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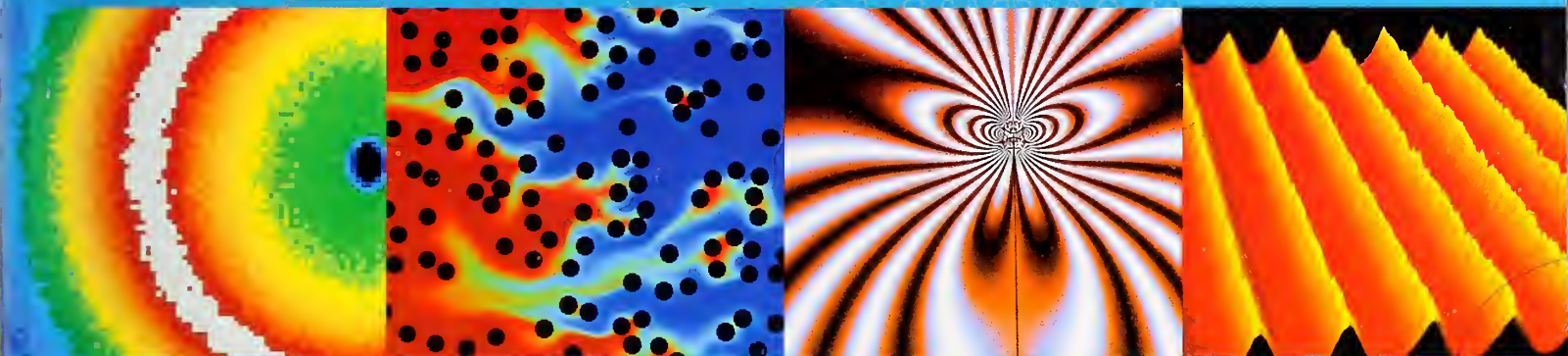


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NIST
PUBLICATIONS

Guide to NIST

National Institute of Standards and Technology



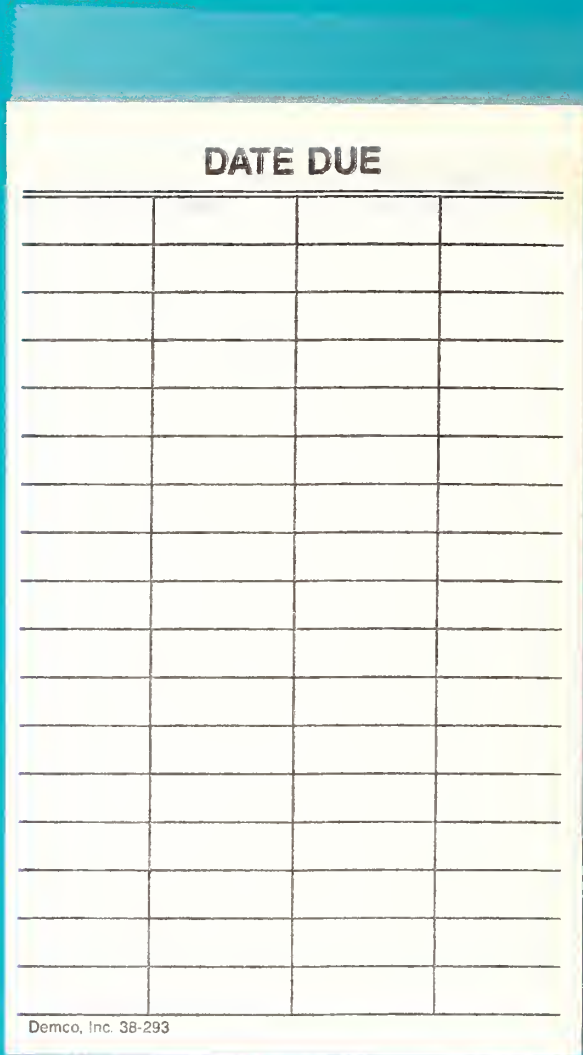
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U.S. DEPARTMENT OF COMMERCE
Technology Administration

On the cover:

NIST scientists and engineers increasingly use computerized graphics programs to visualize scientific data. Shown on the cover from right to left are computer-generated graphics of:

- nanometer-scale lines of chromium deposited on silicon;
- a stress field around a tensile crack tip;
- simulated flow patterns of two fluids mixing within a porous media;
- a neutron diffraction pattern produced by spherical "bubbles" of a surfactant molecules;
- a microscopic "waffle" pattern produced by precisely positioning two different organic compounds to test the feasibility of a new technology for making biosensors;
- benzene molecular rings attached to rhodium, an important element in automobile catalytic converters;
- an atomic force micrograph of a microelectronic transistor; and
- a fractal pattern used to check the quality of a computer code.



FOREWORD

Welcome to the new NIST!

Since 1988 and passage of the Omnibus Trade and Competitiveness Act, the National Institute of Standards and Technology (NIST) has been expanding its outreach efforts to industry. These have included establishment of three relatively new extramural programs—the Advanced Technology Program, providing direct grants to industry for high-risk technology development; the Manufacturing Extension Partnership, a grassroots technology extension service; and the Malcolm Baldrige National Quality Award. The Institute also has substantially increased the number of cooperative programs between industry scientists and engineers and NIST laboratory researchers.

Now we're gearing up for even bigger changes. The Clinton Administration has made improved development, commercialization, and adoption of new technology by U.S. industry a central element of its plan for U.S. economic growth. NIST has a vital role to play in helping turn these plans into reality.

Over the next few years, NIST plans to use requested funding increases to transform itself from primarily a measurement laboratory program with three relatively small extramural programs to a full-service technology development, funding, extension, and quality improvement partner for U.S. industry. To help get that job done, we have begun a major construction and renovation program to bring the Institute's laboratory facilities up to the needs of the 21st century and beyond.

You'll see the beginnings of this transformation within this guide. We've included expanded descriptions of NIST extramural programs, more comprehensive coverage of NIST laboratory projects and facilities, and more detailed guidance on the many different ways—both formal and informal—that industrial and other organizations can work cooperatively with NIST. Also for the first time, the guide includes email addresses for most NIST research contacts listed and information on electronic bulletin boards open to use by the public.

We hope you'll use this guide to find the NIST programs, research projects, products, or services that best match your organization's needs. Then make the most of your federal tax dollars. Work with us to make *all* aspects of U.S. technology—from development to commercialization to adoption by manufacturers—the envy of the world.



Arati Prabhakar, Director
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NIST AT A GLANCE

The National Institute of Standards and Technology was established by Congress "to assist industry in the development of technology ... needed to improve product quality, to modernize manufacturing processes, to ensure product reliability ... and to facilitate rapid commercialization ... of products based on new scientific discoveries."

An agency of the U.S. Department of Commerce's Technology Administration, NIST's primary mission is to promote U.S. economic growth by working with industry to develop and apply technology, measurements, and standards. It carries out this mission through a portfolio of four major programs:

- a rigorously competitive Advanced Technology Program providing cost-shared grants to industry for development of high-risk technologies with significant commercial potential;
- a grassroots Manufacturing Extension Partnership helping small and medium-sized companies adopt new technologies;
- a strong laboratory effort planned and implemented in cooperation with industry and focused on measurements, standards, evaluated data, and test methods; and
- a highly visible quality outreach program associated with the Malcolm Baldrige National Quality Award.

BUDGET

\$609 million

(FY 94 estimated operating resources from all sources)

STAFF

About 3,200 scientists, engineers, technicians, and support personnel, plus some 1,200 visiting researchers each year

SITES

Gaithersburg, Md. (headquarters—234-hectare campus) and Boulder, Colo. (84-hectare campus)

MAIN RESEARCH AREAS IN NIST LABORATORIES

Electronics and electrical engineering
Manufacturing engineering
Chemical science and technology
Physics
Materials science and engineering
Building and fire research
Computer systems
Computing and applied mathematics

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HOW TO USE THIS GUIDE

Finding who or what you need within a federal agency can be a daunting task. This guide is designed to make finding out about programs and contacts at the National Institute of Standards and Technology a little easier.

NIST researchers actively seek out industrial and other collaborators to work on well-defined, cooperative research projects of mutual interest. In addition, NIST researchers collaborate informally with industrial and academic researchers to solve shorter-term technical problems. For an overview of the many different ways NIST may be able to help your organization, see "What NIST Has to Offer" on page 5.

The pages that follow describe more than 250 NIST research projects, grants and industry outreach programs, services, and facilities, followed by contact names, phone numbers, and mail and electronic mail (Internet) addresses for further information. Unless otherwise noted, all addresses listed are at NIST, Gaithersburg, Md. 20899-0001.

This guide is divided into chapters covering each of NIST's major operating units. In addition, each chapter on laboratory research programs includes subheadings for NIST organizational divisions.

A detailed subject index is included on pages 113 to 116. Due to the interdisciplinary nature of NIST's work, many topic areas appear in more than one chapter. For example, research involving polymers is described in different chapters: polymer processing and structure investigations within the Materials Science and Engineering Laboratory and polymer combustion studies within the Building and Fire Research Laboratory.

This guide attempts to include all major NIST program areas. However, no single report can be completely comprehensive. Institute programs change constantly as new research results and technologies become available. If you don't find a topic area that specifically matches your needs, contact the division office for the research area closest to your field of interest. Phone numbers, fax numbers, and electronic mail addresses for division contacts are provided within each chapter.

If you review this guide and you're still not sure which office to call, the NIST Publications and Program Inquiries Unit can probably help you. Contact: Publications and Program Inquiries Unit, (301) 975-3058.

WHAT NIST HAS TO OFFER

Advanced Technology Program

This program provides multiyear funding for high-risk, high-payoff, civilian technology development by individual companies or industry-led joint ventures. See description on page 10.

Manufacturing Extension Partnership

This program provides funding for regionally based extension centers that help small and medium-sized businesses adopt modern technologies. MEP also provides matching grants for state-based technology extension efforts and develops linkages between federal, state, local, and other technology extension efforts. See description on page 13.

Collaborative Research

NIST actively seeks industrial, academic, and non-profit research partners to work collaboratively on projects of mutual benefit. A wide variety of mechanisms are available for carrying out these research collaborations. Special efforts are made to tailor collaborations to specific needs.

Most research collaborations start with one-to-one interactions between industry or other researchers and NIST scientists and engineers. To locate NIST researchers in specific fields of interest, see the project listings on pages 22 to 112. For further information about the process for implementing specific types of research agreements, contact the Technology Development and Small Business Program, (301) 975-3084.

The most common types of arrangements include:

Cooperative Research and Development Agreements (CRADAs)

Typically cover joint research efforts in which both NIST and the cooperating company provide staff, equipment, facilities, and/or funds, in any number of possible combinations, for a project of mutual interest. NIST is currently working with more than 200 research partners on nearly 250 CRADAs in 160 different areas of research. Ninety-five percent of NIST's CRADA partners are U.S. businesses, with about equal numbers from large and small companies.

When companies conduct joint research with the Institute under a CRADA, NIST can protect confidential or proprietary information exchanged during the project, keep research results confidential, and provide exclusive rights for intellectual property developed during the course of the project. Each CRADA is negotiated separately between NIST and prospective partners. Most CRADAs take 6 to 8 weeks to implement. Copies of a model NIST CRADA agreement are available from the NIST Technology Development and Small Business Program, (301) 975-3084.

Guest Researcher Agreements

Typically used when an industrial or other researcher wishes to join an ongoing NIST research effort. The researcher gains access to NIST research staff and facilities and, in return, results from the collaboration are made publicly available. Such agreements cannot protect proprietary information and do not allow cooperating companies to receive exclusive intellectual property rights. Once a NIST research group agrees to host a guest researcher, implementation of such agreements takes only about 1 week. Each year NIST hosts about 1,200 guest scientists and engineers at its Gaithersburg, Md.,

and Boulder, Colo., laboratories. Contact: domestic guest researchers, (301) 975-3084; international guest researchers, (301) 975-4119.

Research and Development Contracts

Used when external organizations contract with NIST researchers to receive specific technical services or results uniquely available at the Institute. The cooperating organization funds the NIST effort on a cost-reimbursable basis. Individual contracts may provide protection of proprietary information under certain circumstances.

Research results are made publicly available, and any intellectual property rights revert to NIST.

Preparation of contracts for such agreements typically takes about 4 weeks.

Informal Collaborations

Informal one-to-one collaborations between Institute and other researchers. Such collaborations often involve exchange of research results and/or samples between NIST and other researchers, rather than transfers of personnel or research funds.

Research Consortia

On research topics of broad interest to a number of different research partners, NIST may sponsor research consortia. Research consortia are usually structured through NIST CRADAs and involve groups of companies and other organizations that exchange data, ideas, researchers, and/or materials among themselves and with NIST to meet agreed-upon research goals. Most consortia require payment of membership fees in exchange for advance knowledge of research results produced by the consortia effort. Currently active NIST-centered consortia open to participation by U.S.-based companies include the following:

Fluid Flow Measurements

Supports research in fluid flow measurements to help industry understand, evaluate, and assess flowmeter performance under non-ideal conditions. Contact: George Mattingly, (301) 975-5939.

Production of Powdered Metals

Applies advanced intelligent processing techniques to improve the quality and productivity of advanced metal powder processing used in making jet engines, high-performance magnets, and other high-technology applications. Contact: Neville Pugh, (301) 975-5960.

North American Integrated Services Digital Network Users' Forum

Promotes the implementation and use of ISDN standards and the development of interoperable systems for the simultaneous transmission of voice, data, and images over high-speed digital networks. Contact: Daniel Stokesberry, (301) 975-3605.

Microwave Monolithic Integrated Circuits

Develops metrology for design and manufacture of microwave monolithic-integrated circuits, especially measurement methods and standards to reduce testing costs. Contact: Gerome Reeve, (303) 497-3557.

Consortium on Automated Analytical Laboratory Systems (CAALS)

Fosters advancement of automated analytical systems to improve laboratory efficiency and data quality and to promote transferability of analytical methods so U.S. companies can compete internationally. Contact: Gary Kramer, (301) 975-4132.

Investigation of S₂F₁₀ Production

Investigates the production of S₂F₁₀ in compressed SF₆ insulated electrical power equipment and provides utilities and other interested parties with information on safe and prudent operation of such equipment. Contact: Joseph Greenberg, (301) 975-2439.

Ceramic Machining Consortium

Develops cost-effective production processes for grinding components made from advanced, structural ceramics, such as silicon nitride and silicon carbide. Contact: Said Jahanmir, (301) 975-3671.

SUCCESS STORIES

For those who need convincing that federal government programs can produce substantial private-sector benefits, consider the following examples from each of NIST's four major program areas.

Advanced Technology Program

- According to a recent survey of initial ATP grant recipients, funding provided by the program enabled a number of companies to pursue research they otherwise would not have been able to do. Typical comments included, "We would not have been able to do this kind of work at all [without the ATP]." ... "and [the ATP] enabled us to keep a highly specialized and trained team together over a long period of time to pursue a technology."
 - Sixty-nine percent of respondents to the survey reported a significant shortening of the R&D cycle over the first year of their funding.
 - All of the single-company award recipients and most of the joint venture participants cited the credibility the company and the technology gained by receiving an ATP award. Smaller companies emphasized that this assisted them in attracting external funding; larger companies found that they received increased support from internal management for the project.
 - Over half of the ATP awards in the first three competitions are led by small businesses. In addition, many more small businesses are subcontractors to the participating organizations. These companies have indicated that ATP funding is critical to their pursuit of the proposed technologies.
- ### Manufacturing Extension Partnership
- Results of a pilot evaluation system with a small number of companies involved in modernization projects with MTC assistance showed that within 2 years these firms, on average, increased employ-

ment by 15 percent, productivity by 7 percent per employee, and sales by 34 percent.

- From January 1989 through June 1991, client companies estimated that the MTCs helped them save a total of \$139 million—or eight times more than the total federal investment of \$18 million during that time.
- Many individual companies have used MTC advice and services to successfully adopt new technologies and increase profits:

Newburgh Molded Products used new processing technology to increase its production volume by two-thirds and reduce waste.

Kintz Plastics bought new automation equipment to cut its production time for making steel and aluminum molds from 8 weeks to 8 days.

Brimfield Precision saved over \$200,000 on the purchase of a new computer-aided design and manufacturing system after trying out several systems at an MTC and choosing a less expensive system than the one they previously thought was necessary.

A South Carolina forklift manufacturer shaved 2 years off the planning and evaluation stage of its transition to a robotic painting and welding system.

A New York-based vitamin manufacturer sped up production and cut its time for filling back orders by better than 50 percent.

NIST Laboratory Research

- U.S. semiconductor manufacturers attributed 4 percent of their productivity growth over a 5-year period and annual savings of up to \$500 million to NIST research.
- A NIST technique for measuring the performance of microwave antennas revolutionized quality control for 11 U.S.

manufacturers. One company estimated that the new technology saved their company \$35 million in testing costs.

- NIST researchers working with an Institute-sponsored consortia developed a computer model that helped one member company, Crucible Compaction Metals, increase the percentage of usable metal powder made at its production facility by over 40 percent.

- More than 50 companies have sent researchers to work with Institute researchers at NIST's Automated Manufacturing Research Facility and more than 20 products and subsystems developed at the AMRF have been commercialized.

- The CEM Corp. credits much of its success in developing new markets for laboratory microwave units to an 8-year successful collaboration with NIST researchers.

- A NIST-developed method for measuring light reflection produces savings of about \$500 million per year for large segments of the U.S. medical, agricultural, food processing, paper, plastics, and building materials industries.

- Laboratory inaccuracies in measurements of cholesterol in blood samples have decreased by half since introduction of NIST Standard Reference Materials for those measurements.

- Axis Instruments is marketing a precision instrument based on a NIST design that makes absolute measurements of the Earth's gravitational field 5 to 10 times more accurately than previously possible.

- Intel's Supercomputer Systems Division has incorporated a NIST-developed performance measurement chip into its Paragon XP/S supercomputers.

- NIST-developed smoke detector performance requirements, installation guidelines, and subsequent studies have helped U.S. manufacturers acquire a 50-percent share of the world market.

- A NIST project with SEMATECH established calibration procedures that markedly improved the accuracy of commercial near-ultraviolet radiometers used in semiconductor photolithography.

- Optical ETC is making microheaters for infrared flat-panel displays using a NIST-developed technology.

- Teradyne Inc. worked with NIST to produce a software package that reduces the number of testing points required for a 13-bit analog-to-digital converter from more than 8,000 to 64.

Malcolm Baldrige National Quality Award

- A 1991 General Accounting Office report calls the Malcolm Baldrige National Quality Award criteria "the most widely used accepted formal definition of what constitutes a total quality management company." "In nearly all cases," the report states, "companies that used total quality management practices achieved better employee relations, higher productivity, greater customer satisfaction, increased market share, and improved profitability."

- In a letter to the U.S. Secretary of Commerce, Solectron Corp., a 1991 award winner, noted, "Since we applied for the Malcolm Baldrige award in 1989, Solectron's sales have increased 316 percent and profit has increased 338 percent in 3 years.... We attribute our financial performance a great deal to the improvement we made through the rigorous examination and feedback from the Baldrige application process."

- Another Baldrige winner, Globe Metallurgical Inc. estimates that its investments in quality have produced a 40-1 return.

- Motorola Inc. considers the criteria for the Baldrige Award so important that it has given its suppliers until 1994 to follow the award criteria or risk losing Motorola as a customer for their products.

Processing of Polymer Blends

Uses NIST measurement tools to develop the data and processing models industry needs to produce new and more economical polymer blends and alloys. Contact: Thomas Yolken, (301) 975-5727.

Advanced Biosensors

Works to hasten development of biosensors that could dramatically change the way laboratories analyze medical, environmental, and industrial samples. Contact: Howard Weetall, (301) 975-2628.

Casting of Aerospace Alloys

Supports efforts to improve understanding and, ultimately, control of the net-shape casting process so that the alloys in finished parts attain the desired structural and performance properties. Contact: Robert Schaefer, (301) 975-5727.

Polymers Processing Measurements

Improves processing techniques used in the manufacture of advanced polymer materials, including on-line measurement technology to monitor polymer processing. Contact: Thomas Yolken, (301) 975-5727.

Intelligent Processing of Ceramic Powders and Slips

Focuses on developing measurement methods for on-line process control and process modeling for advanced ceramic powders and slips. Contact: Subhas Malghan, (301) 975-6101.

Technical Assistance

NIST provides two different forms of assistance to U.S. companies and others seeking advice in specific technical areas.

Direct Assistance from NIST Researchers

Informal technical advice provided without charge by NIST researchers. Often NIST experts can help a company solve a technical problem through one or several phone conversations or a brief visit to the Institute's Gaithersburg, Md., or Boulder, Colo., laboratories. (Institute researchers are not permitted to consult on their own behalf or to receive personal payments for technical advice in areas within NIST's mission.)

See project descriptions on pages 22 to 112 to locate a NIST expert in a specific research field or call the Publications and Program Inquiries Unit for assistance, (301) 975-3058.

Assistance from a NIST Manufacturing Technology or Outreach Center

Formal or informal technical services and advice provided by NIST's regionally based Manufacturing Technology Centers (MTCs) and affiliated organizations. Operated through NIST's Manufacturing Extension Partnership, NIST MTCs and outreach centers give "hands on" technical assistance to small and medium-sized manufacturers and provide referral services to locate additional technical resources. Informal assistance is free; more extensive service may require payment of modest fees. See page 13.

