST to study alloys produced by each of the three major rapid solidification techniques: atomization techniques in which fine liquid droplets are formed and rapidly frozen to produce alloy powder; ribbon techniques in which a very thin liquid stream or ribbon is rapidly solidified; and rapid surface-melting and refreezing techniques in which a directed energy source, such as an electron beam, is scanned across a surface. The emphasis in the NIST work is on measurement and predictive modeling of the rapid solidification processes. Researchers are studying crystalline and metallic glass, as well as the new quasicrystal alloys discovered at NIST. Efforts are under way to apply advanced sensors to an inert gas atomization system to allow feedback and control of this process. Because processing conditions influence alloy homogeneity, microstructure, extended solid solubility, and the production of new alloy phases, control of these features is critical for producing special properties in these new materials.

Contact: John R. Manning, A149 Materials Bldg., 301/975-6157.

Field Corrosion of Metals

The corrosion of metals in natural and manmade environments is very costly to industry and government. For several years, NIST researchers have been involved in developing methods for measuring the corrosion of metals in field conditions, such as steel piling in soil and seawater, electric utility lines in soil, and most recently, steel in concrete. To measure the corrosion of reinforcing steel in concrete bridge decks, NIST scientists have developed a small, portable computer system. With this system, scientists are able to use electrochemical techniques normally limited to the laboratory to measure the corrosion. This new approach, which allows faster, more accurate corrosion measurements, can be used to evaluate the effectiveness of protection systems in place. The system has been applied to several bridges in Maryland and Washington state.

Contact: Edward Escalante, B250 Materials Bldg., 301/975-6014.

Neutron Scattering and Diffraction

Steel Slag Thermochemistry

Thermochemical databases and models are needed by the U.S. steel industry for the design of new or improved steel-making processes. To design such processes, NIST researchers are involved in three programs: measuring refractory and slag thermochemical equilibria, evaluating the scattered literature data, and developing computer models that relate experimental data to industrial conditions. Unique experimental facilities are available at NIST for measuring key phase equilibria and kinetics.

Contact: John W. Hastie, B108 Materials Bldg., 301/975-5754.

Environmentally Induced Fracture of Advanced Materials

Corrosive reactions between the environment and advanced materials can dramatically alter the fracture resistance of the material. To assist in the development of advanced materials, NIST scientists are studying the mechanisms by which environments can induce crack propagation at stresses well below those which cause normal fracture. Researchers are developing experimental techniques to evaluate and quantify the susceptibility of different types of advanced materials. Experiments are being conducted to investigate the mechanisms of hydrogen absorption, dissolution, and environmentally induced cleavage on different types of materials, specifically low-density, high-strength Al-Li alloys; intermetallic compounds; and composites as well as simple model systems.

Contact: Richard E. Ricker, B252 Materials Bldg., 301/975-6023.

Magnetic Materials

As part of the NIST program in magnetic materials, researchers are studying the magnetic properties of alloys and their relationship to metallurgical structure. Composition-modulated alloys, granular metals, metallic glasses, and icosahedral crystals are among the materials being investigated. The magnetic properties are characterized by ac magnetic susceptibility measurements, magneto-optic Kerr effect, and Mössbauer effect observations.

Contact: Lawrence H. Bennett, B154 Materials Bldg., 301/975-5966.

The NIST Cold Neutron Research Facility, designed as a national user facility, will house a number of special instruments with application to a wide range of materials problems.

Activation Analysis

More than 50 billion chemical analyses are performed annually in the United States. NIST helps to ensure the accuracy of these analyses by developing new analytical procedures and improving the reliability and accuracy of present methods. One technique under study is activation analysis, which is a highly sensitive, nondestructive analytical technique not available in most industrial laboratories. Researchers are investigating methods of nuclear analysis utilizing the NIST 20-MW research reactor. Research is performed in all areas of the technique, including the capabilities of cold-neutron activation, the use of sample self-consistent (monitor) activation, determination of new mathematical procedures for the resolution of gamma spectra, the development of prompt-gamma activation techniques, and the use of charged-particle activation techniques. The NIST Cold Neutron Research Facility will include a new neutron depth-profiling instrument and a prompt-gamma activation station. Together, these are expected to form the best capability in the world for chemical analysis with neutron beams.

Contact: Robert R. Greenberg, B108 Reactor Building, 301/975-6285.

Neutron Nondestructive Evaluation (NDE)

Neutron radiography has been a well-established tool for nondestructive evaluation for some time. More recent neutron applications in NDE include neutron diffraction for texture and residual stress determination. All three specialties are available for co-operative R&D utilization and development at the NIST research reactor. In general these techniques parallel their x-ray counterparts; however, in certain cases (e.g., where hydrogenous components are critical or where subsurface texture or residual stress distributions are sought) x rays do not provide the needed sensitivity or penetration.

NIST scientists are continuing their collaboration with scientists from the Smithsonian Institution to examine art works using neutron radiography. They also are working to apply the technique to industry-related problems and to extend the existing capabilities to, for example, backscatter radiography. Scientists from NIST and the Department of Defense (DOD) are continuing to develop and apply neutron diffraction techniques to texture and residual stress characterization. Texture studies have centered on copper, tantalum, and uranium-alloy components for a variety of DOD items; recent work has included ceramic superconductors. Neutron residual stress studies have involved components made of the above metals as well as ceramics, fiber-reinforced ceramic composites, and steel.

Contact: Henry J. Prask, 301/975-6226 or Chang S. Choi, 301/975-6225, A106 Reactor Building.

Neutron Spectroscopy

Researchers at NIST are studying the vibrational dynamics and diffusion of hydrogen in metals and molecular species in heterogeneous catalysts, clays, and other layered materials. Inelastic and quasielastic neutron scattering and neutron diffraction are among the techniques used by the scientists to reveal the bonding states and atomic scale interactions and diffusion paths in such materials.

Studies also are being conducted on the atomic and crystal dynamics in bulk materials and alloys. Recent progress has allowed in-situ spectroscopic studies of hydrogen and molecular species down to 0.1 of an atomic percent. These measurements can provide direct information, for example, on the molecular processes affecting reaction and selective release of chemicals in industrial catalysts and on the local trapping and clustering of hydrogen in metals and semiconductors, which cause embrittlement, corrosion, or changes in electronic properties. NIST scientists are working with researchers from several industrial laboratories to study zeolites and other catalytic materials. Equipment available includes three-axis neutron crystal spectrometers and time-of-flight spectrometers for inelastic scattering, which, along with neutron diffractometers, measure structural and dynamic processes in the time regime from 10^{-10} to 10^{-14} s. Two very-high-resolution inelastic scattering spectrometers will be available at the NIST Cold Neutron Research Facility. Controlled temperature (0.3 -1300 K) and pressure devices are available for changing sample environments.

Contact: J. Michael Rowe, 301/975-6210 or John J. Rush, 301/975-6231, A106 Reactor Building.

Small-Angle Neutron Scattering

Detailed microstructure information is often a key to the prediction or understanding of the performance or failure of structural materials and materials-processing conditions. Researchers at NIST use small-angle neutron scattering (SANS) to characterize submicron structural and magnetic properties of materials in the size regime from 1 to 100 nm. Among the structural features in this size regime that produce SANS diffraction patterns are: small precipitates or cavities in metal alloys, micropores or cracks in ceramics, colloidal suspensions and microemulsions, and polymers and biological macromolecules. These patterns can be analyzed to give information on the size and shape of the scattering centers as well as their size distribution, surface area, and number density.

A number of scientists from the chemical, communications, advanced materials, and aerospace industries are already engaged in SANS research at NIST. Their measurements are carried out with long-wavelength neutrons on the 8-m-long NIST SANS spectrometer which utilizes a 65-by-65-cm position-sensitive detector to record data over the entire small-angle region simultaneously. The

Nondestructive Evaluation

addition of two 30-m SANS spectrometers in the NIST Cold Neutron Research Facility will enhance significantly resolution and sample throughput. Computer-automated apparatus is available for maintaining samples at temperatures from 4 to 700 K and in magnetic fields up to 20 kilogauss. To extract structural information from the data, the researchers analyze SANS patterns with an interactive color graphics system and related programs.

Contact: Charles J. Glinka, 301/975-6242 or James A. Gotaas, 301/975-6243, A106 Reactor Building.

Neutron Diffraction

Precise information on the crystal structure (arrangement of atoms and molecules) in solids is often a key to understanding or improving the properties of modern materials and creating new materials with specific properties. Many important materials—ceramics, catalysts, and rapidly solidified alloys—often can be obtained only in powdered form.

NIST researchers are developing improved methods for accurate structure refinement. A major effort is under way to relate atomic arrangement and superconducting properties in high T_c ceramic superconductors. In addition, a number of industrial scientists are collaborating with NIST staff in neutron diffraction studies of inorganic catalysts, new kinds of ionic conductors for small batteries and fuel cells, improved ceramics for microcircuit substrates and engine components, and high-performance lightweight alloys for advanced aircraft.