Technology Services and Products

NIST provides many different technology services and products to help U.S. industry improve the quality, reduce the cost, and increase the competitiveness of its products. Summaries of the NIST programs providing these services and products appear on pages 16 to 21. Examples include Standard Reference Materials, Standard Reference Data, calibration and laboratory accreditation services, and evaluations of energy-related inventions.

Use of NIST Facilities

The Institute operates more than 40 different research facilities that are accessible to outside researchers for collaborative or independent research. Some are one-of-a-kind facilities not available elsewhere in the United States.

Access to NIST facilities generally occurs through one of four mechanisms: under the provisions of a NIST CRADA or consortium agreement; through a guest researcher

agreement; through contract R&D in which Institute staff members conduct specific experiments or tests at NIST and are reimbursed for their time and supplies; and, for a limited number of facilities, through scheduled appointments for qualified researchers wishing to conduct proprietary research.

Scheduling and priorities for NIST facilities use are determined by the relevant director for each NIST disciplinary laboratory, in some cases assisted by designated user group committees.

An index of NIST facilities appears on page 113. For detailed information on capabilities and availability of individual facilities, call the contact person listed for that facility. For general information on typical facility use agreements, contact the Technology Development and Small Business Program, (301) 975-3084.

Technology Licenses

NIST seeks patents for its product and process inventions with commercial potential. Individuals or companies may obtain a license to use, make, or sell NIST patented inventions, on either an exclusive or nonexclusive basis. Normally licenses are granted only in cases where the licensee agrees that resulting products will be manufactured substantially in the United States.

The goal of NIST's licensing process is to encourage commercial use of NIST-developed technologies.

For a current listing of the more than 120 NIST inventions available for licensing, contact the NIST Technology Development and Small Business Program, (301) 975-3084.

Quality Improvement Assistance

The NIST Office of Quality Programs manages the Malcolm Baldrige National Quality Award and supplies interested businesses with guidelines and criteria important for establishing successful quality management programs. See description on page 15.

Research Grants

Grants supporting research at industry, academic, and other institutions are available on a competitive basis through several different Institute offices. For general information on NIST grants programs, contact (301) 975-6328.

Small Business Innovation Research Program

Funds proposals by small businesses for research and development efforts that fall within areas recommended yearly by the U.S. Department of Commerce. See description on page 21.

Precision Measurement Grants

Supports researchers in U.S. colleges and universities for experimental and theoretical studies of fundamental physical phenomena. Contact: (301) 975-5607.

Fire Research Grants

Sponsors research by academic institutions, non-federal government agencies, and independent and industrial laboratories that supports NIST's fire research laboratory programs. Contact: (301) 975-6854.

Standard Reference Data Grants

Supports research at academic, industrial, and other non-federal institutions to critically evaluate data in chemistry, physics, and materials properties. Contact: (301) 975-2200.

Materials Science and Engineering Grants

Supports work in polymers, ceramics, metallurgy, and neutron scattering and spectroscopy research at academic, industrial, and other non-federal institutions. Contact: (301) 975-5658.

Publications

NIST issues more than 350 publications each year, such as reports on research results and standards, catalogs of products and services, and technical handbooks. NIST staff also author about 1,300 technical journal papers. The Publications and Program Inquiries Unit provides assistance to the public in locating current and past Institute publications, (301) 975-3058.

The Institute also publishes serial publications, including:

Journal of Research of the National Institute of Standards and Technology

Issued bimonthly. Subscription price: domestic—\$27 per year, foreign—\$33.75 per year. Reports NIST research and development results in physics, chemistry, engineering, mathematics, and computer science, with major emphasis on measurement methodology and basic technology underlying standardization. Contact: (202) 783-3238.

Technology at a Glance

Issued quarterly. Free subscription. A four-page, lay language newsletter providing brief updates on NIST research, grants, and other program activities. Includes a NIST contact name for each topic covered. Contact: Gail Porter, (301) 975-3392.

Electronic Information Retrieval Systems

NIST operates a number of different electronic information retrieval systems and bulletin boards designed to encourage dissemination of information on a variety of topics. For assistance locating information on NIST programs *not* provided by these bulletin boards, contact the NIST Publications and Program Inquiries Unit, (301) 975-3058, email: inquiries@enh.nist.gov.

NIST Gopher Information Service

Part of the Gopher system on the Internet. Allows users to search through databases using menus to locate materials of interest. The range of topics included in the Gopher service continually expands. As of late 1993, menu items on the following topics were included: text from this brochure, *Guide to NIST*; Guide to Available Mathematical Software (GAMS); computer security; open systems engineering; Standard Reference Data Program; and NIST phone book and email directory.

To access the NIST Gopher server via Internet:

- from remote log in, type "telnet gopher.nist.gov." At the log in prompt, type "gopher."
- from a gopher client, use the gopher server as "gopherserver.nist.gov" with port 70.

STEP On-Line Information Service (SOLIS)

Provides access to draft standards, supporting documents, and software that contribute to the Standard for Exchange of Product Model Data (STEP).

- Internet access: send an email message to "nptserver@cme.nist.gov". In the body of the message, type "help".
- Anonymous ftp: [ftp ftp.cme.nist.gov](ftp:ftp.cme.nist.gov), name: anonymous, password: <userid>, files to be downloaded are located at "cd pub/step".

Weights and Measures Bulletin Board

Provides information on certificates of conformance, software programs, publication lists, and contacts.

- Modem access: (301) 869-1665 for 1200 baud (data bits: 8/no parity, stop bits: 1)

Computer Security Bulletin Board

Provides information on computer viruses, software reviews, computer security alerts, and publications.

- Modem access: (301) 948-5717 for 300, 1200, or 2400 baud; (301) 948-5140 for 9600 baud (data bits: 8/no parity or 7/even parity, stop bits: 1)

- Internet access: [telnet cs-bbs.ncsl.nist.gov](telnet:cs-bbs.ncsl.nist.gov) or [telnet 129.6.54.30](telnet:129.6.54.30). To download files, Internet users need to use ftp as follows: type "ftp csrc.nist.gov" or "ftp 129.6.54.11." Log in to account "anonymous" using your Internet address as the password. Computer security bulletin board files are located in directory bbs. Or, telnet to the NIST Gopher server. Type "telnet gopher.nist.gov."

Data Management Activities and Applications Bulletin Board

Provides information on activities of the NIST Information Systems Engineering Division, which develops standards and provides technical assistance to government and industry in data administration, data management, technology, computer graphics, and software standards validation.

- Modem access: (301) 948-2048 for 2400 baud, (301) 948-2059 for 300 or 1200 baud (data bits: 8/no parity or 7/even parity, stop bits: 1)

Fire Research Computer Bulletin Board

Features fire computer programs developed by the Building and Fire Research Laboratory at NIST.

- Modem access: (301) 990-2272 for 300, 1200, 2400, or 9600 baud (data bits: 8/no parity, stop bits: 1)

North American Integrated Services Digital Network (ISDN) Users' Forum Bulletin Board

Provides minutes from the North American ISDN Users' Forum, meeting dates and agendas, user applications, analyses, and profiles. When prompted for password, type "dialin."

- Modem access: (301) 869-7281 for 1200 or 2400 baud; (data bits: 8/no parity, stop bits: 1)
- Internet access: [telnet 129.6.53.11](telnet:129.6.53.11)

ADVANCED TECHNOLOGY PROGRAM

Overview

Begun in 1990, the NIST Advanced Technology Program (ATP) promotes the economic growth and competitiveness of U.S. business and industry by accelerating the development and commercialization of promising, high-risk technologies with substantial potential for enhancing U.S. economic growth.

The program provides technology development funding through cooperative research agreements to single businesses or industry-led joint ventures. Applicants must share the costs of ATP projects.

Awards to individual companies are limited to \$2 million over 3 years and can be used only for direct R&D costs. Awards to joint ventures can be for up to 5 years; joint ventures must provide more than 50 percent of the resources for the project. The ATP does not fund product development. It will support development of laboratory prototypes and proof of technical feasibility but not commercial prototypes or proof of commercial feasibility.

The ATP relies on the substantial involvement of industry to define and implement R&D programs that are expected to have a substantial long-term economic impact. The ATP selects specific projects through a rigorous competitive process that includes evaluation of both the technical and business merits of a project. The program has received broad public support from groups such as the Advanced Technology Coalition, which represents over 30 major trade associations, professional societies, and high-technology companies.

Essential Features

In designing the ATP, NIST looked to existing large-scale R&D funding programs with a reputation for results, particularly those of the National Institutes of Health and the Defense Department's Advanced Research

Projects Agency. But the unique mission of the ATP—support for civilian technologies in the nation's competitive interest—required some special features, which have become the hallmarks of the ATP and major factors in its success.

Projects are selected on the basis of both technical and business merit through a fair and rigorous competition.

After each proposal is screened for basic compliance with the ATP's requirements, it is reviewed thoroughly by scientists and engineers expert in the subject area—a common procedure for competitive grant programs. But ATP proposals that score well in this technical review go on to a *further* evaluation of potential economic impact, evidence of significant commitment to the project on the part of the proposer, and other business-related factors affecting the likelihood that successful results will be commercialized.

The scientific and technical reviewers are primarily federal and academic experts to avoid conflict-of-interest problems and protect proprietary information. Business reviews are conducted primarily by business experts from the private sector who agree to avoid conflicts of interest and abide by non-disclosure requirements. Semifinalists receive in-depth oral reviews. Proposals are ranked according to published selection criteria, and funding is awarded primarily on the basis of the ranking. This merit-based selection process has been fully tested and refined and is essential to the effectiveness of the ATP.

The ATP provides direct support to for-profit companies of all sizes.

Commercial organizations know best how to commercialize a promising new technology. With this in mind, the ATP emphasizes direct funding to for-profit companies. Small, medium, and large companies, and

joint ventures led by two or more companies, are eligible for direct funding. Successful ATP project sponsors range in size from start-up companies with a handful of employees to major industrial firms with international scope. Universities, federal laboratories, and non-profit institutions participate in many ATP projects, but as sub-contractors or as members of joint ventures (although non-profit institutions may administer joint ventures).

The ATP has a broad mission to promote large economic benefits for the nation.

The legislative mandate of the ATP is to promote "commercializing new scientific discoveries rapidly" and "refining manufacturing practices." This offers tremendous scope. The objective of some projects is to develop technologies that enable lower-cost, higher-quality, or faster-to-market products. The ultimate objective of others is to develop the know-how to provide new-to-the-world or radically improved products and services. The ATP has a high potential impact on U.S. economic growth because, unlike other federal technology programs, it makes investments explicitly for this reason rather than for some other national goal.

The ATP is market-oriented.

While government provides the catalyst—and in many cases, critical technical support—industry *conceives, manages, and executes* ATP projects. Management of projects is geared to ensure that the work performed is what industry believes should be done and is what it can do best.

The ATP also emphasizes cost sharing—ATP recipients on average pay more than half the total costs of the R&D. This helps ensure that companies have a vested interest in the success of projects and in timely commercialization. At the same time, participation by small companies and start-ups is not precluded, because the single-applicant requirement for cost sharing is that the company cover its indirect costs. Since most start-ups and small companies have low

PAST AWARD WINNERS

A listing of the research goals for past ATP award winners covers a very broad array of cutting-edge technologies.

A sampling of 1992 winners includes multiyear awards to help fund:

- development of thick-film processing technology for radio-frequency components for communications equipment (such as cellular telephone base stations), based on high-temperature superconductors;
- development of technology to "clean" semiconductor wafers of trace metals, particles, and surface damage using dry, gas-phase agents in lieu of wet chemicals;
- demonstration of a revolutionary new design for high-precision, multi-axis machine tools, based on an octahedron frame and a "Stewart platform" actuator;
- improvement in scientific understanding of the relationship between processing, part geometry, microstructure, and part performance for fiber-reinforced molded thermoplastic parts, and application of this knowledge in an integrated thermoplastic engineering design morphology.

- development of a microfabricated chip incorporating synthetic DNA probes, together with necessary sensor and computer technology, for an automated, low-cost DNA sequencer;
- creation of a generic software technology to restore, enhance, or digitally reformat moving pictures, such as sequences from infrared, ultrasonic, or X-ray sensors or motion-picture films;
- application of newly developed production technologies to fabricate high-efficiency long-lived, blue/green lasers and LEDs;
- development of new rapid solidification casting technology to produce thick ribbons of metallic glass sufficiently ductile to be used in high-power electric transformers and motors to reduce wasteful power loss;
- development of the methodology for producing animal-derived extracellular matrix materials as prosthetic materials to support the regeneration of tissues and glands; and
- demonstration of the use of quantum-level "electron trapping optical memory" in a prototype erasable optical disk drive suitable for digital video recording at substantially higher speeds and greater densities than existing optical storage media.

indirect cost rates, this requirement is not prohibitive.

The ATP has a comprehensive plan for monitoring and evaluating its performance.

From the start, the ATP has strongly embraced program evaluation and considers it critical to the development and operation of a results-oriented, efficiently run program. Early on, an evaluation plan was developed and measurable goals were identified against which to track performance. As

the ATP strategic plan is updated, the evaluation plan is revised to ensure that it covers all critical aspects of the program.

Economic Returns

Early results indicate that the ATP is successfully improving the capability of the nation's businesses to capture economic returns from scientific and technological

innovations. (See success stories on page 6.) Two independent studies of projects funded in FY 1991 revealed substantial, early beneficial impacts on participating companies, including:

- expanded R&D activity, particularly the ability to engage in high-risk, long-term research with high-payoff potential;
- cost and time savings, improved productivity, and other benefits from industry-industry, industry-government, and industry-university collaborations;
- improved competitive standing;
- formation of valuable strategic business alliances;
- improved ability to attract investors;
- assistance in converting from defense to commercial applications; and
- acceleration of technology development, leading to improved market share.

General and Program Competitions

The NIST ATP office conducts competitions each year to review submitted proposals and select grantees. The number of projects funded varies with the total program budget.

Two types of competitions are supported: "general" and "program." General competitions are open to all technology areas. Past general competition awards have covered a very broad spectrum of technologies in agriculture, biotechnology, microelectronics, machine tools, advanced automotive manufacturing, advanced materials, information and communication technology, flat-panel display manufacturing, and other areas. (See box above.)

Each program competition focuses on a set of technology and business goals. Program competitions enable the ATP to channel significant support to clusters of related projects, each attacking a critical element and reaping the benefits of this synergy.

Key criteria for selecting program areas include:

- potential U.S. economic impact, including the credibility of the program's proposed pathways to economic growth; the importance of the existing or potential sector affected; and the probability of subsequent commercialization;
- good technical ideas that are "cutting edge," high risk, strategically important, and based on sound scientific and technical concepts;
- strong industry commitment to participate, including breadth and depth of interest and willingness to share costs and to work with the government and other partners; and
- opportunity for ATP to make a major difference by supporting work that is unique or complementary to other industrial and government efforts, that offers timely and significant acceleration of research progress, and that requires a critical mass of funding.

Industry Input

In selecting these broad programmatic areas, the ATP relies on its overall strategy of drawing on industry's ideas. Setting research priorities is a constant, ongoing process based on input from industry. Every program has a finite duration, so there is a constant turnover of programs as some are completed and others started.

Mechanisms for getting industry's input include (among others):

- input from senior industry technical and business managers;
- input from industry associations, trade groups, and professional societies;
- ATP-sponsored technical workshops and conferences; and
- analysis of proposals submitted to ATP in previous competitions.

Beginning in FY 1994, NIST also plans to amplify the ATP's impact on the U.S. economy with several new strategies.

It will take a more active role in building cooperative programs among businesses, universities, and government agencies.

Because of its global view and broad sources of information, the ATP is in a unique position to spot potentially advantageous alliances and bring them to the attention of its industrial partners. For example, the ATP might bring to the attention of a joint venture an outside company whose proposed work appears to mesh well with that of the joint venture. Or the ATP might suggest a strategic alliance between a single-company applicant proposing to develop a new technology and a potential end user of that technology, if such an alliance would increase the chances of a project's success.

Although the final decisions about such alliances will always lie with the companies, recognizing such opportunities gives the program an additional tool to increase the chances of success for its projects and to exploit promising opportunities that emerge.

ATP will assist companies in planning for future commercialization and in developing linkages with investors.

Many of the companies participating in the ATP—particularly small companies—are stronger in their R&D planning and implementation of the R&D plan than they are in their business planning and implementation of that plan. The early-stage, preliminary business plans developed by these companies in their ATP applications often lack sufficient detail to provide the clear path to commercialization required by the ATP and may jeopardize many highly promising projects. The ATP plans to contract with private firms to provide business development support to ATP-funded companies that need such assistance.

The commercialization assistance program will be run initially on a trial basis. Its performance will be monitored and evaluated, and, if successful, it will be continued and expanded to serve all companies that wish to participate.

The program will intensify its outreach efforts.

While well-known to most of the larger technology-oriented companies in the United States, the ATP is less well-known or understood by thousands of small, entrepreneurial companies that play a critical role in technology development and might benefit from its programs. To remedy this, an intensified outreach and marketing program has been started to increase awareness of the program. The outreach program will be coordinated closely with state and local economic development organizations that are in a good position to identify small companies that might have an interest in the ATP.

President Clinton has proposed major increases in ATP funding to increase the number of awards made each year and the breadth of cutting-edge technologies covered. The proposed expansion will allow the program to have a truly national impact on economic growth. The program's ultimate success, however, will depend on continued contributions from U.S. industry in the form of good technical ideas, a willingness to cost share, and the successful commercialization of new technologies developed with ATP funding.

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MANUFACTURING EXTENSION PARTNERSHIP

Overview

The NIST Manufacturing Extension Partnership (MEP) is a nationwide network of organizations to support U.S.-based manufacturers in increasing their competitiveness nationally and internationally through ongoing technological advancement. NIST is building and coordinating the partnership to help smaller manufacturers tap into regional and national sources of information, knowledge, and insight into the use of modern manufacturing and production technologies.

When fully developed, the partnership will meet President Clinton's call for the establishment by NIST of "over 100 manufacturing extension centers nationwide by 1997 to assist manufacturers to modernize their production capability."

The partnership includes four major elements:

- regionally based Manufacturing Technology Centers (MTCs), providing hands-on technical assistance to small and mid-sized manufacturers;
- smaller, satellite operations called Manufacturing Outreach Centers, some affiliated with an MTC;
- the State Technology Extension Program (STEP), providing grants to help states build the infrastructure needed for technology transfer efforts; and
- the Links Program to pull together—both electronically and otherwise—not only the NIST affiliated offices but also all other federal, state, local, and university technology transfer entities into one national network.

The philosophy of the MEP is to take maximum advantage of programs already in place. It avoids duplication of efforts among existing technology assistance organizations and concentrates on matching company needs to available help regardless of the source.

Established in 1992, the MEP builds on the MTC and STEP programs, which were created under the Technology Competitiveness Act of 1988.

Manufacturing Technology Centers

Regionally located and managed centers for transferring manufacturing technology, the NIST MTCs provide major focal points for the partnership. The MTCs are designed to bridge a "technology gap" between sources of improved manufacturing technology and the small and mid-sized companies that need it. The MTCs draw on a wide variety of technology sources, including commercial firms, federal research and development laboratories (such as NIST),

universities, and other research-oriented organizations. They are established in areas with a relatively heavy concentration of industrial firms.

Local management by a regionally based sponsor allows each MTC to tailor its services to the requirements dictated by its location and the type of manufacturing in its client base. In general, the MTCs provide a wide range of services, including individual project engineering, training courses, demonstrations, and assistance in selecting and using software and equipment.

Some of the most important services include factory survey visits, technical training, and direct help with the introduction of modern manufacturing equipment. MTCs also provide access to management, financial,

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marketing, and training services through linkages to other established programs such as the Small Business Development Centers. The MTCs do not conduct research.

The MTCs generally provide facilities that demonstrate various types of computer-aided design and manufacturing software. Some MTCs also offer hardware demonstration facilities, including automated metal working equipment (lathes and milling machines), robotic, and state-of-the-art measuring equipment. (See MTC success stories on page 6.)

Outreach Centers

Smaller than MTCs, Manufacturing Outreach Centers (MOCs) are a new element in the partnership. The MOCs also help manufacturers adopt appropriate, modern technologies, but the services of an MOC generally do not encompass the full breadth of those available through the larger MTCs. In general, MOCs are organized as programs affiliated with existing technical or training institutions such as community colleges, technical colleges, vocational institutions, university manufacturing centers, or state technical assistance centers. MOCs are located in areas with smaller concentrations of industry and focus on delivering services to client firms out of reach of an MTC. These smaller centers may be closely affiliated with a host MTC, or may be independent, with access to technology and management input from non-MTC sources.

NIST will accept proposals for new MTCs and MOCs *only in response to a specific solicitation*. As funds permit, a Request for Proposals is posted in the *Federal Register*.

All solicitations are open and competitive. Specific funding provisions (which may change due to actions by the Congress) and evaluation criteria that apply to the specific solicitation appear in the *Federal Register* notice. In general, proposals are evaluated on:

- knowledge of target firms in the proposed region;
- linkages to sources of technology;
- technology delivery mechanisms; and
- management and financial plans.