State-of-the-art capabilities are available at NIST for measuring and analyzing the crystal and magnetic structure of polycrystalline materials by neutron diffraction. The facilities available for diffraction experiments for both powders and single crystals include a four-circle diffractometer and a multidetector and a high-resolution powder diffractometer, as well as instruments that allow measurements in an energy-dispersive mode.

Contact: Edward Prince, 301/975-6230 or Antonio Santoro, 301/975-6232, A106 Reactor Building.

Nondestructive Evaluation for Ceramics and Composites

Nondestructive evaluation methods are used throughout the manufacturing process to monitor important properties and characteristics of materials. To assist in this process, NIST scientists have developed a new probe for examining ceramics, composites, and other nonconductive materials. The probe is basically an array of capacitive elements, each of which is essentially a parallel plate capacitor unfolded so the two electrodes lie in the same plane. A voltage is impressed across the electrodes, and the resultant current flow between them is measured. The array is placed against the surface of the object to be examined, or displaced from it by a small "lift off" or, in the case of composite materials, the array may be embedded in the composite lay up.

Early work with the capacitive array probe shows that it has good sensitivity to both surface and subsurface discontinuities, such as cracks and voids of submillimeter and even micrometer dimensions. Its capabilities in any given application depend upon the dielectric constant of the material, as well as geometric parameters, and theoretical efforts are under way to guide further development work. Recent studies indicate that the probe has important potential as a sensor for monitoring the sintering of ceramics and the curing of polymers and polymer-based composites because these processes are accompanied by changes in the dielectric constants.

Contact: H. Thomas Yolken, B344 Materials Bldg., 301/975-5727.

Polymers

Composites Processing

Fiber-reinforced composites offer, along with other advantages, versatility in processing combined with high strength and stiffness at low weight. For the current growth in the production of these materials to continue, however, more rapid and reliable processing is needed. To help meet this need, NIST researchers are developing new measurement tools to study the reactions associated with processing to understand the relationships among processing parameters, the microstructure of the fabricated materials, and their performance properties. Such scientific understanding will facilitate both advances in processing methods and implementation of on-line control and automation. The development of this understanding requires researchers to monitor the materials during the curing process to observe simultaneously chemistry, morphology development, flow, molecular network formation, build-up of residual stresses, interfacial effects, and wetting and spreading.

The NIST program currently has 10 different spectroscopic, dielèctric, thermal, and mechanical techniques available for cure monitoring, and others are under development. This diversity of tools provides a unique capability for evaluating and calibrating new measurement methods, for developing process modeling, and for analyzing model thermoset systems. For example, through cooperative projects with NIST, several industries have selected and developed monitoring methods for their particular problems.

Contact: Donald L. Hunston, A209 Polymer Bldg., 301/975-6837.

Polymer Structure

Knowledge of the relationships between mechanical properties of polymers and polymer structure is important to the design and processing of materials for optimal performance. Researchers at NIST are studying semicrystalline polymers, polymer glasses, elastomers, molecular composites, and fibers to develop improved models of mechanical behavior, characterize structure from the atomic- to fine-texture level, and elucidate relationships between mechanical performance and structure.

NIST scientists use a variety of techniques to characterize the structure of polymers in the solid state. Nuclear magnetic resonance spectroscopy is used to determine molecular orientation, molecular dynamics, and microstructure on the 1- to 10-nm scale. Microstructural information is deduced from C-13 lineshapes obtained with magic angle spinning or by proton "spin diffusion" experiments in which domain-size information is inferred from the rates at which proton magnetization diffuses in the presence of magnetization gradients. Fourier transform infrared spectroscopy helps to determine molecular architecture, orientation, and molecular processes, such as measurement of the amount of chain scission associated with mechanical deformation of polymers. Microstructural features, including spherulytic morphologies, lamellar texture, fiber structures, and crystallization habits, are elucidated through optical and electron microscopic studies of polymers. NIST scientists are examining the relationships between mechanical performance of polymers and fine structures by investigating the morphological changes that polymers undergo when they are deformed. Wide- and small-angle x-ray diffraction techniques, which include the use of position-sensitive detectors, are also employed in these investigations.

Contact: Bruno M. Fanconi, A305 Polymer Bldg., 301/975-6769.

Dental and Medical Materials

Modern dental and medical materials utilize numerous substances in an array of combinations. NIST has a comprehensive program aimed at increasing basic understanding of the causes for failure or poor performance of these materials, proposing and testing new material systems, and transferring the resultant science and technology to industry. The program has the active participation of researchers from the American Dental Association, the National Institutes of Dental Research, dental industries, and universities.

Researchers are working in a number of areas. For example, in a tribology study, scientists are examining wear and degradation of materials in various environments, and in a bioadhesion project, they are making new monomers for adhesion to tissues. In addition, improved resins are being synthesized to produce polymers that have improved properties, such as wear resistance, higher strength, resistance to oral fluids, or x-ray opacity. Researchers have developed an in-mouth shield for cancer patients undergoing radiation therapy to protect their healthy tissues from secondary radiation emitted from metallic restorations. With regard to infection control, a unique method that uses gas plasmas to sterilize dental instruments has been shown to be highly effective.

In an effort to improve the strength of dental systems, different combinations of materials are being designed and tested, including ceramic-metal, resin matrix composites, metal-cement, cement-tooth, and composite-adhesive-tooth materials. Weibull statistical analysis is employed to identify the weakest links, and finite-element analysis is applied to define stress states within systems. Scientists working in the area of precision metal casting processes have designed a unique casting monitor that can be used for rapidly solidified alloys.

John A. Tesk sterilizes clinical instruments with a new microwave-generated gas plasma method. The new technique may reduce the damage to expensive instruments caused by repeated exposure to time-consuming, traditional sterilization methods.

Contact: John A. Tesk, A143 Polymer Bldg., 301/975-6801.

Electrical Properties

NIST is conducting a number of studies on the electrical properties of polymers. The research focuses on dielectric measurements, fundamentals and applications of piezoelectric and pyroelectric polymers, measurement of space charge distribution within polymer films, and electro-optic properties of polymers.

Scientists at the Institute have developed instrumentation and data analysis techniques to measure the dielectric constant and loss of polymer films over a frequency range of 10^{-3} to 10^{5} Hz in less than 30 minutes. These developments make it possible to follow changes in the dielectric spectrum as a function of time, processing conditions, or other parameters.

The toughness, flexibility, low dielectric constant, and an acoustic impedance close to water make piezoelectric polymers ideal for many transducer applications. NIST researchers have considerable experience with the fundamental properties of polymers such as polyvinylidene fluoride and its copolymers and can work with industry to develop transducers for novel applications or to assist in measuring the properties of new piezoelectric polymers or composites.

The scientists also have designed instrumentation and data analysis techniques to measure the charge or polarization distribution across the thickness of polymer film by analyzing the transient charge response following a pulse of energy on one surface of the film. This technique has been used to detect the presence of nonuniform electric fields in the poling of piezoelectric polymers and are being used currently to investigate the role of space charge in the dielectric breakdown of polymer insulation.

Organic molecules with highly delocalized π-conjugated electrons offer great potential in the field of nonlinear optics (NLO) due to their relatively large second-order susceptibilities and their picosecond response times. Polymers with highly delocalized electrons (such as polydiacetylenes) are being designed, synthesized, and characterized for their NLO properties. Other polymers are being investigated as a medium in which NLO-active molecules can be dissolved, processed, oriented, and maintained in an oriented configuration for use in NLO devices.

Contact: George T. Davis, B320 Polymer Bldg., 301/975-6725.

Molecular Networks

Thermoset resins are used extensively in practical applications, especially polymer-based composites. However, knowledge of the basic structural entity of these resins, i.e., their molecular network structure, is very limited. NIST researchers have developed a neutron-scattering technique that can be used to determine quantitatively characteristics of the network, including the average distance between crosslinks, the rigidity of the network, the molecular weight distribution between crosslinks, and the topological heterogeneity of the network structure. Current NIST research focuses on developing correlations among chemical compositions, processing conditions, and resulting network structure for epoxy-type polymers. To establish processing-structure-property relationships, these materials are then evaluated to determine performance properties, such as fracture behavior. The neutron-scattering technique is also being used to study how the molecular network deforms when the material is placed under load. These studies help industry by providing guidelines for designing and processing polymers for optimal performance.

Contact: Wen-li Wu, A209 Polymer Bldg., 301/975-6839.