Each MTC or MOC must be sponsored by a U.S.-based, non-profit institution or organization, possibly a state government agency.

The local sponsor must contribute 50 percent or more of the proposed center's capital and annual operating and maintenance costs.

State Technology Extension Program

The State Technology Extension Program (STEP) works with states to develop the "infrastructure" for coordinated manufacturing extension and modernization programs to serve the competitive needs of small and medium-sized businesses. The program emphasizes statewide coordination of existing and newly developed technology assistance programs—such as NIST-funded MTCs and MOCs, university centers, or community college programs—and the development of complementary programs where necessary to ensure more comprehensive statewide delivery of services.

Typical examples might be creating a statewide network of industrial extension agents to provide advice and assistance on implementing new technologies, or a pilot project to provide technology assistance to a particularly important industrial sector in the state.

STEP grant projects must be sponsored by a U.S.-based, non-profit institution or organization, possibly a state government agency. NIST accepts applications for STEP grants *only in response to specific solicitations*, which are published in the *Federal Register*. All solicitations are open and competitive.

STEP grants provide *matching* funds—the sponsor generally is required to put up at least 50 percent of the cost of the proposed project. Specific requirements will vary with each solicitation.

The LINKS Program

Under "LINKS," the Manufacturing Extension Partnership plans to identify sources of assistance, information, and technology, and "network" them in an open system of cooperative "links."

A key feature of LINKS will be a national electronic network that connects all of the partnership's components, including MTCs, MOCs, and other partnering organizations such as federal laboratories, universities, or other federal programs. This electronic network not only will provide for rapid communication but also will provide access to databases and information on a variety of topics, including technologies available from different sources, best manufacturing practices, and listings of technical experts.

Many of these databases exist in an independent fashion already and need only to be tied into the unified LINKS network. In addition to the electronic network, LINKS also will encompass joint projects that can serve extension efforts across the nation. Such activities will include national interactive satellite telecasts on topics of interest to manufacturers, national training programs for extension agents, and development of common tools such as automated software for assisting extension agents in assessing a manufacturer's operations.

MALCOLM BALDRIGE NATIONAL QUALITY AWARD

First presented in 1988, the Malcolm Baldrige National Quality Award has quickly become both the U.S. standard of quality achievement in industry and a comprehensive guide to quality improvement.

Congress established the award to raise awareness about quality management and to recognize U.S. companies that have successful quality management systems. The award was named in honor of Malcolm Baldrige, who served as Secretary of Commerce from 1981 until his death in a rodeo accident in 1987. Baldrige was a strong proponent of quality management and helped draft an early version of the legislation that eventually was named after him.

The award program, developed and managed by NIST with the cooperation and financial support of the private sector, recognizes quality achievements in three categories: manufacturing, service, and small business. Up to two awards can be made in each category.

Applications for the award undergo a rigorous evaluation by an independent review board composed of quality experts from the private and public sectors. Examiners conduct on-site reviews at firms that receive high scores after an initial screening. All applicants receive a written summary that identifies their strengths and points out areas for improvement.

Although the major focus of the award is on results and customer satisfaction, it is *not* given for specific products or services. To win the award, a company must have a world-class system for managing its processes and its people. This system should ensure continuous improvement in its product or service and provide a way of satisfying and responding to its customers.

Tens of thousands of U.S. companies are now using the award's guidelines to evaluate their operations in seven key areas of quality management and performance.

- Leadership. Have senior leaders clearly defined the company's quality values, goals, and ways to achieve the goals? Are senior executives personally involved? Does this involvement include communicating quality excellence to groups outside the company?
- Information and analysis. Is the information used to guide the company's quality management system reliable, timely, and accessible?
- Strategic quality planning. How does the company plan to achieve or retain quality leadership? How are these plans integrated into its overall business planning?
- Human resource development and management. How does the company develop the full potential of its work force?
- Management of process quality. How does the company assure the quality of its goods and services?
- Quality and operational results. What are the company's quality and operational performance results and trends?
- Customer focus and satisfaction. What is the company's relationship with its customers? How does the company satisfy current and future customer needs?

The results of these internal evaluations provide firms with a clear view of where they stand and of how far they must go to achieve world-class levels of quality.

Companies that apply for the National Quality Award must provide the details needed to prove achievement of world-class quality in all seven areas. Facts, not flash, are needed to make it through the tough screening process.

Firms entering the competition pay a fee that covers the cost of the evaluation and feedback reports. Profiles on the quality programs of past award winners are available upon request. Copies of quality management guidelines and award applications are also available.

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PAST QUALITY AWARD WINNERS

Winners of the Malcolm Baldrige National Quality Award include:

1993—Eastman Chemical Co. and Ames Rubber Corp.

1992—AT&T Network Systems Group/Transmission Systems Business Unit, Texas Instruments Inc. Defense Systems and Electronics Group, AT&T Universal Card Services, The Ritz-Carton Hotel Co., and Granite Rock Co.

1991—Solectron Corp., Zytec Corp., and Marlow Industries.

1990—Cadillac Motor Car Division, IBM Rochester, Federal Express Corp., and Wallace Co. Inc.

1989—Milliken & Company and Xerox Corp. Business Products and Systems.

1988—Motorola Inc., Commercial Nuclear Fuel Division of Westinghouse Electric Corp., and Globe Metallurgical Inc.

TECHNOLOGY SERVICES

NIST provides a wide variety of services and programs to help U.S. industry improve its international competitiveness, commercialize new technology, and achieve total quality in all facets of business operations.

Companies spanning nearly all industrial sectors depend on the precision and reliability of NIST measurement services and products to keep their production processes running smoothly, efficiently, and safely. NIST reference materials, data, and calibrations help industry maintain quality control in the production of everything from aerospace alloys to voltmeters to breakfast cereals.

Responding to increased emphasis on quality standards in international markets, NIST provides information and assistance to about 20,000 organizations and individuals every year concerning national and international voluntary and regulatory product standards and certification systems.

In addition, NIST offers a user-friendly environment for businesses interested in cooperative research and development efforts, NIST-developed technologies available for license, guest researcher opportunities, technical information, or technical assessments.

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SERVICES AND PROGRAMS

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SERVICES AND PROGRAMS

STANDARDS ANALYSIS AND ASSISTANCE

Standards Code and Information (SCI) Program staff assist federal agencies and industry with specific technically based trade issues related to standards and conformity assessment. SCI staff develop technical positions for U.S. negotiators in bilateral and multilateral discussions; monitor and report on the adequacy of U.S. participation in international standardization efforts; handle complaints from U.S. industry representatives concerning foreign standards and certification practices; and review and transmit U.S. comments on proposed foreign regulations, especially under its cooperative government-industry program with the Saudi Arabian Standards Organization. The staff also monitor national and international developments related to standards and conformity assessment activities.

SCI staff hold voting membership in various national and international standards committees and participate in interagency task forces and working groups to develop government positions on major international standard-related developments, such as the formation of a European Single Market, the North American Free Trade Agreement, and negotiations under the Standards Code. SCI staff publish information detailing the standards and conformity assessment activities of U.S. private and government organizations as well as international and regional organizations. The program also publishes other reports related to the ISO 9000 Standards Series, U.S. participation in international standardization, the formation of the European Single Market, and other topics.

SCI serves as the secretariat for the U.S. Interagency Committee on Standards Policy and has published guidelines on U.S. government participation in international standards bodies, federal use of third party and self-certification, and its use of laboratory accreditation. It has formed various working groups to deal with issues of multiagency concern related to standards and conformity assessment.

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STANDARDS INFORMATION CENTER

The NIST National Center for Standards and Certification Information is the U.S. focal point for information on standardization programs and related activities at home and abroad. Center staff provide information on U.S., foreign, regional, and international voluntary standards bodies, as well as on mandatory government regulations and conformity assessment procedures for non-agricultural products. As the U.S. member of the International Organization for Standardization Information Network (ISONET), NIST has access to foreign national standards information through approximately 60 other ISONET members and the ISO information center in Geneva, Switzerland. NIST also serves as the U.S. inquiry point under the General Agreement on Tariffs and Trade (GATT) Agreement on Technical Barriers to Trade.

At the center, NIST maintains an extensive collection of reference materials, including U.S. military and other federal government specifications, U.S. industry and national standards, international standards, and selected foreign national standards. Staff members respond to requests for information either directly or by identifying the most appropriate source of information. They also prepare directories and indexes of specialized standards information, arrange for translations of foreign standards, and issue periodic publications explaining ongoing developments in domestic and international standards activities.

Two telephone hotlines located within the center offer weekly updates on draft European standards [(301) 921-4164] and on proposed foreign regulations that may significantly affect trade [(301) 975-4041].

Information for the latter hotline is supplied by the GATT Secretariat in Geneva.

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WEIGHTS AND MEASURES

Helping federal, state, and local governments ensure equity in marketplace measurements is one of NIST's longest running and best-known programs. It includes an accreditation program for state weights and measures laboratories in the areas of mass, length, and volume, as well as providing test protocols, training, and ongoing laboratory assistance.

NIST sponsors the National Conference on Weights and Measures, a standards development organization, which involves over 3,000 industry and regulatory agency representatives. Program staff manage the

National Type Evaluation Program, which, at manufacturers' expense, evaluates commercial measuring devices against national and/or international standards. Staff produce numerous training manuals, handbooks, and other publications, and they operate an electronic bulletin board to provide the weights and measures community with a mechanism for rapidly exchanging information. (See listing for bulletin board on page 9.)

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STANDARDS MANAGEMENT

NIST manages U.S. technical representation and participation in the International Organization of Legal Metrology (OIML) and administers the U.S. Department of Commerce's Voluntary Product Standards (VPS) program.

OIML is a treaty organization with a membership of 51 voting and 37 non-voting nations. OIML's objective is to enhance trade by harmonizing national regulations governing performance requirements for measuring instruments used for equity in commerce, for assurance of public and worker health and safety, and for protection of the environment. To realize its objective, OIML develops International Recommendations and International Documents for adoption and use by member nations. These publications include requirements for testing and verifying the performance of measuring instruments. In managing this program, NIST obtains technical advice and support from U.S. trade associations, instrument manufacturers, academia, and federal and state regulatory agencies.

Under the VPS program, NIST provides the secretariat for the development and maintenance of voluntary standards for selected products, with the costs paid by proponent trade associations or other groups. Current standards concern softwood lumber, construction and industrial plywood, wood-based structural-use panels, and glass bottles for carbonated soft drinks.

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NATIONAL LABORATORY ACCREDITATION

The NIST National Voluntary Laboratory Accreditation Program (NVLAP) rigorously evaluates the competencies and technical qualifications of public and private laboratories for providing testing and calibration services. An accredited laboratory must meet all requirements of national consensus standards as well as international accreditation requirements of the International Standards Organization (ISO Guides 25 and related standards).

For a fee, NVLAP currently accredits qualified laboratories that offer services in the following testing areas: product testing (acoustics, carpets, paints, paper, plumbing, seals, sealants, insulation), computer networks, construction products (cement, concrete, etc.), electromagnetic compatibility, energy-efficient lighting, fasteners and metals (chemical, dimensional, metallurgical), telecommunications, and personnel radiation dosimetry. Accreditation is also available in the following calibration areas: dimensional, electrical, radiation, mechanical, thermodynamics, and time and frequency.

Any interested laboratory, organization, or agency can apply for accreditation in these and other areas. Requests for expanded program services will be evaluated on a case-by-case basis. Among the many benefits of NVLAP accreditation are certification of proficiency with a quality-assurance check on laboratory performance, substantive advice for improving performance, and national recognition of competency. Accreditation also helps users—from industry, government, and elsewhere—identify providers of high-quality testing and calibration services.

The program staff publish an annual directory of NVLAP-accredited laboratories.

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OFFICE OF RESEARCH AND TECHNOLOGY APPLICATION

The Office of Research and Technology Application assists U.S. industry in identifying, accessing, and applying NIST and other federally developed technology. The staff also participate in and develop workshops, conferences, and seminars that bring federally developed technology to the attention of companies that can benefit from it.

The office staff works with federal, state, and local technology outreach and economic development programs, as well as professional and scientific societies and trade associations, to help them assist industry with the application of NIST and other federal technology. The staff can guide

industry and other customers to a spectrum of technical assistance services, ranging from information, patents available for license, cooperative research and development agreements, use of unique facilities, specialized technical workshops, and scientific and engineering expertise.

The office director is the NIST representative to the Federal Laboratory Consortium.

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TECHNOLOGY DEVELOPMENT AND SMALL BUSINESS PROGRAM

The Technology Development and Small Business Program serves as a central NIST technology transfer office. The office helps develop R&D relationships between NIST and industry, and it is also responsible for patenting and licensing technologies developed with NIST partners and by NIST laboratories.

The office is the point of contact for U.S.-based organizations interested in:

- exploring the various ways of working with or accessing NIST's R&D capabilities, including obtaining technical assistance from NIST experts in specific fields;
- setting up R&D partnerships with NIST laboratories, such as bilateral or consortia cooperative R&D efforts, through cooperative research and development agreements (CRADAs), domestic guest researcher agreements, or other formal arrangements;
- obtaining licensing rights to NIST-patented technologies; and

- accessing NIST's world-class measurement facilities through facility use agreements or proprietary measurement agreements.

Working with NIST has helped individual U.S.-based firms leverage their R&D efforts, develop new products, improve production processes, improve quality control measurements, and enhance existing product performance. Collaboration with NIST has helped consortia and other industrial groups to develop technical consensus; develop generic technologies with broad, industry-wide applications; or pool a critical mass of industrial participants for effective technology implementation.

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STANDARD REFERENCE DATA

Working closely with industry, NIST provides well-documented numeric data to scientists and engineers for use in technical problem-solving, research, and development. These recommended values are based on data extracted from the world's literature, assessed for reliability, and then evaluated to select the preferred value. The evaluations are carried out through a network of data centers, projects, grants, and cooperative programs.

Standard Reference Data (SRD) have a variety of uses in industrial applications and are available as databases for personal computers, as well as in other computerized forms, and as publications. Common applications include use for calibration points (such as spectral wavelengths and transition energies) and as input to the design of new processes and materials. Among the many subjects covered are analytical chemistry, atomic and molecular physics, chemical kinetics, fluid mixtures, thermochemistry, materials properties, phase equilibria, and biotechnology.

To increase the usefulness and accessibility of data, NIST has developed a series of personal computer databases with interactive programs, search routines, and other calculational and graphical software features. Most databases are updated yearly, adding more data and more software capabilities.

Another major dissemination vehicle is the *Journal of Physical and Chemical Reference Data*, a bimonthly journal published jointly with the American Chemical Society and the American Institute of Physics.

A free catalog of NIST SRD data products and services is available.

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STANDARD REFERENCE MATERIALS

Now numbering more than 1,200 and steadily growing to meet the needs of industry, Standard Reference Materials (SRMs) are a diverse collection of solids, liquids, and gases certified for their chemical composition or physical properties. With an SRM, companies can verify the accuracy of analytical or other measurement methods under development or calibrate established measurement systems to ensure consistently accurate performance of equipment and operators. Specific types of SRMs range from linewidth standards for producing integrated circuits, to metal alloys for checking quality control in steel production, to radio-pharmaceuticals for calibrating medical equipment.

NIST's SRM catalog provides a complete listing of available reference materials along with a description of their certified properties. In addition, the *Handbook for SRM Users* offers practical guidance on the use of the materials, describes the fundamental elements and concepts of quality control and measurement processes, provides advice on using control charts and statistical tools to evaluate measurement quality and uncertainty, and includes articles on quality assurance, sampling, and validation of analytical instruments.

The SRM program staff also publish timely information on reference materials, offer telephone consultations on SRM uses, and organize seminars to advise industry on SRM applications.

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CALIBRATION SERVICES

NIST provides more than 500 different services to ensure that manufacturers and other users of precision instruments achieve measurements of the highest possible quality. These services, which satisfy the most demanding and explicit requirements, link a customer's precision equipment or in-house standards to national standards. For calibrations and special tests, NIST personnel check, adjust, or characterize an instrument, device, or set of in-house, or transfer, standards. Customers are assured that measurements are consistent with national standards and adequate for their intended use. Besides individual equipment items, NIST measurement assurance programs calibrate entire measurement systems.

The full range of NIST calibration services ensures the accuracy and compatibility of measurements used in day-to-day quality-control applications. The services, available for a fee, encompass seven major areas: dimensional measurements; mechanical, including flow, acoustic, and ultrasonic; thermodynamics; optical radiation; ionizing radiation; electromagnetics, including direct current, alternating current, radio frequency, and microwave; and time and frequency.

The program staff publish a regularly updated catalog describing available services, fee schedules, and detailed descriptions of calibration protocols. Staff members offer telephone consultations on the use of services and on the importance of traceability to national standards, and they make presentations to industry groups and other organizations.

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A104 TRF Building

TECHNOLOGY EVALUATION AND ASSESSMENT

NIST offers technology evaluation and consulting services, on a cost-reimbursement basis, to client institutions or organizations. Evaluation is free where the technology qualifies for consideration under the Energy-Related Inventions Program. All technologies are evaluated on the basis of technical and commercial feasibility, and all evaluations are held in strict confidence.

In cooperation with the U.S. Department of Energy (DOE), NIST evaluates new product or process ideas for their potential to improve energy efficiency, reduce energy costs, or increase energy supply. Inventions may be submitted to the program at any stage of development. All inventors are informed, in detail, of the results of the free evaluations.

Inventions that satisfy NIST criteria are recommended to DOE, which may decide to support development and commercialization. Since 1975, DOE has awarded nearly \$35 million to move NIST-recommended inventions closer to commercialization. In addition, inventors may use the NIST recommendation report to help attract private investment capital.

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INFORMATION SERVICES

The Office of Information Services maintains a comprehensive international collection of information in scientific disciplines such as metrology, mathematics, physical sciences, computer science, and materials science. The staff serve the technical information needs of NIST scientists and engineers and communicate the results of NIST research to scientific and engineering communities worldwide.

The office staff participate in national and international publications and technical information networks and consortia, as well as a document exchange program to ensure that NIST publications are available to scholars, scientists, engineers, industry researchers, and others. An inquiries service and information staff assist the public in obtaining information about past and present NIST programs, publications, and special projects.

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OPPORTUNITIES FOR INNOVATION

The Opportunities for Innovation (OFI) Program assists small to medium-sized technology-based companies in the formation of R&D strategic partnerships with leading manufacturing corporations. To accomplish this goal, a series of regional OFI workshops is organized by NIST in cooperation with states and regional partners to

promote deployment of advanced technologies by small to medium-sized businesses. These workshops cover selected technologies, such as sensors, advanced manufacturing, biotechnology, pollution prevention, optoelectronics, and others, where R&D opportunities exist for small firms. The workshops also provide a forum for exchange of information on "niche" technologies available from the participating smaller businesses and on opportunities for joint R&D partnerships with the leading manufacturing corporations. The technical part of the OFI workshops is supported by OFI monographs written by industrial experts and consultants commissioned by NIST. Information on financing opportunities for small and medium-sized businesses through the Small Business Administration and state-based resources is also provided to participants of OFI workshops.

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METRIC PROGRAM

The NIST Metric Program helps implement the national policy to establish the metric system as the preferred system of weights and measures for U.S. trade and commerce. The Metric Program coordinates the metric transition activities of all federal agencies. It provides leadership and assistance on metric conversion and metric usage to federal agencies, state and local governments, standards organizations, trade associations, and businesses. The program also disseminates educational information to increase understanding of the metric system and to identify and remove barriers to metric usage.

The 1988 amendments to the Metric Conversion Act of 1975 require federal agencies to use the metric system in procurements, grants, and other business activities. Executive Order 12770, "Metric Usage in Federal Government Programs," issued in 1991, reaffirms the legislation by instructing the federal agencies to implement formal plans for using the metric system and by requiring the federal agencies to report metric progress annually. The order authorizes the Secretary of Commerce to direct and coordinate the federal agency metric transition and to assess progress in annual reports to the President. The NIST Metric Program carries out the direction and coordination responsibilities of the Secretary.

Because of the metric system's importance as an international standard, its use in product design, manufacture, marketing, and labeling is essential for U.S. industry's success in the global marketplace. The use of

the metric system in federal agency programs relating to trade, industry, and commerce is intended to support industry's voluntary adoption of metric usage and to help catalyze a broader metric transition that will achieve the full economic benefits of metric usage.

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SMALL BUSINESS INNOVATION RESEARCH PROGRAM

The Small Business Innovation Research (SBIR) Program provides funding on a competitive basis to small businesses that can carry out research on topics of interest identified by participating federal agencies. Each year, the Department of Commerce issues a list of recommended R&D topics. There are two phases of awards: In Phase I, awardees can receive up to \$100,000 to establish the technical feasibility of a proposed project. Successful Phase I participants may compete in Phase II for up to \$750,000 to support further development of the work. Funds available at each agency for SBIR are directly tied to the agency's extramural research funding level. Accordingly, NIST's program has been expanding in recent years.

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ELECTRONICS AND ELECTRICAL ENGINEERING LABORATORY

In consultation with industry, NIST electronics and electrical engineering researchers tailor Institute programs to meet the most critical measurement needs in the manufacture of semiconductor, magnetic, radio-frequency, microwave, optical, optoelectronic, and superconducting products, as well as electrical power systems.