Polymer Blends

Blending polymers has become an effective method for producing high-performance engineering polymers. The fundamental data required to design a manufacturing process include the equilibrium phase diagram, the energetic interaction parameter (compatibility) between the blend components, diffusion coefficients, and the interfacial tension. At NIST small-angle neutron scattering has been used to measure the interaction parameter and phase diagram of polymer blends. NIST scientists have developed forced Rayleigh scattering and temperature-jump light-scattering techniques to measure polymer-polymer diffusion and other parameters which control phase separation kinetics and morphology.

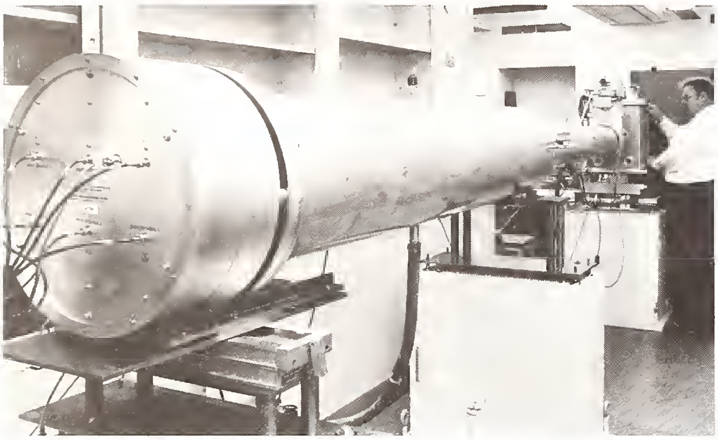
Currently, Institute researchers are testing various kinetic theories of phase separation and late-stage coarsening and are studying the control of morphology and mechanical properties of microphase-separated polymer blends. As part of this program, they are working with industry to study the homogenization and phase coarsening of rubber blends.

Contact: Charles C. Han, B210 Polymer Bldg., 301/975-6771.

Small-Angle X-Ray Scattering

Small-angle x-ray scattering (SAXS) is used to characterize structural elements of polymers, ceramics, and metals in the 1-nm to 100-nm size range. This technique has been used successfully at NIST to study phase separation, crystallite morphology, molecular dimensions, void formation, pore characteristics, and other elements. A state-of-the-art 10-meter SAXS facility has been constructed at NIST for such studies and is available for cooperative research. This SAXS facility uses a 12-kW rotating anode source, pinhole collimation, and a two-dimensional position-sensitive detector to provide high resolution and simultaneous recording of all scattering data over the entire small-angle region. In addition, a computer-assisted interactive data reduction and analysis program is available with color graphics display for the two-dimensional image. Structural and dimensional information can be extracted using available model analysis and curve-fitting procedures.

Radiation Research



The small-angle x-ray scattering facility is used by NIST polymer physicist John Barnes to obtain information on the microstructures of polymer blends to develop polymer alloy phase diagrams.

Additional equipment is available for characterizing the crystallite orientation distribution of semicrystalline polymers using pole figure techniques. Workers from Mobil Chemical Company's research and development laboratory have used the SAXS and pole figure facilities to characterize their processes for producing tear-resistant polyethylene films.

Contact: Charles C. Han, B210 Polymer Bldg., 301/975-6771.

Fluorescence Monitoring

NIST researchers are evaluating fluorescence spectroscopy, which is used to characterize the structural and dynamic properties of polymer molecules. Fluorescence quenching is employed, for example, to monitor the uniformity of mixing in polymer blends and in particle-filled polymer melts. In addition, excimer fluorescence is utilized to monitor the cure of thermoset resins, while fluorescence anisotropy is used to monitor the non-Newtonian flow of polymer solutions and melts. At NIST, the measurements are carried out with a spectrofluorimeter and a nanosecond spectrofluorimeter. In combination with optical fibers, which are used to get the exciting light into the interior of a composite part, the fluorescence techniques are attractive for process monitoring of composites.

Contact: Francis W. Wang, B320 Polymer Bldg., 301/975-6726.

Luminescence Spectral Radiometry

Luminescence techniques have broad application in virtually every scientific field, including radiation measurement, remote sensing, quantitation of biomolecules by intrinsic luminescence and immunoassay techniques, and characterization of laser, semiconductor, and superconductor materials. The accurate spectral radiometric quantitation of excitation and emission radiations is an exacting task requiring painstaking radiometric measurements and knowledge of the fundamental chemical and physical processes represented by these radiative transitions. Standard lamps, both radiance and irradiance, and silicon detector radiometry provide the accuracy base for the spectral and quantum efficiency measurements. Luminescent phenomena under investigation at NIST are photo-, chemi-, thermo-, electro-, and bioluminescences. These designations usually indicate the source of the excitation energy. The NIST researchers are conducting luminescence radiometric research in the near-ultraviolet, visible, and near-infrared spectral regions and are developing accurate standards and measurement procedures for these regions. Facilities available for this research are various laser and lamp sources, the NIST reference spectrofluorimeter, and a low-light-level spectroradiometer now under construction.

Contact: Ambler Thompson, B306 Metrology Bldg., 301/975-2333.

Thermal Radiometry

NIST researchers are investigating the use of thermal imaging cameras as a temperature-measuring tool. These devices may prove to be very useful in determining the quality of products and in investigating changes in different processes. Research projects under way involve the development of large-area blackbodies, use of Pt-Si as detector standards, and the characterization of thermal imaging cameras. Equipment available at NIST includes several heat-pipe blackbodies, a Pt-Si camera, and an infrared radiometer.

Contact: Robert Saunders, A221 Physics Bldg., 301/975-2355.

UV Radiometry

The measurement of terrestrial solar irradiance in the UV-B spectral region is being investigated by NIST researchers in order to provide improved techniques and standards in this region. Their work is of importance not only to scientists studying biological effects but to researchers investigating the aging of materials by uv light. Specific projects include the development of a reference spectral radiometer, broadband detectors, and source standards in the region. A high-accuracy spectrometer, standard detectors, and standard sources are available for this research.

Contact: Robert Saunders, A221 Physics Bldg., 301/975-2355.

Accelerator Research

The NIST accelerator research program is aimed at developing advanced particle accelerators for applications in free-electron lasers (FEL's), production of monoenergetic x rays, and dosimetry.The program focuses on designing, constructing, and commissioning the NIST racetrack microtron (RTM), which will accelerate electrons in a continuous train of pulses to energies of up to 185 MeV by recirculation through a 12-MeV, continuous-wave linac. Results of preliminary evaluations surpass the design goals of beam quality by almost a factor of two.

The unique characteristics of the RTM beam—±20-keV full-energy spread, ±10-keV energy stability, 10–μm normalized emittance, 100-percent macroscopic duty factor, and 100-kW average power—open up a range of innovative applications. The major planned application is to drive the NIST free-electron laser (FEL), an intense source of radiation with wavelengths tunable between 200 nm and 10 μm. Researchers are developing a new, continuously pulsed, 5-MeV injector with several amps of peak current to facilitate lasing. They also are studying, both theoretically and experimentally, beam breakup in the RTM. Improved techniques for measuring the properties of high-quality, relativistic electron beams will be developed. Completion of construction and performance tests at full energy are scheduled for 1990.

Contact: Mark A. Wilson, B119 Radiation Physics Bldg., 301/975-5605.

Coherent X-Ray Sources Based on High-Quality Electron Beams

Recent advances in electron accelerators have provided high-quality, continuously pulsed electron beams without using storage rings, opening up a host of possibilities for new types of intense, coherent x-ray sources. Insertion devices are presently used in highly expensive, multi-GeV storage rings for coherent production of x rays. Despite small electron-beam dimensions, the need to maintain the lifetime of the stored beam necessitates large clear apertures and precludes interception of the beam. However, these restrictions do not apply if the beam is not reused. In this case, much smaller structures, even interceptive ones, can be used to produce coherent x rays at beam energies well below 1 GeV.

The racetrack microtron (RTM) under construction at NIST provides a unique opportunity to develop such innovative sources.The expected beam size and divergence at 185 MeV are ±160 μm and ±160 μrad. X-ray production mechanisms accessible with a beam of this quality include radiation from miniature undulators, transition radiation, channeling radiation, and parametric x-ray generation. Although the full range of beam energies will not be available until 1990, researchers are using the 17-MeV beam now available for an experiment with an undulator with a submillimeter magnetic period.

Contact: Philip Debenham, B119 Radiation Physics Bldg., 301/975-5602.

Free-Electron Laser

A free-electron laser (FEL) facility under construction at NIST will be operated as a user facility for research in physics, chemistry, biophysics, material sciences, and medical sciences. The electron source for the FEL is the NIST racetrack microtron (RTM). Because the RTM will provide a continuous train of pulses and will have a wide energy range, the FEL will have unique characteristics. It will be tunable over the range of 200 nm to 10 μm with average power of 10 W to 200 W, and the temporal structure will be a continuous train of 3-ps pulses at 66 MHz.