These researchers develop improvements in quality control and cost effectiveness for both current and next-generation semiconductors; produce methods that help increase the efficiency of optical fiber networks; and operate specialized computer facilities to develop new standards and performance measures for flat-panel displays and high-definition television systems.

They also conduct fundamental studies on promising future technologies such as high-temperature superconductors and hybrid computer chips that utilize both electronic and lightwave signals.

This laboratory provides the fundamental basis for all electrical measurements in the United States.

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COOPERATIVE RESEARCH OPPORTUNITIES

Electricity

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- 23 Metrology for Flat-Panel Displays
- 23 Automated Electronics Manufacturing Program
- 24 Electrical Metrology with Optical Sensors
- 24 Gaseous Electronics
- 24 Synthesis of Precise Signals
- 24 Testing Electronic Systems
- 25 Fast Pulse and Waveform Acquisition Standards
- 25 Self-Calibrating Systems
- 25 Advanced AC-DC Voltage and Current Measurements
- 25 Josephson-Effect Voltage Standards
- 26 Resistance Standards and Materials
- 26 Quantum Hall Effect
- 26 Applying High-T_c Superconductors to Precision Electrical Measurements

Semiconductor Electronics

- 27 Silicon Characterization
- 27 Compound Semiconductors and Semiconductor Microstructures
- 27 Molecular Beam Epitaxy
- 28 Semiconductor Spectroscopy
- 28 Semiconductor Devices
- 28 Power Semiconductor Electronics
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- 29 Advanced Integrated-Circuit Test Structure Metrology
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- 29 Building-In Reliability

Electromagnetic Fields

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- 30 Electromagnetic Characterization of Materials
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- 33 Semiconductor Processing Research Laboratory
- 34 Superconductor Integrated-Circuit Fabrication Laboratory
- 34 High-Voltage Measurement Facility
- 34 Transistor Safe Operation Test System
- 35 High-Accuracy Ellipsometer
- 35 Near-Field Scanning Facility for Antenna Measurements
- 36 Ground Screen Antenna Range
- 36 Mode-Stirred Chambers
- 37 Transverse Electromagnetic Cells
- 37 Electromagnetic Anechoic Chamber

COOPERATIVE RESEARCH OPPORTUNITIES

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VIDEO PROCESSING

Data compression, motion encoding, scan-rate conversion, and other video processing research topics are being explored at NIST using a massively parallel video supercomputer, the Princeton Engine. The Princeton Engine, developed by the David Sarnoff Research Center, Princeton, N.J., is a 14-giga-instruction-per-second image-processing system capable of simulating video rate signals, including conventional National Television Standard Code and high-definition video, in real time. Because the engine is programmable, it can be used to evaluate software prototypes of video processing components rapidly and at a cost below that of building hardware.

The Princeton Engine consists of 1,024 parallel processors, where each 16-bit processor has its own ALU, multiplier, and 128 kilobytes of local memory. Each processor operates on one picture element per video scan line, and all processors execute the "same" instructions. Wideband input and output channels accept and produce a number of analog and digital video formats. For many applications, video data can be processed and output at the same rate as they are input, that is, in real time. For longer algorithms up to 7 seconds of video data may be acquired in real time, stored in local memory, and, once processed, displayed at the original data rate.

Programming is accomplished using a subset of the C language having special constructions for parallel operation. Video recorders, multiscan monitors, high-definition monitors, and additional video support equipment are available.

NIST researchers are interested in using the Princeton Engine laboratory for a wide variety of collaborative research projects. Such collaborations would focus on precompetitive research with broad applications in advancing the state of the art in high-definition systems.

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METROLOGY FOR FLAT-PANEL DISPLAYS

Researchers at NIST are developing the measurement technology for the characterization of advanced image display systems. A set of meaningful performance specifications is needed that can be used to assess display quality and that can be applied across the wide spectrum of display technologies that either are available or will shortly become available. Display quality issues are not simply a matter of light measurement, power efficiency, display environment, or signal quality. Rather, many of these factors act in concert to affect display quality, with an important addition—the complexities of human visual perception. Research topics include the development of radiometric and colorimetric measurements of emissive and non-emissive displays, the

automation of such measurements, investigation of the visual perception of the eye, and modeling of display characteristics using the Princeton Engine video supercomputer.

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AUTOMATED ELECTRONICS MANUFACTURING PROGRAM

The Automated Electronics Manufacturing Program (AEMP) at NIST is working with industry to build the infrastructure for an electronic marketplace and to demonstrate and apply this technology to the electronics industry. AEMP researchers are leading a demonstration team within the national industry/government Electronic Commerce of Component Information (ECCI) program. The objective of ECCI is to show the viability of today's technology coupled with emerging standards to broker electronic component information across a national information highway. Another enabling technology for electronic commerce is a complete and consistent suite of standards for the exchange of electronic product data descriptions. AEMP is involved in efforts to "harmonize" existing, overlapping standards (such as EDIF and IGES), to help industry test for compliance with those standards, and to work with industry to develop standards in critical areas where none exist.

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ELECTRICAL METROLOGY WITH OPTICAL SENSORS

Measurements involving high voltage or combined high-voltage and high-speed phenomena are costly and difficult to perform because of the cost of high-voltage sensors, high-voltage insulation requirements, and electromagnetic interference. Yet nearly every item installed in an electric power generation and distribution network must undergo acceptance tests at high voltage and withstand accidental high-voltage surges as well as natural ones.

Optical and electro-optical techniques offer possibilities of overcoming the disadvantages of conventional sensors. Researchers at NIST are developing electro-optical methods as part of a program to develop theory, methods, and physical standards for measuring electrical quantities and phenomena in advanced high-voltage/high-power systems.

Experimental research includes development of Kerr effect techniques to measure high-voltage transients and electric fields in insulation systems. Devices based on the Faraday effect in optical fibers and glass rods are evaluated as substitutes for conventional current transfers and shunts in high-voltage applications. High-speed photography, image-preserving optical delay systems, optical multichannel analyzers, lasers, and sensitive detectors are used to study electrical breakdown phenomena in real time involving nanosecond time resolutions. Theoretical studies are focused on the use of finite-element code for electric-field computation and computer-aided data acquisition and analysis.

Anticipated benefits include measurements and tests to evaluate more reliably the performance of high-voltage power equipment and thus increase its efficiency. Better understanding of safety margins and on-line performance monitoring will enable the equipment to operate at higher loads and facilitate the introduction of new, more

effective, and environmentally more acceptable insulation materials. The direct beneficiaries will be the electric utility industry, its equipment suppliers, and the pulsed-power community that uses high-voltage techniques in high-energy physics, space, and defense applications.

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GASEOUS ELECTRONICS

NIST scientists are developing measurement methods to characterize gaseous dielectrics for high-voltage power systems. Emphasis is on investigation of phenomena that affect reliability and safety associated with operation of gas-insulated systems, such as production of toxic byproducts in electrical discharges. Theoretical work addresses Boltzmann equilibrium statistics, chemical kinetics code, and computer-aided data acquisition and analysis. Experimental work focuses on high-voltage ac and dc tests, gas chromatograph and mass spectrometer techniques for chemical characterization, and partial discharge measurements. Researchers are investigating rf discharges used for processing electronic materials, including the study of plasma diagnostics and kinetics as they apply to the plasma processing of semiconductor materials.

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SYNTHESIS OF PRECISE SIGNALS

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 and producing both sinusoidal and arbitrary waveforms. 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.

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TESTING ELECTRONIC SYSTEMS

NIST scientists are developing new testing approaches for electronic systems to minimize the attendant testing costs while assuring product quality. Program emphasis is on development and application of generic error modeling methods for describing the systems to be tested. Once an accurate model is available, it can predict the performance of a device based on the fewest possible number of tests. Theoretical work centers on dimensionality selection for empirical models to minimize prediction errors, and on the assignment of uncertainties and confidence limits when making predictions based on empirical models. Results

of this work are being used by the semiconductor industry to reduce the costs of testing mixed-signal integrated circuits.

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FAST PULSE AND WAVEFORM ACQUISITION STANDARDS

NIST has an active program to provide a basis for characterizing both the time domain and frequency domain performance of sampling and digitizing systems, including A/D converters, sampling oscilloscopes, and waveform recorders. Theoretical and experimental research establishes test methods, reference waveforms, and state-of-the-art sampling technology to support these systems. Research areas include optoelectronic and electro-optical techniques for sampling and pulse generation in the 1- to 5-picosecond regime; advanced signal processing methods, including deconvolution, phase-plane compensation and spectral estimation; and ultrahigh accuracy techniques to support modern sigma-delta sampling technology.

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SELF-CALIBRATING SYSTEMS

Self-calibration features are ubiquitous in modern instrumentation, but their overall effects are often poorly understood. NIST researchers are developing a model-based theory of self-calibrating systems that should lead to more efficient and accurate implementation, better understanding, and realistic programs for calibration support.

Major goals are the development of a high-level representation scheme capable of describing the data characteristics and information flow of self-calibrating systems, and the development of an analysis engine to extract performance information.

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ADVANCED AC-DC 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.

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JOSEPHSON-EFFECT VOLTAGE STANDARDS

High-accuracy voltage-standard systems have proliferated among many industrial, government, and international standards laboratories with the advent of the Josephson-array device. Within this NIST laboratory, there are three array voltage-standard systems in operation, including a fully automated 10-V array system. Guest researchers can gain hands-on experience with array system operation and verification, as well as cooperate on studies into both precision voltage metrology and Josephson-array physics.

The metrology goals are to improve measurement precision to better than one part in 10^8 in applications of direct system-to-system intercomparisons and lab-to-lab volt transfers, achieve greater reliability in automation algorithms, and further the development of solid-state reference standards and precision digital voltmeters.

The physics research addresses the effects of electromagnetic noise on the stability and accuracy of the Josephson quantized-voltage steps, studies the boundaries of chaotic behavior in junction-junction interactions, and explores other possible array device applications, such as the generation of ac signals through frequency modulation of the millimeter-wave drive frequency.

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RESISTANCE STANDARDS AND MATERIALS

Component precision resistors of both film and wire construction have found widespread use as references and dividers in precision instrumentation, such as digital multimeters and calibrators. The quality of these resistors and their level of immunity to the effects of environmental parameters, such as temperature and mechanical shock, have enabled the 3-month performance of these instruments to begin to approach that of the standards most commonly used to calibrate them. This fact and the desirability of calibrating such instruments where they will be used has heightened the need for a next generation of resistance standards—standards whose performance in adverse conditions would eclipse that of existing standards in a laboratory environment.

NIST scientists are beginning a program to develop new standards with sub-ppm performance, both short- and long-term, under field conditions. To do so, the electrical/physical properties of a number of alloys are being investigated, and new resistor designs are being formulated and tested. Future efforts will investigate metallurgical techniques such as rapid quenching, ion implantation in semiconductors and glasses for resistors $>10^7 \Omega$, and Evanohm or Nichrome film deposition on Si substrates. The desired output will be fixed-value standards in the range from 1Ω to $10^{12} \Omega$ with sub-ppm per year drift rates, temperature coefficients less than $0.1 \text{ ppm}/^\circ\text{C}$, and low power and voltage coefficients. A metallurgical facility with the capability of monitoring the electrical properties of materials during annealing and a silicon processing

facility are available along with access to precision resistance measurement systems and the national resistance standards.

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QUANTUM HALL EFFECT

The quantum Hall effect now provides the basis for the national unit of resistance. The realization of the resistance standard in the laboratory presents many interesting problems; researchers at NIST are investigating the physical principles underlying the effect, understanding sample-specific artifacts, and improving the measurement systems. Research is being conducted on the range of parameters over which the quantum Hall effect provides the most accurate and reproducible standard of resistance.

Using GaAs heterostructures grown at NIST, researchers are using a dedicated class-10 clean room facility to investigate different methods of making contacts to the devices that will have very low resistances (in the milli-ohm range) even at temperatures below 4.2 K and in high magnetic fields.

Research also is being conducted on determining the degree to which the device resistance is independent of its material and manufacturing variables by comparing the resistances of devices made from different materials.

Recent research at NIST has opened up the possibility that quantum Hall devices may be a source of very-high-frequency phonons when large current densities are passed through the devices.

NIST researchers also are working to improve and simplify the measurement systems used to calibrate resistors; a new He-3 refrigerator and 16-T magnet facility have been developed for use with a new cryogenic current comparator. This enabled the accuracy of NIST calibrations to be increased severalfold.

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APPLYING HIGH- T_c SUPERCONDUCTORS TO PRECISION ELECTRICAL MEASUREMENTS

NIST and other national standards laboratories for years have used cryogenic current comparators (CCCs) to make ratio measurements of voltage, current, and resistance with accuracies of 0.01 ppm or better. This approach has not found widespread commercial use because the cryogenic current comparator must be operated at liquid-helium temperatures, which presents a variety of operational difficulties. Moreover, existing comparators are working prototypes rather than completed instrumentation systems and, accordingly, are difficult to use.

Recent advances in superconductivity technology have made the application of high-temperature superconductors practical. In at least one case, an integrated circuit SQUID magnetometer, similar to devices used in CCCs to detect low levels of magnetic flux, has been built that operates at liquid-nitrogen temperatures. Thus, the possibility for developing a commercial instrument based on a CCC has now been opened. Such an instrument might be run with a refrigerator at liquid-nitrogen temperature

This development and the possibility of commercialization make it feasible to automate the basic CCC design, which then will be more attractive for general calibration use. NIST scientists are now engaged in designing, building, and testing CCCs to support measurements of the new national resistance standards based on the quantized Hall effect. This involves establishing a few select ratios that range from 1:1 to 100:1. Future efforts will include the development of CCCs with selectable ratios over a somewhat larger range.

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SEMICONDUCTOR ELECTRONICS

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SILICON CHARACTERIZATION

NIST conducts research on 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 using 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 non-destructive methods. Measurement techniques include four-probe, spreading resistance, and capacitance-voltage; Fourier transform infrared spectroscopy; deep-level transient spectroscopy; and photoluminescence.

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COMPOUND SEMICONDUCTORS AND SEMICONDUCTOR MICROSTRUCTURES

The electronics industry now requires light-emitting and detection devices and ultra-high-speed structures that cannot be fabricated from silicon. Compound semiconductors including III-V binaries and alloys, such as GaAs and AlGaAs, and II-VI materials, such as CdTe and HgCdTe, are employed to complement the functions of the Si circuitry. In addition, special and unique electronic and structural properties can be obtained using artificially structured materials, such as quantum wells and superlattices. Efficient exploitation of these novel materials and structures in the production of useful electronic devices requires detailed studies to understand the fundamental physics involved as well as the characterization of possible device structures.

Scientists and engineers at NIST currently are involved in producing and characterizing III-V binary and alloy materials and device structures using optical techniques such as ellipsometry, photoreflectance, Raman scattering, and photoluminescence; variable temperature and variable magnetic field Hall-effect measurements; resistivity measurements; capacitance-voltage profiling; deep-level transient spectroscopy; photoconductivity and X-ray diffraction; and rocking curve studies with conventional and synchrotron radiation sources.

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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 that 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 high-energy electron diffraction (RHEED). Studies are under way to correlate RHEED oscillation intensity measurements with material quality and growth parameters. The MBE program is an inter-

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SEMICONDUCTOR SPECTROSCOPY

Spectroscopic studies in the visible and near visible regions of the electromagnetic spectrum are invaluable in investigating both materials- and device-related properties. The ability to couple to electronic states of interest in device applications and their non-destructive nature make spectroscopic analyses attractive research and analytical tools. Studies currently under way at NIST focus on the electronic and structural behavior of semiconductor materials, such as Si, GaAs, and HgCdTe; microstructures, including quantum wells and superlattices; and photonic and electronic devices. Excellent spectroscopic facilities are available to perform high-resolution photoluminescence, Raman scattering, reflection, absorption, spectroscopic ellipsometry, and modulation spectroscopic measurements, such as electroreflectance and photorelectance. The equipment used includes one of the highest

resolution ellipsometers in the world, excitation lasers, spectrometers, cryostats, and associated optical and electronic instruments.

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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 that 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.

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POWER SEMICONDUCTOR ELECTRONICS

Power electronics is an enabling infrastructure technology that significantly enhances capabilities across a wide range of industrial sectors, including manufacturing, transportation, consumer electronics, defense, and information systems. NIST researchers are working on semiconductor device problems as they relate to the design and reliability of power electronic systems. For instance, electrothermal power device models are being developed and verified for use in power system simulators. Included is the novel concept of physics-based, compact thermal models for device packages and heat sinks for inclusion in the simulators. Verified parameter extraction procedures are an important part of the effort. The results of this task will lead to improved circuit and system design capability for systems such as electric vehicles and large and small motor drives. Another task is development of characterization methods for the thermal properties and limits of safe operation of devices such as the IGBT, power ICs, and power-circuit modules. Laboratory capabilities include extensive electrical and thermal characterization facilities, infrared microradiometry, and a unique non-destructive test system. Successful completion of this work should lead to more reliable power devices and to improved measurement methods in general.

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SEMICONDUCTOR THIN-FILM METROLOGY

The electrical, optical, and mechanical properties of thin films are important in many phases of semiconductor manufacturing and in device and circuit operation. NIST researchers are developing procedures for measuring these properties and devising artifacts for instrument calibration. Currently, staff members are improving ellipsometric measurements of thickness for thin films on semiconductors, specifically SiO₂ on Si. Other films of interest include nitrides, thick oxides, layered structures important in silicon circuit manufacturing, and photoresist. For quality control and technology transfer, it is essential that all steps of the IC production process be absolutely calibrated. NIST provides artifacts traceable to national standards of length that industry uses to calibrate its equipment and processes.

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ADVANCED INTEGRATED-CIRCUIT TEST STRUCTURE METROLOGY

Integrated-circuit (IC) test structures and test methods developed by NIST are used widely by the semiconductor industry and other government agencies. These devices can be used to characterize IC manufacturing processes, to evaluate the effectiveness of semiconductor processing equipment, to obtain crucial parameters for process or circuit simulators, to perform product acceptance tests, and to determine the reliability of the products manufactured. NIST work involves test structure design, modeling,

data acquisition, and data analysis. Institute engineers are investigating pattern recognition techniques for the rapid diagnosis of IC manufacturing processes. They also are developing new structures for nanometer-level metrology and for establishing methods to determine the reliability of thin films used in state-of-the-art microcircuits.

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INTEGRATED MEASUREMENT SYSTEMS

Microelectromechanical systems (MEMS) incorporate new sensors and actuators in integrated-circuit (IC) technology for low-cost and portable precision measurement applications. Areas of interest include standardization, environmental monitoring, and control in biomedical, military, and space applications. Systems aspects address the development of new circuits for control, communication, self-test, and self-calibration of complex micromechanical-based systems. Standards aspects address the need for test structures and methods for evaluation and reliability of micro-mechanical-based devices. Custom and commercial foundry-compatible techniques are developed and utilized for device fabrication, and computer-aided design methods and standard design libraries are developed for rapid commercialization and technology transfer.

This new MEMS fabrication methodology is used to produce integrated microsensor systems that can be used to monitor and control IC processing. An increasing demand is placed on microelectronic devices to be more reliable, especially as their size decreases and the density of these devices increases on an IC chip. Reliability characterization based on post-manufacture stress tests and burn-in cycles becomes extremely undesirable in terms of test time and cost for these advanced ICs. A new approach for reliability characterization is to monitor and control the process parameters that affect the reliability of the device. Currently, NIST is developing an integrated microsensor system for the in-situ monitoring of a sputter metallization process. This system will provide real-time measurements of metallization resistivity and substrate temperature that can be used as feedback to control the process. Other microsensor structures for measuring gas composition also are being developed.

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BUILDING-IN RELIABILITY

Advances in microelectronic circuit density, complexity, and reliability, as well as greater demands for ever shorter times to develop and market new products, are forcing the U.S. semiconductor industry to use a new approach to reliability. The traditional, reactive approach of using screen and accelerated-stress tests is becoming increasingly impractical to assure the reliability of microelectronic products because too many parts and too much time will soon be required.

NIST is working with the semiconductor industry to implement the new "Building-In Reliability Approach," which emphasizes understanding and controlling the causes for reduced reliability. A pilot project is under way to demonstrate how this new approach can be used to identify and control key input process parameters affecting product reliability. The process being investigated is one for depositing the thin-film metal used to make electrical interconnects in microelectronic circuits. The microelectromechanical systems (MEMS) fabrication methodology is being used to develop an integrated microsensor system for in-situ monitoring of the thin-film metal sputtering process used widely in the industry. The system is being designed to provide real-time measurements of metal film resistivity and substrate temperature that can be used as feedback to control and to identify key input parameters of the sputtering process.

NIST has begun this project in response to industry-identified needs for guidance and for "success stories" that can be used to develop and implement this approach expeditiously.

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ELECTROMAGNETIC FIELDS

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ADVANCED MICROWAVE/MILLIMETER-WAVE METROLOGY

Rapidly developing microwave technology requires the support of advanced measurements and standards. The microwave industry and the Department of Defense rely on NIST for calibrations of transfer standards to provide accurate, traceable measurements required for product development, performance evaluation, quality assurance, and commercial interchangeability.