Collaborative opportunities exist in both the development and the use of the FEL. The FEL will have sufficient small-signal power gain to lase in the ultraviolet, but the lower wavelength limit of 200 nm to 300 nm will depend strongly on mirror performance. NIST researchers will be investigating the development of low-loss, high-power mirrors; laser diagnostics and stabilization; optimization of harmonic radiation (for wavelengths as low as 30 nm); Q-switched mode of operation; and optical pulse compression. They are especially interested in dynamical studies which exploit the temporal structure of the FEL.

Contact: Ronald G. Johnson, B110 Radiation Physics Bldg., 301/975-5568.

Spectral Radiometry

Research and development programs at NIST span a broad spectrum of activities associated with the measurement of optical radiation, including spectral radiance measurements and new techniques for spectrophotometric measurement of dense optical media. These activities cover the ultraviolet spectral region from 200 nm to the far infrared region and include the development of appropriate detector methodology to perform the measurements and relate them to the U.S. radiometric measurement base. Specific research and development projects involve low background infrared calibrations in a cryogenic environment, solid-state photodiode metrology, applications of detector metrology to all areas of radiometry, development of an absolute cryogenic radiometer, and application of laser heterodyne technology to optical density measurement.

Several well-equipped laboratories for optical measurements in the uv and visible spectral region are available for use, and new facilities are being developed which will enable scientists to research both detector development and optical properties of materials in the infrared spectral region.

Contact: Al Parr, A221 Physics Bldg., 301/975-3739.

Radiation Processing

To enhance quality-control methods used in industrial radiation processing of foods and in the production and use of medical devices, electronic components, and polymers, NIST researchers are developing standardization and measurement assurance methods related to industrial high-dose applications of ionizing radiation. As part of this program, Institute scientists are investigating radiation chemical mechanisms and kinetic studies applied to chemical dosimetry systems in the condensed phase, including liquids, gels, thin films, and solid-state detectors.

They also plan to examine sensor materials such as doped plastics, solid-state matrices, fiber optics, organic dye solutions, semiconductors, scintillators, biopolymers, amino acids, metalloporphyrins, and organic or inorganic aqueous solutions and gels. A number of analytical methods will be used, including transmission and fluorescence spectrophotometry, electron spin resonance spectrometry, and chemiluminescence spectrophotometry as well as fiber optics analysis, microcalorimetry, pulse radiolysis, laser-induced photochemistry, and conductivity measurements. Various

On the automated spectral comparator facility, physicists Jeanne Houston and Chris Cromer align the silicon photodiode light traps that are used in photodetector research and calibration.

x-ray and gamma-ray sources and electron accelerators with energies in the 0.1- to 10-MeV range are used in this work. Conventional ultraviolet, visible, and infrared spectrophotometers and spectrofluorimeters, high-intensity gamma-ray sources, pulsed and continuous beam electron accelerators, and organic-chemical analytical equipment are also available.

Contact: William L. McLaughlin, C209 Radiation Physics Bldg., 301/975-5559.

Autoxidation/ Antioxidants

The kinetic and mechanistic aspects of autoxidation in foods, organic materials, and biochemical systems; the design of appropriate antioxidants to prevent the deleterious effects of oxygen; and the extension of the lifetime of chemical and biochemical systems are important to many food, drug, and medical industries. NIST researchers are investigating the free-radical chemistry of organic molecules and biochemicals susceptible to autoxidation and free-radical mechanisms and reaction rates of oxidants, particularly key components of foodstuffs and other life-supporting substances. In addition, the effects of oxygen pressure, temperature, additives, and concentrations on the optimization of these parameters and the development of products less sensitive to oxidation are being studied.

NIST researchers are seeking industrial collaboration in the analysis of short- and long-term intermediate species in pulse-irradiated oxygenated organic and aqueous solutions; derivation of kinetic data and unraveling of auto- and radiation-stimulated oxidation processes; and design of new antioxidants to protect against food spoilage, carcinogenesis, atherosclerosis, and nitrosamine formation in foods. Kinetic and analytical chemical technologies, such as GC/MS, HPLC, spectroscopy, chromatography, electrophoresis, and ESR spectroscopy; high-intensity gamma-ray sources, and pulsed- and continuous-beam electron accelerators; and various organic-chemical analytical equipment are also available.

Contact: Michael G. Simic, C214 Radiation Physics Bldg., 301/975-5558.

Industrial Radiologic Imaging

The use of penetrating radiation for imaging is one of the most powerful investigative techniques available to industry for maintaining or improving the quality of products. Designers, aware of this, are creating components that facilitate such nondestructive testing. Research is under way at NIST to allow better quantification of radiographic images. Particularly relevant to image evaluation are computer-based systems that permit pseudo three-dimensional images and the implementation of image processing on these or traditional images in real time or near real time.

The NIST research focuses on image processing for improved imaging of low contrast for noisy images; adaption of tomographic equipment to industrial needs and measurement of the performance characteristics of such systems; and development of reliable techniques for image storage and retrieval. Available equipment includes x-ray sources, low-energy electron accelerators, gamma-ray sources, and state-of-the-art radiologic imaging devices.

Contact: Charles E. Dick, C215 Radiation Physics Bldg., 301/975-5580.

Neutron Fluence Measurement and Neutron Physics

NIST researchers are studying industrial applications of neutron fluence and dose determination in the neutron energy region from thermal to 20 MeV. They are developing effective methods to transfer personnel protection technology to the private sector. This research provides a basis for standardizing personnel protection control procedures in nuclear reactor and in high-energy accelerator operations. Specific research involves the measurement of reference standard neutron reaction cross sections; characterization of reference fission deposits; development of neutron detectors with fast timing; and calibrations using standard neutron and gamma-ray fields. Equipment available includes a 100-kV ion generator-based 2.5-MeV neutron source, a 3-MV pulsed positive-ion accelerator, and a 20-MW nuclear reactor.

Contact: Oren A. Wasson, B111 Radiation Physics Bldg., 301/975-5567.

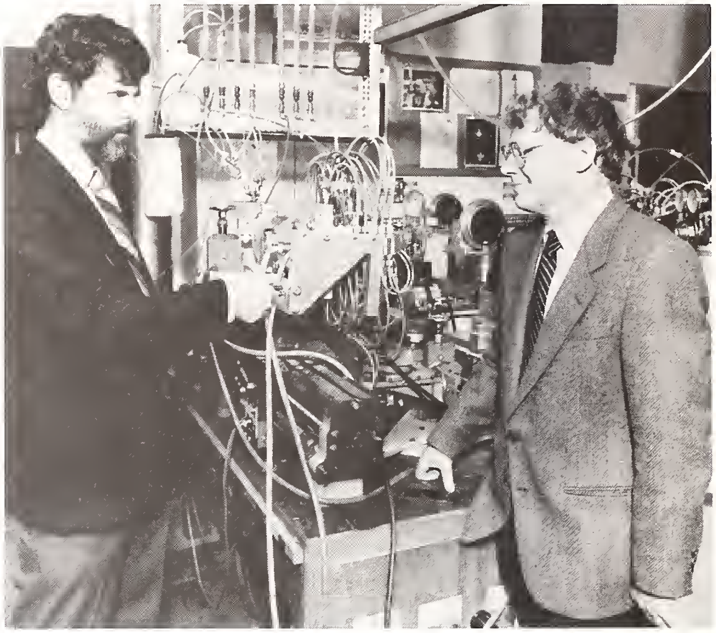
Standard Reference Data

Computerization of Standard Reference Data

Using computers to provide timely and inexpensive access to reliable chemical, physical, and materials data contributes greatly to increased productivity and lower manufacturing costs of industrial operations. The NIST Standard Reference Data program works closely with industry to develop the tools and standards necessary for computerizing industrial technical data—the numbers, graphics, tables, and text that convey research results.

The National Standard Reference Data System, coordinated by NIST, is a focal point in the United States for the evaluation of chemical, physical, and materials properties data. The NIST Standard Reference Data program has made a commitment to provide national leadership in the computerization of evaluated data, including database design, database and data exchange standards, and data dissemination. NIST research combines expertise in the physical sciences with specialized knowledge in computer science. Areas of activity include preparation of databases of evaluated data and predictive software for use on personal computers, conversion and combination of published data compilations into searchable databases, standardization of formats for scientific and engineering information, development of expert systems, and establishment of distributed systems linking scientific databases. The computer and telecommunications capabilities at NIST offer challenging alternatives for the handling of these projects, with state-of-the-art mainframes, minis and micros, database management systems, graphics, and applications software available.

Contact: Malcolm W. Chase, A323 Physics Bldg., 301/975-2200.



Jeffrey Fuhr (left), a physicist in the NIST Atomic Transition Probabilities Data Center, demonstrates the wall-stabilized arc to W.L. Wiese, head of the data center. The arc is used to measure atomic transition probabilities for use in plasma modeling and analysis, including fusion research as well as laser physics and astrophysics.

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