For measurements of attenuation as well as impedance and scattering parameters, NIST researchers have developed automated and highly accurate techniques using six-port network analyzers. Accurate techniques for microwave power measurement using primary microcalorimeters and transfer standards, as well as noise measurement based on the evaluation of standard noise sources, have been developed. Calibration services based upon these methods form a critical element in the nation's microwave electronics infrastructure.

To support the latest technologies, measurement capabilities are currently being enhanced. Power and impedance standards are being greatly improved. Advanced wide-band six-port automatic network analyzers and techniques for measuring the noise figure of active devices are under development. Measurement services are being extended to cover millimeter waves as well as subminiature coaxial connectors.

The group also develops metrology for industrial use, particularly in microelectronics. NIST researchers support the monolithic microwave integrated circuit and high-speed microelectronics industries through research and the development of on-wafer metrology. This work is supported by fabrication facilities, which include the facility to manufacture coplanar and microstrip calibration standards. Industrial applications of the results are ensured by close collaboration with industry.

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ELECTROMAGNETIC CHARACTERIZATION OF MATERIALS

It is widely recognized that critical needs exist for accurate data on the electromagnetic properties of certain materials used extensively throughout the aerospace, microwave, electronics, and communications industries. The Electromagnetic Properties of Materials Program at NIST seeks to support industry by evaluating and improving measurement techniques, by providing well-characterized reference materials, by providing measurement services, and by organizing measurement intercomparisons. Current capabilities include room temperature measurements of complex permittivity and permeability for bulk materials in the spectral range, 100 kHz to 18 GHz, as well

high-precision cavity measurements of low-loss dielectrics near 10 GHz. NIST plans to extend measurement capabilities, for both bulk and thin-film materials, into the millimeter range with coverage at elevated and cryogenic temperatures. Adequate and more accurate materials characterization data will help industry obtain optimal component and system performance with greatly reduced costs for corrective redesign.

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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 refining 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 that are meaningful, technically practical, and reliable. These techniques could then

be incorporated into voluntary standards by both U.S. and international standards organizations.

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ANTENNA MEASUREMENTS

Researchers at NIST are developing reliable techniques and standards for measuring key performance parameters of antennas and components used with satellites, Earth terminals, radars, and communications systems. Near-field scanning is now used routinely to characterize microwave and millimeter-wave antennas. NIST researchers are focusing on developing and implementing techniques to correct for errors in the scan surfaces and applying all near-field techniques to higher frequencies. Software for the analysis of spherical near-field data recently has been rewritten and improved. Other research areas include spacecraft and phased-array antenna measurements, antenna diagnostics using near-field techniques, and antenna systems measurements using celestial radio sources.

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MAGNETICS

Magnetic materials have a great variety of uses, such as in magnetic recording and other computer-related applications, transformers, motors, sensors, and medical systems. The trend in magnetic recording is toward high information density and higher access speed, both of which are increasing rapidly. As information storage becomes more dense, smaller read/write heads are required. The materials properties for very small components change drastically from properties in the bulk. New measurement methods are required to determine these properties in very small specimens and on very small scales.

NIST researchers address these problems by developing methods to characterize magnetic materials such as ferromagnetic and magnetoresistive films, recording tapes and disks, ferromagnetic steels, very weakly magnetic alloys, amorphous ribbons, spin glasses, ferrites, and permanent magnets. Structures of interest include magnetic thin films, coupled magnetic layers and multilayers, and particulate composite materials. New, improved, and traditional techniques are used, including vibrating-sample, SQUID, and Hall-probe magnetometers, as well as alternating-field techniques such as ac susceptometry, B-H loops, and rf permeability. Novel imaging by magnetic force microscopy is used extensively. Attention is given to calibration accuracy, measurement

precision, and instrument development. The research has broad application, from magnetic technologies to basic understanding of materials properties.

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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 (HTS). Research programs at NIST involve measurement techniques for critical current, critical magnetic field, ac losses, magnetic hysteresis, and electron tunneling. Specialized experimental work is being performed to determine the effect of strain on the superconducting properties of low-temperature commercial conductors and HTS materials.

The correlation between deposition parameters of laser-ablated HTS thin films and the resulting morphology and quality of the films is studied. In 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 has been produced for use in calibrating critical-current measurement apparatus. A new reference material for large currents is being developed.

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OPTICAL ELECTRONICS

The accurate characterization of optical electronic devices is crucial to several industries, including lightwave communications, lasers, and optical fiber sensors. NIST staff are developing metrology to support lightwave communications in areas of optical fibers, sources, detectors, and integrated optic components. Measurement capabilities are aimed at evaluating components at the research and commercial level. Semiconductor materials are grown by chemical beam epitaxy, and fabrication facilities exist for integrated optics on glass and crystalline substrates. National standards have been established for evaluating laser power and energy meters; high-speed detectors are characterized by a number of time and frequency domain methods. Novel sensors based on optical fibers are being used to detect voltages, currents, and other physical quantities. Cooperative research with NIST in the above areas results in new measurement procedures, new technology, and calibration services. The nature of this NIST research is applied, so opportunities for commercialization are excellent.

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LOW-TEMPERATURE ELECTRONICS

Cryogenic, and especially superconducting, electronics provide remarkably high speed and sensitivity, coupled with exceptionally low-power dissipation. NIST uses the unequalled performance of low-temperature electronics to supply U.S. industry with standards and measurement capabilities ahead of state-of-the-art conventional, room-temperature technologies. NIST maintains a world-leading program through its complete facility for fabricating large-scale superconducting and normal metal integrated circuits. A similar capability has been developed for circuits of growing complexity made from high-temperature ceramic superconductors.

NIST research spans the range from very basic studies of ultra-small tunnel junctions to a superconducting series array voltage standard in operation at almost three dozen laboratories around the world. The work has established numerous world performance records over the years with such devices as analog-to-digital converters, samplers, electrometers, microwave and infrared detectors, lithographed antennas, and magnetic flux detectors using SQUIDS. NIST efforts support private industry through cooperative research and assistance with measurement techniques.

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RESEARCH FACILITIES

SEMICONDUCTOR PROCESSING RESEARCH LABORATORY

As integrated circuit (IC) sizes increase to more than 1 cm^2 and feature sizes within the circuits decrease to less than $1 \mu\text{m}$, critical demands are placed on the measurement capability required to control and monitor IC fabrication successfully. To meet the demand, NIST researchers are developing state-of-the-art measurement procedures for microelectronics manufacturing.

The semiconductor processing research laboratory provides a quality physical environment for a variety of research projects in semiconductor microelectronics as well as in other areas of physics, chemistry, and materials research. The laboratory facilities are used for projects addressing many areas of semiconductor materials and processes, including process control and metrology, materials characterization, and the use of integrated circuit materials and processes for novel applications.

The laboratory complex occupies about 72 square meters, approximately half of which is composed of clean rooms. Within the clean rooms, work areas are maintained at class 10 or better. The facility is designed so that the work areas can be modified easily to accommodate the frequent equipment and other changes required by research.

CAPABILITIES

The laboratory has a complete capability for IC fabrication. Principal processing and analytical equipment is listed below. The capabilities are expanded and improved continuously to meet the technological challenges.

- Diffusion, Oxidation, and Annealing. Six furnace tubes for up to 75-mm-diameter wafers and nine tubes for up to 100-mm-diameter wafers.
- Photolithography. Research mask aligner (proximity and contact) for wafers up to 100 mm in diameter and irregularly shaped samples and $10\times$ direct-step-on wafer system for 75-mm-diameter wafers. Photoresist spin coating and developing and related chemical processing, including oxygen plasma stripping.
- Film Deposition. Low-pressure chemical vapor deposition systems for depositing silicon nitride, polysilicon, and low-temperature silicon dioxide. Rf and dc vacuum sputtering of metals and dielectrics. Electron beam and hot filament vacuum evaporation of metals.
- Etching. Wet and dry etching processes. Reactive ion beam etcher capable of ion milling and chemical etching with gases such as freon, sulfur hexafluoride, oxygen, and chlorine.
- Ion Implantation. Multipurpose 200-KeV ion implanter.
- Analytical Measurements. Thin-film reflectometry and other thickness measurements, optical microscopy, and grooving and staining. Automated and manual probe stations for current-voltage measurements and capacitance measurements as a function of voltage, frequency, and time.

APPLICATIONS

Small quantities of specialized semiconductor test specimens, experimental samples, prototype devices, and processed materials can be produced. The processes and processing equipment can be monitored during operation to study the process chemistry and physics. The effects of variations in operating conditions and process gases and chemical purities can be investigated. Research is performed under well-controlled conditions.

A research-oriented facility, the laboratory is not designed to produce large-scale ICs or similar complex structures. Rather the laboratory emphasizes breadth and flexibility in order to support a wide variety of projects.

Currently, research projects address many aspects of microelectronic processing steps and materials as well as silicon micro-machining. Examples include: metal-oxide-semiconductor measurements; metal-semiconductor specific contact resistivity; uniformity of resistivity, ion-implanted dopant density, surface potential, and interface state density; characterization of deposited insulating films on silicon carbide; ionization and activation of ion-implanted species in semiconductors as a function of annealing temperature; electrical techniques for dopant profiling and leakage current measurements; and processing effects on silicon-on-insulator materials. A simple CMOS process has been established.

AVAILABILITY

Laboratory staff welcome collaborative research projects consistent with the research goals of the NIST semiconductor program. Work is performed in cooperation with the technical staff of the laboratory.

The most productive arrangements begin with development of a research plan with specific goals. The commitment of knowledgeable researchers to work closely with NIST staff and the provision of equipment and other needed resources are required. Because hazardous materials are present, laboratory staff must supervise all research activities.

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SUPERCONDUCTOR INTEGRATED-CIRCUIT FABRICATION LABORATORY

NIST maintains a complete fabrication laboratory for superconducting integrated circuits. Devices employing both low- and high-temperature superconductors are supported. Demonstrated capabilities include the fabrication of 20,000-junction Josephson 10-volt array standards, using niobium trilayer technology. Individual facilities include a digital pattern generator, a wafer stepper having submicrometer resolution, laboratory-scale electron-beam lithography apparatus, thin-film deposition and etching systems, and requisite accompanying processing tools. These facilities are available on a limited basis in support of collaborative research with NIST.

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HIGH-VOLTAGE MEASUREMENT FACILITY

NIST maintains a high-voltage measurement facility in which researchers develop and evaluate measurement techniques needed for the efficient, reliable transmission and distribution of electric power (including for defense purposes). Major programs now being pursued using this facility are the measurement of transient voltages and currents; the development of techniques to quantify pre-breakdown and breakdown phenomena in liquid and gaseous dielectrics; and the measurement of low-frequency electric and magnetic fields.

CAPABILITIES

With existing power sources, direct voltages of 300 kV, 60-Hz alternating voltages of 175 kV, and standard lightning impulses of 500 kV can be produced. Selected waveforms, such as microsecond duration trapezoidal waveforms up to 300 kV and gated 60-Hz waveforms up to 100 kV, are also available. Supporting equipment includes high-voltage standard capacitors rated at 200 kV; high-accuracy, current-comparator bridges for 60-Hz measurements; a precision dc divider rated at 200 kV; dividers to measure standard lightning impulses up to 1-MV peak; partial discharge measurement systems; high-speed cameras and supporting optical equipment (including an image-preserving optical delay); a computer-controlled system to measure the electric field in transformer oil; a gas-chromatograph/mass-spectrometer system; and a system to produce a known electric field and current density in air at atmospheric pressure.

Measurement systems are available to measure pulsed voltages and currents with characteristic times ranging from nanoseconds to milliseconds. These systems include Rogowski coils and capacitive probes as well as the necessary recording equipment to acquire and store digital records. These conventional measurement systems are supplemented by optical sensors and couplers.

APPLICATIONS

- Instrumentation and Component Evaluation. Impulse, ac, and dc dividers; electric and magnetic field meters; capacitors; transformers; lightning arresters; and ion counters.
- Dielectrics Research and Development. Chemical degradation studies; measurement of the fundamental processes of discharge initiation; onset and magnitude of partial discharges; space charge measurement; and streamer propagation studies.

AVAILABILITY

The high-voltage facility is used by NIST staff and by guest researchers from industry, universities, and other federal agencies. Use of the facilities must be scheduled in advance. Because of the complexity of the system, typical use of the facility is in the form of a collaborative investigation with NIST staff.

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TRANSISTOR SAFE OPERATION TEST SYSTEM

A unique test system that automatically determines the turn-off limits for bipolar transistors and MOS-gated devices (MOSFETs and IGBTs) is available to scientists, engineers, and technicians for characterizing devices at currents between 1 and 100 A and voltages from 60 to 2000 V. The system is non-destructive for all bipolar devices and often non-destructive for MOS-gated devices. The system works by turning on the device (either with a gate voltage or current) into an inductive load and then turning off the device by reversing the gate current or voltage. The drain or collector voltage rises rapidly as the current attempts to decrease because of the inductive load. The predominant failure mode in this application is a rapid collapse of the voltage and associated current construction, which usually causes device failure due to melting. The system senses the voltage collapse and removes all of the current from the device in less than 50 ns, thus preventing destruction in bipolars and either preventing or reducing damage in MOS-gated devices. The system is under the control of a computer via an IEEE 488 interface. Tests can be set up and run automatically;

non-destructive tests, an entire area of operation using a single device can be and in a few minutes.

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HIGH-ACCURACY ELLIPSOMETER

Ellipsometry is an important non-destructive optical technique used throughout the semiconductor industry in determining critical thicknesses and uniformities of a variety of semiconductor materials. The high-accuracy, single-wavelength ellipsometer at NIST has been used primarily in the certification of Standard Reference Materials (SRMs) in the 2530 series. These SRMs are certified for measured ellipsometric parameters Δ and Ψ , as well as the derived thickness and refractive index of a range of silicon-dioxide layer thicknesses on a silicon substrate. This unique instrument is capable of making measurements at a multiplicity of incident angles with an accuracy of position to within $\pm 0.004^\circ$. Current projects utilizing this capability include the continuing certification of these SRMs as well as a variety of projects that observe the effect of various growth techniques of silicon dioxide on silicon, different preparations of the silicon substrate prior to oxidation, alternative methods of treating the silicon-dioxide surface prior to measurement, and long-term effects on the quality of the oxides. Extension of these efforts as they pertain to other semiconductor systems is planned. NIST welcomes the oppor-

tunity to collaborate on projects related to the current studies and to provide a measurement capability that is truly unique.

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NEAR-FIELD SCANNING FACILITY FOR ANTENNA MEASUREMENTS

This automated facility is designed to measure the near-zone phase and amplitude distributions of the fields radiated from an antenna under test. Mathematical transformations are used to calculate the desired antenna characteristics.

CAPABILITIES

Near-field data can be obtained over planar, cylindrical, and spherical surfaces; the planar technique is the most popular. Efficient computer programs are available for processing the large quantities of data required.

When operated in the planar mode, the facility is capable of measuring over a 4.5-m \times 4.5-m area with probe position errors of less than ± 0.01 cm. Improved position accuracy is possible with further alignment, especially over smaller areas. Antennas with apertures up to about 3 m in diameter can be measured with a single scan. The facility has been used successfully over the frequency range 750 MHz to 75 GHz. It incorporates provisions for scanning larger antennas in segments.

APPLICATIONS

- **Antenna Characteristics.** The facility is used primarily for determining the gain, pattern, and polarization of antennas. Accuracies are typically ± 0.15 dB for absolute gain and ± 0.10 dB/dB for polarization axial ratio. Patterns can be obtained down

to the -50 dB to -60 dB levels with side lobe accuracy typically about ± 1.0 dB at the 40 dB level. (The exact uncertainties depend on the frequency, type, size of antenna, and other factors.) Near-field data also can be used to compute near-field interactions (such as mutual coupling) of antennas and radiated field distributions in the near zone.

- **Antenna Diagnostics.** Near-field scanning is also a valuable tool for identifying problems and for achieving optimal performance of various types of antenna systems. It has been used to advantage in locating faulty elements in phased-array antennas and for adjusting feed systems to obtain the proper illumination function at the main reflector. Phase contour plots of the near-field data also can be used to determine surface imperfections in reflectors used for antennas or compact ranges.

- **Probe Calibrations.** A spherical probe calibration facility serves as a far-field range for measuring the receiving characteristics of probes used to obtain near-field data. These measurements are required to determine the probe coefficients, which, in turn, are used to calculate accurate, probe-corrected, far-field gain and pattern characteristics of an antenna.

AVAILABILITY

Two kinds of arrangements can be made to use this facility. NIST staff can perform specified tests or measurements on a reimbursable basis. In this case, the customer has no direct use of the facility; all measurements are performed by NIST staff and the customer is issued a test report. As an alternative, work may be performed on a cooperative basis with NIST staff. This arrangement permits the user the advantage of developing firsthand knowledge of the measurement processes, and the user is responsible in large part for the accuracy of test results. In either case, arrangements

need to be made well in advance, and reimbursement is required for the facility use and time of NIST staff involved.

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GROUND SCREEN ANTENNA RANGE

The ground screen antenna range is an open area test site.

CAPABILITIES

The ground screen consists of 6.35-mm mesh galvanized hardware cloth stretched over a level concrete slab. The screen is 30.5 m wide \times 61 m long and is spring loaded around the perimeter to ensure uniform tension, a flat surface, and adequate compensation for thermal expansion. The overall size of the ground screen permits far-field measurements in the high-frequency portion of the spectrum, and the mesh dimension provides for an efficient ground plane well into the ultrahigh frequency region.

APPLICATIONS

The range can be used for the following:

- antenna calibrations;
- antenna patterns at any polarization;
- electromagnetic susceptibility measurements;
- electromagnetic radiated emission measurements;
- calibration of field intensity meters; and
- wave propagation studies in frequency or time domains.

AVAILABILITY

This facility is used heavily in performing calibrations for industry and other government agencies. It is available for independent or collaborative work.

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MODE-STIRRED CHAMBERS

NIST researchers have designed and constructed mode-stirred (reverberating) chambers to measure radiated electromagnetic emissions, susceptibility of electronic equipment, and shielding effectiveness of materials and cable/connector assemblies. A mode-stirred chamber is an electrically large (in terms of wavelength), high-quality cavity whose boundary conditions are varied by means of a rotating conductive tuner or stirrer. The time-averaged field inside such a cavity, when a sufficient number of modes are excited, is formed by uniformly distributed plane waves coming from all directions. This causes the polarization of the field to vary randomly, hence eliminating the need for, or the utility of, physical rotation of test objects in the field. A microwave oven is a simple example of a mode-stirred chamber without measurement support instrumentation.

CAPABILITIES

The mode-stirred chamber simulates near-field conditions for tests at frequencies from 200 MHz to 40 GHz. High-level test fields (up to 1000 V/m) can be generated efficiently over a large test volume in the chamber, or the chamber can be used to measure low-level radiated emissions (total radiated power down to -100 dBm) from equipment under test with minor instrumentation changes. Equipment as large as 1.5 m \times 2.0 m \times 3.0 m can be tested.

APPLICATIONS

In addition to performing radiated-emission or susceptibility measurements of electronic equipment, the mode-stirred chambers can measure the shielding effectiveness of gasketing, composites, and other materials used for radio-frequency shielding applications. The chambers also can be used to measure the shielding effectiveness of wiring harnesses and electrical cables, connectors, and assemblies.

LIMITATIONS

The usable lower frequency is limited by insufficient mode density, tuner effectiveness, and ability to excite uniformly all modes in the chamber. These factors are a function of both chamber geometry and size. Measurement uncertainties vary from ± 10 dB at 200 MHz decreasing to ± 4 dB from approximately 1.0 GHz to 18 GHz. Directional characteristics of an antenna or test equipment placed inside a mode-stirred chamber are lost, resulting in the need to estimate their free-space maximal gain as a function of frequency in order to correlate results obtained by open-field tests. However, tests can be performed cost effectively in a shielded environment, with sufficient accuracy to make these facilities very attractive for diagnostic testing and for minimizing the need for expensive testing in facilities such as anechoic chambers.

AVAILABILITY

Two mode-stirred chambers are available: one that is 2.74 m \times 3.05 m \times 4.57 m and smaller version, 1.16 m \times 1.425 m \times 1.47 m. NIST staff are available for collaborative programs or to advise and interpret measurement results. Independent testing also can be arranged.

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TRANSVERSE ELECTROMAGNETIC CELLS

NIST researchers have designed and constructed several transverse electromagnetic (TEM) cells that are available for use. A TEM cell is a device for performing radiated electromagnetic emission and susceptibility measurements of electronic equipment. Its design is based on the concept of an expanded transmission line operated in a TEM mode. The cell is a two-conductor system with the region between the inner and outer conductors used as the test zone. The tapered sections at both ends are required to match the cell to standard 50 Ω coaxial cable connectors.

CAPABILITIES

The cell provides a shielded environment for testing without introducing multiple reflections experienced with the conventional shielded enclosure. It simulates very closely planar far field in free space and has constant amplitude and linear phase characteristics. The external electromagnetic signals will not affect the measurement of low-level radiated emission from the device under test. The high-level test field generated inside a cell for radiated susceptibility tests will not interfere with external electronic systems.

APPLICATIONS

In addition to radiated electromagnetic compatibility/interference testing, other applications of the TEM cells include the calibration of antennas and the study of biological effects of radio-frequency radiation.

LIMITATIONS

The usable frequency range is limited by an upper bound determined by the appearance of the lowest high-order mode. The volume available for testing purposes is inversely proportional to this upper frequency limit. The size of the device to be placed inside a TEM cell for testing should be small relative to the available test volume in order that the field structure associated with the ideal TEM mode existing in an empty cell not be significantly perturbed.

AVAILABILITY

Several TEM cells with five different sizes and five upper frequency limits in the 100 MHz to 1 GHz range are available. In collaborative programs, NIST staff are available to advise and interpret measurement results. Independent testing also can be arranged.

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ELECTROMAGNETIC ANECHOIC CHAMBER

The electromagnetic (EM) anechoic chamber at NIST is a facility for generating standard, well-characterized electromagnetic fields. Such fields are fundamental to the research, development, and evaluation of antennas, field probes, and EM material properties.

CAPABILITIES

EM fields up to 100 V/m can be established in the chamber over the broad frequency range from 200 MHz to 40 GHz, and up to 200 V/m for certain frequency bands above 1 GHz. A majority of the individual systems composing the measurement system are under computer control, thus enhancing statistical control of the measurements. The chamber dimensions are 8.5 m \times 6.7 m \times 4.9 m.

APPLICATIONS

The EM chamber is used in areas such as:

- research, development, and evaluation of new EM-field-generation and measurement methods;
- antenna and field-probe development and evaluation;
- calibration of field measurement instruments;
- susceptibility testing of electronic equipment;
- shielding effectiveness and material parameter studies; and
- special tests for government agencies, industry, and universities.

AVAILABILITY

This facility is used heavily in performing calibrations for industry and other government agencies. It is available for independent or collaborative work with NIST.

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MANUFACTURING ENGINEERING LABORATORY

NIST engineers and scientists are developing many of the tools for automated intelligent-processing systems that will soon be the core of all world-class manufacturing operations. These components include intelligent machines; advanced sensors for real-time in-process measurements; software for precision control of machine tools; and information technology for integrating all elements of a product's life cycle, from planning and design through marketing and customer support.

The Manufacturing Engineering Laboratory provides technical support for industry groups that develop standards for measurements, measurement techniques, hardware, software, and data interfaces. It operates the Automated Manufacturing Research Facility, a unique national resource for studying a wide range of manufacturing topics. Laboratory researchers also work at the forefront of the emerging field of nanofabrication, developing measurement tools for the atomic-scale production technologies of the future.

Laboratory staff members work closely with their industry counterparts, from the planning of research projects to the dissemination of results.

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COOPERATIVE RESEARCH OPPORTUNITIES

Precision Engineering

- 38 Atomic-Scale Measuring Machine
- 39 Advanced Optical Systems
- 39 Measuring Patterned Layers on Integrated Circuits
- 39 Measuring Surface Roughness

Automated Production Technology

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- 40 Machine-Tool Performance Evaluation and Accuracy Enhancement
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- 41 Intelligent Machine Controls
- 41 Sensory Processing and World Modeling for Intelligent Control
- 41 Off-Line Programming of Robotic Systems
- 41 Robot Metrology
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- 45 Automated Manufacturing Research Facility
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COOPERATIVE RESEARCH OPPORTUNITIES

PRECISION ENGINEERING

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ATOMIC-SCALE MEASURING MACHINE

By the year 2001, uncertainty requirements for dimensional metrology of step heights, surface roughness, linewidth, and line spacing for the integrated circuit and optics industries will be 0.1 nm to 1 nm. Furthermore, these uncertainties need to be held over areas ranging from several square millimeters to fractions of a square meter. To address these needs, NIST is building the molecular measuring machine (M^3). M^3 will be capable of positioning and measuring to atomic-scale accuracies over an area of 25 cm². It incorporates a scanning tunneling microscope into a unique system design that includes a very stiff core structure, carriages for moving the probe over the sample, interferometry for measuring probe and sample position, and two stages of isolation from seismic and acoustic perturbations. Construction and testing are under way.

After construction is completed, M^3 will serve as an independent means for characterizing distances, geometries, and distortions of highly ordered arrangements of atoms on single-crystal surfaces. M^3 also will serve as an exploratory tool for building mechanical and electrical structures in the nanometer-size range. Among the organizations collaborating on the construction of M^3 are several major universities and

ational laboratories as well as Watson
research Center, AT&T Bell Laboratories,
and Zygo Corp.

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ADVANCED OPTICAL SYSTEMS

Advanced optical systems increasingly are
designed around high-accuracy, aspheric
optical elements. Measuring the figure error
of generalized aspheres to the required accu-
racy is a complex and unsolved problem.
NIST is embarking on a program to charac-
terize the systematic errors of commercial,
phase-measuring interferometers used for
surface figure metrology and to develop
techniques to use these instruments for
aspheric metrology. The goal of the pro-
gram is to close the gap between the resolu-
tion and the accuracy of phase-measuring
interferometers. NIST researchers are work-
ing with personnel at Wyko Corp. and Zygo
Corp., which manufacture these inter-
ferometry systems.

NIST researchers already have demonstrated
significant sensitivity to fringe density of
the measured figure error for several com-
mercial phase-measuring interferometer sys-
tems. They are working to build a dedicated
test facility for future systematic investiga-
tions. The results of this work will make it
possible to manufacture lightweight, high-
performance optical systems for space-based
applications and multilayer mirror systems
for projection X-ray lithography.

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MEASURING PATTERNED LAYERS ON INTEGRATED CIRCUITS

NIST researchers are developing techniques
for measuring the critical dimensions of
patterned layers on integrated circuits. The
work involves theoretical projects on the
formation of images in the optical and
scanning electron microscopes as well as
experimental and design projects on the
construction of new metrology instruments
for the calibration of standards. The project
was initiated about 15 years ago at the
request of the semiconductor industry.

The ever smaller dimensions on integrated
circuits have created a demand for new and
improved techniques of measurement and
their related standards, especially as feature
sizes approach and become smaller than the
wavelength of light used in conventional
optical metrology instruments. The dimen-
sions of present interest range from about
0.5 μm to 30 μm and will extend to smaller
dimensions in the future. A series of three
linewidth/pitch Standard Reference Mate-
rials for photomasks is presently in produc-
tion. Research is in progress to develop new
and improved standards for use in instru-
ments utilizing optical or scanning electron
microscopy.

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MEASURING SURFACE ROUGHNESS

The need for effective, on-line control of
surface texture is increasing. For example,
many U.S. automobile companies are begin-
ning to see superior coatings as a potential
competitive advantage over foreign competi-
tion. One of the keys to achieving this
advantage is better on-line surface measure-
ment methods. NIST is using contacting

and optical profiling techniques as well as
optical scattering to develop such methods
(which will be sensitive to the functionality
of the components). The researchers
already have used an experimental light-
scattering instrument and a long-range
scanning tunneling microscope to generate
accurate descriptions of light scattering
from rough metal parts and from glossy
paper. They currently are studying the
effects of using a light-scattering system to
inspect glossy paper during manufacturing.
The researchers plan to adapt this system
for other materials and manufacturing proc-
esses. They also intend to build a remotely
controlled profiling instrument. These
advances will provide a better under-
standing of the relationship between process
parameters and surface finish. NIST
researchers currently are working closely
with academia, the automotive and paint-
ing industries, and standards committees.

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AUTOMATED PRODUCTION TECHNOLOGY

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QUALITY IN AUTOMATION PROGRAM

This program is an effort to achieve higher
part accuracy from existing discrete-parts
manufacturing equipment. A four-layer,
closed-loop, control architecture has been
proposed. Three layers are being imple-
mented: real-time (RT), process-

intermittent (PI), and post-process (PP) control loops. The RT and PI loops implement algorithms to predict and/or measure machine- and process-related systematic errors and compensate for them via real-time tool path modification and NC program modification. The PP loop is used to verify the cutting process and to tune the other two control loops by detecting residual systematic errors measured on the finished parts, correlating these errors to the uncompensated machine- and process-related errors, and modifying the control parameters of the other loops accordingly.

Feature-based error-analysis techniques are being developed to identify the residual systematic errors of the system. NIST researchers are working with industry and academia to use DMIS-defined features in their analyses. They are developing tools for feature segmentation of part geometries to improve analyses of the manufacturing process. They also are developing a quality database using feature types and the errors measured on these features as key fields.

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MACHINE-TOOL PERFORMANCE EVALUATION AND ACCURACY ENHANCEMENT

Deterministic manufacturing is a concept based on the premise that most errors in manufacturing are repeatable, thus predictable. Errors that are predictable can be measured and corrected, thereby improving quality through better control of the existing manufacturing equipment. Machine tools are computer-controlled, multi-degree-of-freedom structures that have inherent quasistatic and thermally induced geometric errors. Complete characterization of

these errors is being investigated to evaluate and enhance performance under changing thermal conditions. This process is complicated and time consuming.

NIST researchers are working with industry and academia to optimize this process to make it feasible for even small manufacturers. NIST, industry, and academia worked together to develop the industry standard for machining center performance evaluation (ASME B5.54). Compensation of machine-tool errors is an area of continuing interest. Researchers are developing generic electronic hardware to implement error compensation without any intrusion into the existing machine-tool controllers. They also are working to speed up the on-machine part inspection by introducing fast probing and powerful data analysis capability at the machine-tool level.

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PRECISION PISTON TURNING

The Precision Piston Turning Project is a cooperative research effort between NIST, General Motors Corp., Ford Motor Co., and Giddings and Lewis, with funding through the National Center for Manufacturing Sciences. The primary objective is the transfer of NIST's expertise in machine tool enhancement and technology to U.S. industry. This goal currently is being achieved by researching and applying enhancement methods for a Giddings and Lewis Piston Turning Machine, model 3000.

This project is comprised of several activities. The first task was performed in 1992, when a research team from NIST traveled to Giddings and Lewis' Fraser, Mich., plant to analyze the design of a prototype of the 3000. Using infrared technology and contact temperature sensing devices, an investigation of the thermal behavior of the

machine tool was performed. Based on analysis of the data collected during this investigation, several design changes were recommended. These changes were implemented on the machine tool, which was sent to NIST for a more rigorous thermal analysis.

NIST is now performing a full geometric-thermal characterization of the machine, using laser interferometry and other advanced sensors. The characterization is performed by monitoring the error motions existing in the machine tool as it is brought to a variety of thermal states. The thermal states are quantified by the use of remote temperature sensing devices attached at various locations on the components and structure of the machine. The end result of this characterization is a geometric-thermal error map of the piston turning machine. This error map can then serve as the database for real-time error compensation.

Benchtop analysis of two key machine components is also under way. These components are the linear actuators, which control cutting tool position, and the spindles, which rotate the parts. In general, the pistons machined on this tool are elliptical in shape. The designs of the linear actuators and spindles are being analyzed, and their performance is being tested to identify further areas in which machine accuracy can be enhanced.

This project is expected to have several benefits for the U.S. automotive industry. The performance of this particular machine tool will be improved, yielding both higher productivity and better piston quality. Of additional benefit to industry will be the knowledge gained by the industrial partner in the project in the areas of thermal balance and thermal gradient control within the machine tool, error characterization, and error compensation.

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ROBOT SYSTEMS

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INTELLIGENT MACHINE CONTROLS

The concept of advanced real-time, sensory-based control of machines has been a goal of researchers and system developers for over a decade. However, the lack of a structured, theoretical approach for designing and developing such systems has limited severely the number and sophistication of applications seen in operation today. Based on years of research and development in real-time, sensory control of robots and manufacturing systems, NIST is conducting the research necessary to develop a standardized architecture for implementing intelligent machine control. This architecture has been adopted by such organizations as the National Aeronautics and Space Administration, the U.S. Army, and a number of corporations.

NIST's current research seeks to expand and document a formal mathematical theory for the control of intelligent machines and to verify these theories using testbeds involving both simulation and actual controller hardware. Advanced control concepts, involving planning, sensory processing, world modeling, and knowledge representation, are being investigated. Several independent development projects are under way to demonstrate implementations of these control principles on functioning machines. They involve automated manufacturing, robotic deburring, space robotics, construction,

remotely operated land vehicles, underground mining, and undersea vehicles.

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SENSORY PROCESSING AND WORLD MODELING FOR INTELLIGENT CONTROL

Intelligent control of machines requires a detailed knowledge of both the machine and its operating environment. Since these are both dynamic in nature, it is necessary to measure, analyze, and comprehend changes in real time to achieve intelligent, sensory-based control of machines. NIST has a number of projects focused on developing advanced sensory-processing and world modeling capabilities. Sensory-processing research includes work on specialized vision systems, real-time image processing, and sensor data fusion. Vision systems being investigated include non-uniform resolution, active scanning of the fovea over points of interest, and active control of multiple cameras.

Under investigation are image-processing techniques for obtaining dense range maps from image flow and from stereo images. World modeling research is concentrating on data structures that can represent both spatial and symbolic information about surfaces, objects, and regions of space. Methods are being developed for comparing world model and sensory data so that one could, for example, generate a map overlay that is registered with and tracks camera images in real time. Also being developed are Kalman filtering techniques for updating the world model based upon sensory data.

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OFF-LINE PROGRAMMING OF ROBOTIC SYSTEMS

Off-line programming (OLP) systems are used to generate robot programs without the use of the actual robot. OLP has two advantages over the traditional teaching-dependent programming method: It improves safety, and system downtime is reduced because the robot is not involved in developing and debugging programs. Unfortunately, most commercially available OLP systems rarely produce the final robot control programs.

Research at NIST has focused on the use of OLP to generate directly robot control programs to determine robot trajectories for part handling and deburring. Since the models of the robot and the workstation layout never exactly match the actual equipment, there can be significant errors between the OLP-generated robot positions and the actual points through which the robot will move. To compensate for this, NIST has developed several sensor-based approaches for automatically calibrating or registering the OLP model of the robot and workstation with the real systems. This permits automatic generation of reliable robot programs in a matter of seconds or minutes instead of the hours or days required for manual teaching.

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ROBOT METROLOGY

Characterizing the performance of a robotic system is important in understanding the limitations of the system and in optimizing its operation. Although several U.S. and international standards committees are working on measuring robot performance, no standard robot acceptance and characterization tests currently exist. Research is

ongoing at NIST to develop and validate standard test procedures for measuring robot performance. NIST has been working closely with the Robot Industries Association subcommittee on developing such tests.

Currently, a laser-tracking interferometer system, originally designed and developed by NIST and now available commercially, is used to make these measurements. This system provides very accurate position measurements of 1 to 2 parts in 100,000 and an angular accuracy of 1 to 2 seconds of arc. Also under development is a low-cost robot calibration system that consists of a series of string encoders mounted to a fixture. This system provides a relatively inexpensive robot calibration system with an accuracy of ± 0.127 cm. Currently, research is being conducted to characterize the performance of this system and to expand its capabilities from measurement of three degrees-of-freedom to a full six degrees-of-freedom.

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MOBILE ROBOTIC SYSTEMS

NIST has been conducting a joint research program with the U.S. Army on the development of a mobile robotics platform for military applications, and with the Department of Transportation (DOT) Intelligent Vehicle Highway Systems (IVHS) program on the development of a vision-based vehicle mobility control system for autonomous driving.

As part of the Department of Defense's (DOD's) Robotics Testbed Program, NIST is involved in specifying the basic control system architecture for the mobile vehicles that are to be used in tactical applications. This control system handles autonomous subsystem integration and communication

with the remote operator station. The goal of the program is to have a standard architecture that could be adopted by the military for all of its robotics applications, thereby significantly reducing integration costs and allowing subcomponents to be transferred between different robotics systems.

NIST's support of the DOT IVHS program includes applying technology developed under the DOD program to the needs of the private sector. The goal of the IVHS program is to increase highway safety and traffic flow, while reducing driver workload.

NIST has developed and demonstrated a vision-based approach for autonomous road following under the Advanced Vehicle Control Systems element of the IVHS program. Demonstrations of autonomous driving have been conducted on a test course at NIST; on a local Maryland highway; and on a closed-loop test track at the Montgomery County, Md., Police Training Academy. The current system uses the painted stripes on the road to steer the vehicle along the center of a lane. The vision processing cycles at 15 Hz and can drive the vehicle at 55 mph in bright sunlight, on cloudy days, in the rain, and at night. Future work will include the development of more robust and reliable approaches for extreme variations in outdoor conditions. Other research includes development of vision processing and control approaches for autonomous car following. This technology is of interest to both the Army and DOT. Convoying or platooning of vehicles is envisioned for future automated transportation systems.

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ROBOTIC DEBURRING OF MACHINED PARTS

Engineers at NIST are developing an automated system that produces precision chamfers on aircraft engine components fabricated from titanium and inconel. The chamfers, or beveled edges, must be placed on parts such as turbine engine blades and hubs to relieve potential areas of stress concentration and ease assembly. The system, called the advanced deburring and chamfering system (ADACS), consists of a six-axis electric robot fitted with an actuated chamfering tool. This tool is capable of high-speed force control within a small work area.

The approach is to use the industrial robot as a coarse positioning device, while relying on the actuators and force sensors of the tool to provide control of cutting force and stiffness at the part edges. The tool compensates for robot inaccuracies and other factors, such as part misalignment and large tolerances. The system has maintained chamfers of 38 μm on titanium while traversing corners, in spite of part positioning errors on the order of several millimeters. The ADACS builds on two techniques pioneered in the NIST Automated Manufacturing Research Facility: a technique to generate robot trajectories off-line from CA data, and a technique to integrate a variety of sensors into the robot-control system.

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ROBOTIC CRANE TECHNOLOGY

Shipbuilding, aircraft manufacturing, and building construction operations rely on cranes with a single cable for lifting heavy loads. The problem with this approach is that the load is free to rotate and swing with the slightest side force. NIST has designed

crane that provides a very stiff load platform that can be used to lift heavy loads or as a base for mounting a conventional industrial robot. The design consists of a triangular platform suspended from six wire cables. By adjusting the length of each cable from independently controlled winches, it is possible to position the platform accurately. As long as the cables remain in tension, this configuration provides a significant improvement in stiffness and positioning capability over conventional cranes. NIST is building several testbed systems to investigate the performance of this crane design.

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FACTORY AUTOMATION SYSTEMS

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PRODUCT DATA EXCHANGE STANDARDS FOR THE APPAREL INDUSTRY

Numerous vendors supply computer-aided apparel design and pattern-making equipment. Each vendor's equipment represents the design and pattern data in a unique or proprietary file structure, preventing the direct electronic exchange of data among different organizations. NIST is helping the apparel industry to develop standards for product data exchange. NIST researchers have developed a prototype computer program for translating apparel pattern data between different file storage formats. The program demonstrates the feasibility of using a single, standard, interchange for-

mat. The program implements an information model also developed at NIST.

The software was developed as part of an ongoing project at NIST to extend the emerging international Standard for the Exchange of Product Model Data to apparel applications. The work is partially sponsored by the Defense Logistics Agency and is being carried out in cooperation with the Computer Integrated Manufacturing Committee of the American Apparel Manufacturing Association. In the short term, the goal is to develop a neutral data format for exchanging two-dimensional pattern data between apparel CAD systems. In the longer term, researchers plan to develop an information model that can be used to encompass the entire apparel life cycle.

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INSPECTION AND TOLERANCES RESEARCH

To establish a unified framework of U.S. and international standards dealing with mechanical tolerance issues, NIST scientists are carrying out a program of research and technology development in inspection and tolerances. These activities are aimed at developing a common technical basis for tolerance standards. The efforts involve development of emerging standards on dimensional measurement methods, particularly regarding coordinate measuring machine (CMM) methods.

The standards of interest include standards for tolerance models, inspection performance, mathematics of tolerances, and statistical tolerance methods. Examples of critical emerging and draft standards are the Standard for the Exchange of Product Model Data, the Mathematical Definitions of Dimensions and Tolerances, and Performance Testing of Coordinate Measuring

Machine Software. The work also involves participation on standards committees, research on measurement methods, and interaction with other government agencies to assess and improve the performance of CMMs used in their laboratories and production facilities.

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NATIONAL PDES TESTBED

Product data is an integral part of the information shared across computer applications and organizations, i.e., it is a crucial part of any integration scheme. Currently, no commercial products exist that allow systems to share information in a standard way and, consequently, to be integrated. STEP (the Standard for the Exchange of Product Model Data), when implemented, will simplify this integration problem. NIST is developing the National PDES Testbed to provide technical leadership and a testing-based foundation for the rapid and complete development of STEP. (PDES stands for "Product Data Exchange using STEP.") Major objectives of the testbed project include: the identification of computer software applications that will use STEP, the specification of technical requirements for these applications, the evaluation of the proposed STEP standard with respect to application requirements, the design and implementation of prototype STEP applications, the establishment of configuration management for STEP specifications and certain supporting software, and improved interactions between organizations working to develop STEP.

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RAPID RESPONSE MANUFACTURING INTRAMURAL PROJECT

The NIST Rapid Response Manufacturing (RRM) Project is sponsored as an intramural project through the NIST Advanced Technology Program office. The project is managed and executed through the Factory Automation Systems Division. The principal objective of the project is to establish collaborations with National Center for Manufacturing Sciences (NCMS) RRM consortium members and to leverage NIST skills and technologies to ensure the advancement of RRM capabilities. The project builds expertise and increases awareness of engineering and manufacturing technologies being applied to improve the process of rapid response manufacturing. The RRM consortium intends to enhance and adopt key technologies, including variant design, rapid prototyping, design visualization, and generative NC to enable use of advanced, highly integrated systems for manufacturing.

The three primary focus areas of the RRM Intramural Project include research and development, RRM testbed laboratory, and technology transfer.

R&D efforts will increase the knowledge and skills of NCMS RRM consortium members and NIST personnel through assessments of the current state of the practice and state of the art in key technologies. The R&D program supports and accelerates development of the engineering and manufacturing technologies required by the NCMS RRM consortium. The NIST RRM testbed laboratory will be established as a neutral facility where NCMS RRM and NIST collaborators can investigate interoperability between systems, experiment with the use of standards, and perform exploratory system integration studies. The NIST RRM testbed will emulate the system architecture proposed for the NCMS RRM integrated-engineering environment. This laboratory will allow collaborators to

identify issues with technology and standards applied to RRM applications and to address information technology barriers to RRM. Technology transfer activities are an important part of NIST's mission and will also play a significant role in this project. Several project activities are included in this focus area, including cooperative research and development, industry workshops, NCMS RRM committee participation, and consultation with other NIST research projects.

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DESIGN RESEARCH LABORATORY

As automated design becomes more and more prevalent, researchers are, of necessity, becoming more interested in the "process" of design. Furthermore, the emphasis on concurrent engineering is making this an iterative and integrated process, rather than a one-shot, stand-alone process. Several research questions remain. Can software tools be developed to create and maintain candidate designs in digital form? Can data structures for representing and updating the knowledge contained in these designs be developed? Can formats for exchanging that knowledge across manufacturing functions be devised? To address these and other interesting questions, NIST is building an engineering design laboratory equipped with state-of-the-art computers and software.

NIST researchers are investigating the issues involved in integrating a variety of commercial and university "design" tools. They also have begun a project aimed at capturing and representing "design knowledge and intent" in a manner compatible with the emerging Standard for the Exchange of Product Model Data. The work currently is focused on rigid mechanical parts, includ-

ing assemblies. NIST researchers are working with several major universities through the Defense Department's Advanced Research Projects Agency.

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COMPUTER-AIDED MANUFACTURING SYSTEM ENGINEERING

Just as computer-aided design and engineering tools have revolutionized product design during the past decade, computer-based tools for production system engineering can revolutionize manufacturing. A new type of computer-aided engineering environment is envisioned, which will improve the productivity of manufacturing/industrial engineers. This environment would be used by engineers to design and implement future manufacturing systems and subsystems.

The overall goal of computer-aided manufacturing system engineering is to lower manufacturing costs, reduce delivery times, and improve product quality through the coordinated development and use of advanced tools. The project is aimed at advancing the development of software environments and tools for the design and engineering of manufacturing systems. NIST researchers are placing an emphasis on providing an integrated framework, operating environment, common databases, and interface standards for a wide variety of emerging tools and techniques for designing, modeling, simulating, and evaluating the performance of manufacturing processes, equipment, and enterprises.

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RESEARCH FACILITIES

AUTOMATED MANUFACTURING RESEARCH FACILITY

The Automated Manufacturing Research Facility (AMRF) was established by NIST in 1982. The facility has been co-sponsored since 1983 by the Navy and serves as one of several Centers of Excellence supported by the Navy's Manufacturing Technology Program. NIST and other government agencies also co-fund research within the AMRF.

The objective of the AMRF is to develop automated manufacturing technologies that can improve the competitiveness of both the commercial and defense industrial bases. A key element of the AMRF is a research testbed, completed in 1986, producing technical results that are being transferred to the Navy and industry. Specific areas of research and development at the AMRF include advanced manufacturing systems, quality and inspection, integrated engineering tools, intelligent controls, sensor-based automation, and precision machining. These AMRF program activities have resulted in many technical accomplishments, collaborations, patents, standards, major awards, and, ultimately, commercial products.

The workstations of the AMRF are being used in active research programs by NIST researchers, industrial research associates, guest researchers, university personnel, and scientists and engineers from other government agencies.

CAPABILITIES

The facility currently supports research in machine tool technology, robot systems, metrology, motion control, sensors and sensory processing, accuracy enhancement, real-time control, computer-aided engineering tools, production scheduling and con-

trol, factory networks, process planning, and inspection technology. The facility is particularly suited for studying interfaces between production equipment and information systems.

AVAILABILITY

This facility has substantial potential for use by researchers from industry, academia, and other government agencies to pursue joint programs with NIST research personnel. Most successful work to date has involved close working relationships between NIST and a collaborator for periods of 6 months or more.

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ACOUSTIC ANECHOIC CHAMBER

This facility is used to perform acoustical measurements under free-field conditions, usually at moderate to very small sound pressures. These measurements include calibrating the free-field amplitude and phase responses of sound transducers, such as microphones and loudspeakers, and determining acoustic intensity in well-defined sound fields.

The facility is a vibration-isolated shell-within-shell structure. All interior surfaces of the inner shell are covered with a sound-absorptive treatment consisting of custom-designed, triple-density wedge modules. The chamber dimensions, measured wedge tip to wedge tip, are 6.7 m × 10 m × 6.7 m, defining a volume of 450 m³. A wire-mesh floor permits access to instrumentation within the chamber.

Accessories include signal, control, and power lines as well as instrumentation supports on all six interior surfaces. Air-

conditioning ducts are acoustically treated and vibration isolated. Temperature and humidity within the chamber are independently controlled by the heating, ventilating, and air-conditioning (HVAC) system.

CAPABILITIES

The chamber provides a highly anechoic sound field and a very small mechanical ambient noise level. The wedge modules are designed to absorb 99 percent or more of the normally incident sound energy at frequencies above 45 Hz. If increased acoustical isolation from the HVAC system and a uniform temperature within the chamber are required simultaneously, the air flow to the chamber interior can be turned off while controlled air flow continues between the inner and outer shells.

APPLICATIONS

The chamber is used to calibrate and to characterize acoustical instruments and their directionality under free-field conditions at moderate to very small sound pressures, to measure non-linear distortions, and to determine self-noise equivalent free-field sound pressures. The chamber is used for basic research aimed at developing methods for calibrating microphones of standard and non-standard geometries, for calibrating sound intensity probes and other transducer arrays and instruments, and for determining acoustic intensity.

AVAILABILITY

This facility has substantial potential for use by researchers in industry, universities, and other government agencies. Scheduling arrangements can be made for collaborative programs and individual research.

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CHEMICAL SCIENCE AND TECHNOLOGY LABORATORY

The Chemical Science and Technology Laboratory develops the calibration and measurement standards for a wide range of instruments and processes important to the chemical-manufacturing, energy, health-care, biotechnology, food-processing, and materials-processing industries.

It produces Standard Reference Materials and Standard Reference Data needed to achieve ever lower detection limits and to improve the quality, productivity, and efficiency of chemical measurements. The laboratory also is working with industry to increase efficiency, cut costs, and improve competitiveness through development of new sensor technologies, quantitative compositional mapping methods, analytical techniques, and novel processes. An important focus is the development of environmental technologies to monitor the environment and to minimize waste produced by manufacturing processes.

The laboratory maintains the national system of chemical measurement and coordinates the system with those of other nations.

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COOPERATIVE RESEARCH OPPORTUNITIES

Biotechnology

- 47 Protein Characterization by Two-Dimensional Electrophoresis
- 47 DNA Chemistry
- 47 Nuclear Magnetic Resonance
- 48 Bioprocess Engineering Measurements
- 48 Biomolecular Electronics
- 48 Biosensor Technology
- 49 Center for Advanced Research in Biotechnology

Chemical Kinetics and Thermodynamics

- 49 Chemical Thermodynamics
- 49 Chemical Kinetics

Inorganic Analytical Research

- 50 Atomic Spectroscopy
- 50 Analytical Mass Spectrometry
- 50 Electroanalytical Research
- 50 Activation Analysis

Organic Analytical Research

- 50 Capillary Electrophoresis
- 51 Bioanalytical Sensors
- 51 Supercritical Fluid Extraction
- 51 Laboratory Automation and Robotics for Organic Analysis
- 52 Supercritical Fluid Chromatography
- 52 Fundamental Chemical and Physical Processes in Chromatography
- 52 Trace Organic Analysis Using High-Resolution Chromatography
- 52 Methods and Standards for Drugs-of-Abuse Testing
- 53 Mass Spectrometry of Biomolecules
- 53 Trace Gas Measurement Techniques
- 53 Instability of Compressed Gas Mixtures

Process Measurements

- 54 Refrigeration
- 54 Flow Measurement Research and Standards
- 54 High-Temperature Reactors
- 55 Chemical Sensor Research
- 55 Chemistry of Supercritical Water Oxidation Processes
- 56 Chemistry of High-Temperature, Gas-Phase Materials Synthesis
- 56 Dynamic Pressure and Temperature Research
- 56 Chemical-Vapor Deposition Reaction Kinetics and Flow Modeling
- 56 Particulate and Droplet Diagnostics in Spray Flames
- 57 Temperature Sensor Research

Surface and Microanalysis Science

- 57 Microbeam Compositional Mapping
- 57 Atmospheric and Chemometric Research
- 58 Magnetic Engineering

Thermophysics

- 58 Properties of Fluids and Fluid Mixtures
- 59 Thermophysical and Supercritical Properties of Mixtures
- 59 Membranes Separation Technology
- 59 Modeling of Transport Phenomena with Moving Boundaries
- 60 Properties of Atmospherically Safe Refrigerants
- 60 Pressure Standards
- 60 Vacuum and Leak Standards

RESEARCH FACILITIES

- 61 Water Flow Measurement Facility
- 61 Fluid Metering Research Facility
- 61 Nitrogen Flow Measurement Facility
- 62 Neutron Depth-Profiling Facility

COOPERATIVE RESEARCH OPPORTUNITIES

BIOTECHNOLOGY

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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.

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 that will be used

to assess the abilities of existing and new electrophoretic techniques to separate and detect proteins.

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DNA CHEMISTRY

Working in several areas of DNA chemistry, NIST scientists are actively manipulating DNA to produce proteins, developing methods for measuring DNA damage at the molecular level, and developing methods for characterizing DNA, including profiling.

NIST scientists are developing experimental methods to measure DNA damage in mammalian cells exposed to free-radical-generating systems, such as ionizing radiation, elevated oxygen pressure, redox-cycling drugs, and a number of carcinogenic compounds. Free radicals produced in-vivo are thought to be mutagenic and carcinogenic. Measurement of DNA damage at the molecular level in mammalian cells is a prerequisite to understanding the chemical mechanisms of damage by free radicals. Techniques used for measuring DNA damage include gas chromatography, mass spectrometry, HPLC, and NMR spectroscopy.

NIST scientists are working on new methods for DNA profiling, ranging from developing well-characterized DNA fragment standards for restriction fragment length polymorphisms to performing research for rapid determination of DNA profiles by polymerase chain reaction amplification and automated detection of fragments. In addition, cooperative development of short-term repeat technology and attendant standards is sought. Techniques for DNA detection include sensitive staining of electrophoretic

gels, use of chemiluminescence, and enhanced methods for capillary electrophoresis.

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NUCLEAR MAGNETIC RESONANCE

Programs are under way in which NIST scientists are using nuclear magnetic resonance (NMR) spectroscopy to study simple peptides and proteins, aminoglycoside and macrocyclic antibiotics, carbohydrates, glycoproteins, and DNA. The studies are facilitated by research materials isotopically labeled with carbon-13 or nitrogen-15, which are prepared by synthetic or biosynthetic methods.

The researchers are making extensive use of two-dimensional NMR methods, including homonuclear and heteronuclear chemical shift correlation and J-resolved techniques, nuclear Overhauser measurements in the rotating frame, and indirect detection. Measurements of chemical shifts and coupling constants provide information on the structures, stereochemistry, and conformations of biomolecules. Determination of nuclear Overhauser effects and relaxation times allows the imposition of distance constraints for three-dimensional structure analysis and characterization of molecular dynamics, respectively.

In the future, researchers plan to use three- and four-dimensional NMR techniques to investigate higher molecular weight biomolecules. Detailed knowledge of the three-dimensional structures and conformations of the biomolecules is important to an increased understanding of biochemical reaction mechanisms, enzyme specificity, drug-protein/DNA binding, and molecular-recognition processes.

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BIOPROCESS ENGINEERING MEASUREMENTS

NIST scientists are actively involved in the development of theories, measurement methods, models, and databases for upstream and downstream bioprocessing.

To accurately measure cell parameters and product amounts during fermentation for bioreactors—upstream processing—researchers are making precision thermodynamic measurements and developing sensor technologies. Downstream processing research includes the development of fundamental transport data and experimental methods and models for separation of proteins and other biomolecules from complex mixtures. Among the methods under study are aqueous two-phase partitioning systems, chromatography, and electrophoresis technologies.

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 biotechnology. 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.

Light-scattering studies are being made on biomacromolecular solutions to characterize their transport and thermodynamic properties. Models and experimental methods, needed to obtain the necessary data, are being developed to characterize aqueous two-phase separation techniques. NIST scientists are using small-angle neutron scattering to characterize chromatographic media in concentrated polymer solutions.

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BIOMOLECULAR ELECTRONICS

Biological molecules have many properties that may allow them to act as substitutes for present-day electronic components. Studies are under way in laboratories around the world to develop molecular wires, gates, information storage devices, and even simple computers.

NIST scientists are studying the light sensitive protein bacteriorhodopsin (BR) as a potential repository of information. These studies require methods for immobilization of BR and characterization of its physical and chemical properties. In addition, NIST scientists are attempting to control the rate at which this molecule moves from one transition state to the next. In this manner it is believed that optical methods may be developed for the storage and retrieval of information using BR in the form of an "optical disk."

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BIOSENSOR TECHNOLOGY

Biosensors use a biocomponent for the rapid, sensitive, and specific determination of an organic or biological compound. These devices, which can be utilized for on-line measurements in real time, have potential for widespread use in biomedical, clinical, environmental, and industrial monitoring.

Basic problems associated with biosensor technologies must be overcome, however, to ensure successful commercialization. NIST scientists are examining the mechanisms of protein immobilization and stabilization on surfaces. Optical fiber techniques are being developed for making non-intrusive, rapid and selective measurements. Fluorescence techniques, as well as Raman and resonance Raman spectroscopy, are used to determine the characteristics of amino acids, small peptides, and small organic molecules as an aid to eventually providing improved sensor specificity and selectivity. Molecular diffusion, rotational mobility, complexation, and photochemical interaction also are being examined.

NIST scientists are developing amplification technologies, including liposome-encapsulated molecules, multiturnover enzyme reactions, and ion-exchange polymer-modified electrodes. Such methods and devices provide the potential for extremely sensitive devices.

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CENTER FOR ADVANCED RESEARCH IN BIOTECHNOLOGY

the Center for Advanced Research in Biotechnology (CARB) in Rockville, Md., recently established by NIST, the University of Maryland, and Montgomery County, Md., researchers study protein structure/function relationships. They are focusing on the measurement of protein structure by X-ray crystallography and nuclear magnetic resonance spectroscopy as well as 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 protein crystallography, NMR spectroscopy, molecular biology, and physical biochemistry. Its computer facilities include a variety of computational and high-resolution graphics workstations as well as access to the NIST Cyber 205 supercomputer.

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CHEMICAL KINETICS AND THERMODYNAMICS

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CHEMICAL THERMODYNAMICS

NIST researchers use precision oxygen-bomb and fluorine-bomb calorimeters to determine data on enthalpies of combustion, from which enthalpies of formation can be derived. The addition of a new low-temperature heat capacity calorimetry facility now gives the NIST thermodynamics laboratories the capacity to carry out the full range of measurements necessary to predict chemical equilibrium constants for systems of interest. The focus is on the determination of thermodynamic properties of materials of importance to modern technologies and of unique compounds that can be obtained only in small quantities, as well as on the certification of Standard Reference Materials. The Chemical Thermodynamics Data Center carries out expert evaluations of thermodynamic data on organic and inorganic compounds. Current interests include comprehensive evaluations of the thermodynamic data for species involved in the reactions related to the destruction of ozone in the upper atmosphere, and of data for organic compounds. The latter work has the long-range goal of producing reliable estimation schemes for predicting the properties of species for which measurements are not available.

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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, 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 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 data (including kinetic data and spectral data for analytical chemistry) as well as the design of databases and relevant software.

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ATOMIC SPECTROSCOPY

Atomic spectroscopy methods are probably the most widely used analytical techniques in industry today. Considerable research is required 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 the inductively coupled plasma as an atomic excitation source. Additional research concerns the use of uv-vis Fourier transform spectroscopy for optical line assignments of atomic transitions in commonly available atom sources. X-ray fluorescence is used for homogeneity testing and certification of a wide variety of metals, ceramics, and other materials.

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.

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ANALYTICAL MASS SPECTROMETRY

Analytical mass spectrometry has played a key role in industries, such as the semiconductor industry, that require accurate measurements of trace elements in raw materials, products, and product containers. The NIST inorganic mass spectrometry program is developing analytical capabilities for making highly accurate determinations of trace inorganics using stable isotope dilution.

Areas of research include developing instrumentation in thermal ionization, inductively coupled plasma ionization, and photoionization mass spectrometry, as well as devising methods for highly accurate measurement of absolute isotopic abundances. Methods are also developed for generating and characterizing pure reagents and for performing ultratrace chemical analyses.

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ELECTROANALYTICAL RESEARCH

Electroanalytical research is vital to the development of methods and materials for environmental and clinical determinations. A broad range of electroanalytical and chromatographic techniques, such as voltammetry, coulometry, and ion chromatography, are used by researchers at NIST for analysis and research. Research on standardization of pH and electrolytic conductance leads to the certification of new classes of Standard Reference Materials.

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ACTIVATION ANALYSIS

Nuclear methods of analysis provide unique approaches to quantitative analysis. In this research, methods of nuclear analysis are investigated utilizing the 20-megawatt NIST research reactor. All areas of the technique are researched, including the use of cold neutrons, the use of monitor activation, radiochemical separations, the use of focused neutrons, the development of prompt gamma-activation techniques, and neutron-depth profiling.

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CAPILLARY ELECTROPHORESIS

The exciting new technique of electrophoresis in small-diameter capillaries provides a tremendous opportunity for basic research into the fundamental properties and interactions of ions and neutral molecules. The association of analyte ions via simple electrostatic attraction, or more stable complexation, may be studied directly by the effect on the electrophoretic mobility of the ions. Hydrophobic interactions between neutral molecules and charged micellar surfactants can be investigated using micellar electrokinetic capillary electrophoresis (MECE).

through the use of electrolyte modifiers, such as urea and methanol, MECE can be extended to very non-polar molecules. Surfactants with more specific interactive character, such as aromaticity and chirality, need further exploration. Other "physical" modifications also promise to increase the applicability of capillary electrophoresis (CE). Soluble polymeric gels can be used to provide molecular weight discrimination for biomolecules, where differences in charge may be too small to allow direct CE separation.

Detection in CE is also a hot research area. The small sample size and capillary dimensions make sensitive detection difficult. Electrochemical detection in CE by the use of microelectrodes does not suffer from the dimensional liabilities normally associated with the use of small capillaries. Using knowledge gained from the recent exploration of oxidative detection via carbon fiber and platinum electrodes, researchers also could be able to carry out reductive detection at mercury film electrodes. Sensitive optical CE detection using axial absorbance, as well as laser-source thermal lens and fluorescence modes, is of current interest at NIST.

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BIOSENSORS

Biosensors are a new 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 sensing devices because of their binding specificity, the strength of their interactions, and their potential for

use in conjunction with a wide variety of amplification schemes. Immunological, enzymatic, and receptor-ligand interactions are being explored as the basis for analytical measurement.

NIST researchers are using a variety of optical techniques for detection. Detection can be based on changes in size and rotational mobility of analytes or binding agents upon interaction, or it can be the result of enzymatic activity that occurs due to analyte binding, causing enhanced fluorescence or absorbance signals. Amplification can be achieved with release to liposome-encapsulated molecules or multiturnover enzyme reactions. Combining high specificity for analytes with amplification provides the potential for extremely sensitive devices.

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SUPERCRITICAL FLUID EXTRACTION

NIST researchers are studying the basic mechanisms responsible for analyte release in supercritical fluid extraction (SFE) processes. They are designing experiments to determine the role of pressure, temperature, and extractant fluid composition on the equilibrium and kinetic processes of analyte release from both simple model and complex environmental matrices.

Research in this area also encompasses the practical application of analytical SFE to a wide variety of sample matrices; the modeling of the analyte-trapping process and concurrent design/optimization of trapping media; hardware and software development for automated extraction systems for on-line chromatographic analysis; investigations of intermediate analyte class separations based on solid-phase adsorbents, following the extraction; and the design of expert systems for the optimization of SFE

system performance. Analyte/matrix combinations being studied include polycyclic aromatic hydrocarbons and polychlorinated biphenyls in such matrices as sediments, soils, and air particulate matter; fat-soluble vitamins in foods and serum; and drugs of abuse in body fluids and hair.

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LABORATORY AUTOMATION AND ROBOTICS FOR ORGANIC ANALYSIS

NIST has joined with industry and other government agencies in a cooperative project to develop automated analytical devices for organic analysis based on new chemistries and apparatus, as well as on laboratory robotic systems. One project focuses on the development of an on-line system for extraction of solid samples (using supercritical fluids and volatile liquids) with deposition onto a short chromatographic column, followed by selective elution for conventional chromatographic analysis. Also, researchers are studying the use of a state-of-the-art laboratory robotic system for automated sample preparation of samples for clinical and environmental analysis.

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SUPERCRITICAL FLUID CHROMATOGRAPHY

Supercritical fluid chromatography (SFC) in both capillary and packed columns has been shown to offer several advantages when compared with liquid and gas chromatography for high-efficiency separations of non-volatile, reactive, or thermally labile molecules. NIST scientists are investigating the variables that influence retention, selectivity, recovery, and efficiency of SFC separations; the use of SFC as an analytical technique for providing high-efficiency separations and accurate quantitative analysis of complex mixtures; and the use of supercritical fluids for extraction of solid and liquid samples emphasizing on-line extraction and analysis of microsamples.

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FUNDAMENTAL CHEMICAL AND PHYSICAL PROCESSES IN CHROMATOGRAPHY

Solute retention in chromatographic systems is the result of a complex assortment of molecular interactions between the solute, the stationary phase, and the mobile phase. The diversity of these interactions can be used to optimize separations for different classes of compounds by varying separation parameters, such as stationary phase and/or mobile phase composition, and column temperature. An understanding of these fundamental retention mechanisms facilitates the optimization of separations in gas chromatography (GC), liquid chromatography (LC), and supercritical fluid chromatography (SFC).

Recent LC research has focused on the design of chemically bonded stationary phases (such as monomeric and polymeric C₁₈ phases and charge transfer phases), which offer unique capabilities for the separation of isomeric compounds and compound classes. Polycyclic aromatic hydrocarbons have been used as model solutes for investigating retention mechanisms. Since these compounds are highly isomeric, retention effects resulting from differences in solute shape can be isolated by studying isomer sets.

Molecular modeling of solutes and stationary phase species holds the potential to provide further insight into retention mechanisms. Similar approaches can be taken to characterize retention processes in GC and SFC. A comparison of the retention behavior for isomer sets in GC, LC, and SFC may prove useful in developing a unified understanding of chromatographic retention processes.

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TRACE ORGANIC ANALYSIS USING HIGH-RESOLUTION CHROMATOGRAPHY

NIST research in high-resolution chromatography is focused on the development of gas chromatography (GC) and liquid chromatography (LC) methods for the determination of individual organic compounds in complex mixtures. Research areas in GC include:

- development of systematic chromatographic approaches for sample preparation/cleanup and analyte preconcentration prior to GC analysis;
- development of multidimensional chromatographic procedures using stationary phases of differing selectivity;
- use of simultaneous multiple and/or selective detection systems (such as mass spectrometric, electron capture, and atomic emission detectors); and
- development of on-line extraction and analysis of solid microsamples.

Recent activities have emphasized the measurement of trace levels of environmentally significant compounds, including polychlorinated biphenyls and polycyclic aromatic hydrocarbons, in natural matrices such as sediment, tissue, and airborne particulate matter.

Using LC, researchers will focus on the following approaches to analyzing complex mixtures: solid-phase extraction on short columns as an isolation/cleanup/preconcentration step; development of multidimensional LC procedures to isolate and quantify selected compounds; selective detection systems (such as uv, fluorescence, electrochemical, mass spectrometric, chemical derivatization); and the development of microcolumn LC procedures.

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METHODS AND STANDARD FOR DRUGS-OF-ABUSE TESTING

To reduce the use of illegal drugs, particularly in work-related activities, many employers are now performing drug tests on

employees and prospective employees. Most of these tests involve analysis of urine samples for traces of drugs or metabolites.

Because tests used to screen urine samples for drugs are subject to cross-reactivity from other substances, it is strongly recommended, and in many cases mandated, that positives from the screening procedure be subjected to confirmatory analysis by gas chromatography/mass spectrometry (GC/MS). The GC/MS methods are used not only to confirm the presence of drugs but also to determine quantitatively if concentrations of the drugs are above specified cut-off levels. Laboratories performing these confirmatory analyses must ensure that their methods produce accurate results.

To support accuracy in drug testing, NIST scientists are developing a series of urine-based Standard Reference Materials with appropriate concentrations of drugs of abuse. Drug levels are certified by a combination of two independent methods, one of which is generally GC/MS. Research is going to develop alternate methods to complement GC/MS.

Considerable attention is now focused on an alternate matrix for drug testing. Human hair provides a long-term record of drug use, in contrast to urine, which provides a record of only the previous 48 hours to a few hours. NIST scientists are investigating analytical aspects of hair analysis for drug abuse. Research areas include the extraction of drugs from hair, measurement methods, the effects of hair treatments on drug levels, and differentiation between hair externally contaminated with drugs and hair with drug levels acquired through internal use.

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MASS SPECTROMETRY OF BIOMOLECULES

Major advances in mass spectrometry have improved its capabilities for characterizing biomolecules. Techniques such as fast-atom bombardment, electrospray, matrix-assisted laser desorption, and others permit the accurate determination of molecular weights of peptides and small proteins previously unmeasurable by mass spectrometry.

Molecular weights greater than 100k daltons are now being determined with accuracies far exceeding those of other techniques. Advances in structural determinations of biomolecules include the use of collision-induced dissociation and photodissociation for determining sequence information for peptides and oligonucleotides. Considerable attention now is focused on coupling these new mass spectrometric techniques with developments in capillary electrophoresis and microscale liquid chromatography.

Scientists at NIST are investigating these new techniques to understand their capabilities and apply them to biomolecule characterization. They are particularly interested in applying these techniques to the quantitative analysis of species not previously amenable to mass spectrometric analysis. These capabilities should result in the development of reference materials to support industries involved in biotechnology and biomedical research.

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TRACE GAS MEASUREMENT TECHNIQUES

Accurate measurement of gaseous species is of great importance to many industries for applications ranging from 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 because of 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.

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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 various 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.

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REFRIGERATION

Cooling superconducting electronics, magnetic devices, and highly sensitive infrared detectors require specialized refrigerators capable of reaching cryogenic temperatures. Other applications, such as satellite cooling or gas liquefaction, demand long-term reliability and maintenance-free operation. Advances in the 1980s led to widespread interest in many regenerative-cycle refrigeration systems for these applications, including the use of pulse-tube refrigerators. NIST is the world leader in pulse-tube refrigeration research and is developing

extensive engineering databases for these devices and other regenerator applications.

In pulse-tube studies, NIST scientists have developed the orifice pulse-tube refrigerator (OPTR), which has reached temperatures of 60 K in a single stage. Using thermoacoustic drivers (TADs) in place of mechanical compressors, an OPTR was designed with no moving parts. A patent, a Strategic Defense Initiative Office innovative technology award, and an R&D 100 award have been received for this device, called a TADOPTR. Recently, the TADOPTR was proposed for liquefaction of natural gas at remote well sites, where about 30 percent of the gas produced would be burned to run the TAD, providing cooling to liquefy the remaining 70 percent.

Substantial research efforts have been applied to the development of improved regenerators for refrigeration systems. NIST researchers have assembled the world's largest database for adsorption of low-temperature gases on carbon. NIST computer models of regenerator performance are the only optimization tools available to designers of regenerators.

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FLOW MEASUREMENT RESEARCH AND STANDARDS

The accelerating costs of scarce fluid resources and valuable fluid products—particularly petrochemical fluids—are causing increased concerns about the performance of flowmeters. 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 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 the evaluation, the appropriate range of calibration will be done on the developed standards so that performance can be assured at specific levels. Current fluid-metering research programs use laser Doppler velocimetry (LDV) techniques to focus on the flows 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.

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HIGH-TEMPERATURE REACTORS

Chemical and associated industries produce enormous amounts of byproducts. To avoid wasting industrial resources and polluting the environment, the impact of these byproducts must be minimized. The solutions are minimizing waste at the source; modifying industrial processes; recovering energy and chemicals for reuse; and converting pollutants to acceptable species. For all of these solutions, thermal treatments offer the most promising approach. Hence

There is an urgent need for detailed mechanistic elucidation of fundamental thermal processes, such as pyrolysis and oxidation, that govern chemical conversion and destruction of both model compounds and actual industrial byproducts.

NIST maintains two instrumented facilities that are exceptionally promising for efficient pyrolytic and oxidative destruction of a wide variety of chemical compounds: a fluidized bed reactor and a plug-flow reactor designed for long residence times (seconds) at elevated temperatures. The research centers on kinetic studies, both global and mechanistic, of destruction of model compounds representative of major industrial byproducts, the most prominent of which are chlorinated hydrocarbons and nitrogen-containing species (amines and nitrocompounds, for example). The scientists are investigating: 1) the effects of temperature, residence time, and composition of reactor fluids on both the destruction efficiency of the model compound and formation and disappearance of intermediate products; and 2) the effects of highly corrosive reactor environments on structural materials. Diagnostic instrumentation includes both on-line sampling with subsequent analysis by several analytical techniques (GC, MS, and FTIR) and in-situ analytical systems.

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CHEMICAL SENSOR RESEARCH

To understand the performance of thin-film sensors, NIST scientists are conducting research aimed at improving the sensitivity, selectivity, stability, and accuracy of their response, as well as developing concepts for new sensing and measurement techniques.

Research investigations focus on mechanisms governing surface adsorption and desorption processes, interfacial diffusion, adhesion mechanisms, and surface morphology as these relate to sensing in chemical, biochemical, and physical systems.

Analytical methods are used to relate the structure and composition of sensing devices to fabricating parameters and performance as well as to develop mechanistic performance models. Research areas include thin-film thermocouples and resistance devices, moisture and pH sensors, gas phase chemical sensing based on tin and other metal oxides, and self-assembled monolayer-based structures. Fabrication facilities available include magnetron sputter deposition of metals and metal oxides and gas reactors.

NIST scientists also are investigating the feasibility of thin-film systems as improved chemical sensors. Their research efforts employ an array of surface spectroscopic techniques to determine the electronic properties of thin-film and single-crystal specimens. Among the techniques used are X-ray and uv photoemission and thermal desorption spectroscopies, SIMS, and in-situ electrical measurements. Recent research activities have focused on the use of self-assembled organic monomolecular films as adhesion layers for future multilayer sensing structures for chemical and biochemical materials.

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CHEMISTRY OF SUPERCRITICAL WATER OXIDATION PROCESSES

Supercritical water oxidation (SCWO) is a new technology with high promise as a safe, efficient process for the minimization and destruction of hazardous materials. It is a totally contained process that takes place in water above its critical point, that is, at pressures greater than 22 MPa and temperatures above 374 °C. Under these conditions, many reactions proceed unusually rapidly, producing benign end-products carried in the output water stream. Industrial implementation of SCWO has lagged, in part because of an inability to prescribe the process variables, such as the temperature, pressure, flow rates, and concentration of oxidants, required for safe, efficient waste destruction. These, in turn, demand understanding of fundamental thermodynamic and kinetic processes in supercritical media.

NIST researchers are seeking to supply both the understanding and data necessary to support reliable process modeling for SCWO. The experimental work centers around reactors for studies of chemical kinetics and durability of materials, as well as a unique flow reactor, which provides optical access for in-situ measurements of density, chemical species, temperature, and product/reactant concentrations. The researchers currently are studying the ammonia destruction reactions as functions of temperature, pressure, and added oxidant.

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CHEMISTRY OF HIGH-TEMPERATURE, GAS-PHASE MATERIALS SYNTHESIS

The semiconductor, coatings, and ceramics industries require high-performance thin films, particles, and fibers. This demand for materials with micro-engineered mechanical, electrical, and optical properties has placed greater emphasis on the development of new processing methods and on the need for increased fundamental understanding of materials-fabrication processes.

NIST researchers are seeking an understanding of high-temperature materials synthesis in a fast-flow reactor that provides reaction temperatures in excess of 1500 K and residence times as short as 10 ms, allowing extension of conventional chemical kinetics to temperature regimes representative of the chemistry in materials processing. The reactor has provisions for molecular-beam sampling of gas-phase species, including clusters, with subsequent mass spectrometric analysis. It also is equipped with optical excitation and diagnostic probe beams.

Currently, NIST scientists are researching the homogeneous (gas-phase) and heterogeneous (thin-film and cluster/aerosol) chemistry of silicon oxide. They are comparing measurements of species and growth kinetics to the predictions of chemical reaction and fluid flow models developed for the process. This approach identifies rate, purity, or defect-limiting steps in the process.

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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 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 ns at accuracy levels of 5 percent appear feasible. Through the 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.

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CHEMICAL-VAPOR DEPOSITION REACTION KINETICS AND FLOW MODELING

Chemical-vapor deposition (CVD) is an important process used to grow thin films in the manufacture of microelectronics devices, as well as to produce high-performance coatings. CVD involves com-

plex gas-phase chemistry, surface chemistry, and mass and heat transport processes. These highly coupled processes control the quality, uniformity, and yield of the deposited layers. NIST researchers are developing and testing numerical models that can be used to design and control CVD processing reactors. These models account for gas-phase chemistry, particle formation, heat and mass transport, and surface deposition leading to the formation of thin films.

The modeling effort is coordinated with a measurement program to supply the required chemical kinetics and materials-growth information and to validate the modeling results in a materials-synthesis flow reactor. The measurement program includes optical and mass spectrometric diagnostics of the gas phase and post-production evaluation of particle and film growth.

An interactive, graphics-based chemical kinetics program has been developed. Researchers are constructing a supporting thermochemical and kinetics numerical database, and they are developing two-dimensional heat and mass transport models, which simulate reactor geometries relevant to practical devices.

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PARTICULATE AND DROPLET DIAGNOSTICS 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 effi-

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 non-intrusive 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 extinction measurements to determine the effect of fuel chemistry, particularly in the case of multicomponent fuels, on spray atomization, combustion efficiency, and formation of soot and gaseous pollutants.

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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, and resistance thermometers of various types. 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 industrial grade thermometers. NIST is planning a series of new materials and techniques to provide highly precise and accurate temperature measurements.

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SURFACE AND MICROANALYSIS SCIENCE

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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 truly 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 are 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, a laser Raman microprobe of NIST design, and extensive computer facilities, including image processing.

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ATMOSPHERIC AND CHEMOMETRIC RESEARCH

Current regional and global concerns with the impact of human activities on the environment, including environmental contamination and wastes, atmospheric pollution, and potential effects on health and climate make it imperative to determine with a high

degree of accuracy the individual sources of noxious species. State-of-the art research, pioneered at NIST, makes possible unique source identification by application of the most advanced microchemical and isotopic analytical techniques, including accelerator mass spectrometry and high-precision gas isotope ratio mass spectrometry.

Complementing advanced isotopic-chemical characterization of atmospheric gases and particles is basic research in chemometrics, which represents the synthesis of chemical knowledge and measurement with modern statistical and computational methods. Work in this area is directed toward improving the quality of chemical measurements generally through advanced design, measurement and data analysis quality assurance, and graphical multivariate data exploration.

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MAGNETIC ENGINEERING

Magnetic thin films play a key role in many information storage products, and improved performance of these products depends in large part on the ability to engineer improved manufacturing processes for these films. At present, a wide knowledge gap exists between the magnetic thin films produced with great precision and studied in great depth by the basic research community and the magnetic thin films manufactured by industry in the development of new commercial products.

NIST has designed and built a novel instrument which will bridge the gap between these communities. The instrument provides for magnetic thin films to be produced by industrial manufacturing methods and investigated by the most advanced techniques of the basic research community. The instrument is equipped for magnetic

thin-film deposition by the three basic methods: magnetron sputtering, electron beam evaporation, and molecular beam epitaxy. The composition and atomic microstructure of the films is studied by X-ray photoelectron and Auger electron spectroscopy, ion scattering spectroscopy, reflection high-energy electron diffraction, low-energy electron diffraction, sputter depth profiling, spectroscopic ellipsometry, and scanning tunneling microscopy. The magnetic properties of the films are studied in a superconducting magnet by a magnet-optical Kerr spectrometer and a 6-point contact magnetoresistance probe. A major advantage of this instrument is that all of these features are available in situ.

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PROPERTIES OF FLUIDS AND FLUID MIXTURES

The thermophysical properties of fluids and fluid mixtures are essential for process design and control in the chemical, natural gas, aerospace, environmental, and energy-related industries. The properties of fluids research program involves experimental and theoretical research and computer simulation studies on the thermodynamic and transport properties of pure fluids and fluid mixtures. A primary goal of this

program is to develop highly accurate predictive models for the thermophysical properties of fluids and fluid mixtures. This is accomplished through an integrated program of measurements, theory, and correlation. Key ingredients of this program include measurements of the thermodynamic and transport properties of pure fluids and mixtures. Apparatus are available for state-of-the-art measurements of pressure-volume-temperature relations, sound speeds, heat capacities, dielectric constants, viscosities, phase equilibria, and thermal conductivities over wide ranges of operating conditions. Included in this work are measurements in the critical and extended critical region. In concert with the experimental work, theoretical studies are directed toward the development of wide-range predictive models and computer code.

A wide variety of research, both experimental and theoretical, is directed toward the understanding of complex fluid behavior, the microscopic structure of fluids, and the liquid-solid phase boundary. Included are studies of non-Newtonian fluids, colloidal suspensions, shear-induced chemical reactions, supercooled fluids and melting phenomena, and macromolecules. A unique shearing cell is available for neutron scattering studies at the NIST reactor.

Molecular-level computer simulation has proved an essential technique for utilizing statistical mechanics-based models of condensed matter. Molecular dynamics studies, involving both equilibrium and non-equilibrium systems, have been conducted. Computer simulation studies are important in interpreting and understanding the results of experimental studies in fluids and in developing predictive models of fluid properties. Other theoretical studies include dynamic and static critical region models (emphasizing mixtures), extended corresponding states, equations of state, kinetic

theory of gases and dense fluids, theory of the glassy state, properties of mixtures of dissimilar compounds, phase transitions, and structure-based modeling.

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THERMOPHYSICAL AND SUPERCRITICAL PROPERTIES OF MIXTURES

Chemical process technology requires accurate knowledge of various thermophysical properties of pure, polyfunctional chemicals and their mixtures. NIST research focuses on the most important of these properties—equilibrium phase composition, density, vapor pressure, and enthalpy. NIST researchers are developing predictive methods for the properties of chemically dissimilar compounds, especially complex mixtures and aqueous solutions. Another project is aimed at developing accurate predictive models for the thermodynamic and transport properties of near critical and supercritical mixtures. This work includes T_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 super-

critical mixtures and theoretical studies to focus on applying extended corresponding states to supercritical systems.

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MEMBRANES SEPARATION TECHNOLOGY

Membranes are used increasingly in separation processes, novel synthesis processes, and as process sensors. To add to the science and engineering base of membrane technology, NIST scientists are working on methods of measuring and correlating structure/transport property relationships in phase-separated polymers such as ionomers. This methodology should also be applicable to interpenetrating polymer networks and polymer blends. The model applications include acid gas and water separation of water and organics from liquid and vapor streams (pervaporation processes). Recognizing the need to provide improved engineering models for design of integrated processes, NIST staff are developing test protocols, facilities, and process design models. Current models have been generated that improve the determination of mass transfer boundary layer effects in gas and liquid membrane contactors. The fouling of membranes in pressure-driven liquid processes is a critical process difficulty. Researchers are studying the fundamental steps of irreversible protein adsorption as a model

system. Recent results have led to the development of an approach for surface modification, which is still under study but has provided substantial improvements in early testing.

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MODELING OF TRANSPORT PHENOMENA WITH MOVING BOUNDARIES

As technology progresses, it is increasingly more difficult to create unifying theoretical descriptions of important processes and phenomena. Numerical software for simulating and analyzing fluid flow with associated heat- and mass-transfer is an increasingly important tool for understanding the complex physical environments that arise in engineering applications.

NIST has developed a highly flexible numerical library to model transport phenomena in a wide range of applications. This software has two key features: the capability to address problems with moving boundaries such as interfaces; and an object-oriented design allowing it to be efficiently tailored for a very wide range of applications. The software design optimizes the ability to add quickly code modules implementing new numerical algorithms to address our future needs. The net result is an evolving capability to address complex problems in detail. Sample applications include simulating chemical vapor deposition for the design and characterization of a commercial reactor and modeling the manufacture of supported membranes to understand the mechanisms and conditions that lead to defects.

NIST researchers are currently building a library of chemical reactions that can be incorporated into the mass-transport equations. Planned enhancements include capabilities to model interfacial physics, including phase changes.

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PROPERTIES OF ATMOSPHERICALLY SAFE REFRIGERANTS

Chlorofluorocarbons (CFCs) have been used widely for the past 50 years as refrigerants; as foam-blowing agents in building insulation, furniture, and car seats; and in many other applications. Recent evidence has shown, however, that CFCs are breaking down the stratospheric ozone layer that protects the Earth from harmful levels of ultraviolet radiation. Alternative chemicals must be found to replace the existing fluids as quickly as possible.

To replace the CFCs, accurate knowledge of the thermophysical properties of the substitutes 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.

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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 sub-atmospheric to 700 MPa 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 the 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 to understand these effects. Examples include 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.

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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 operated from 10^{-3} to below 10^{-9} std cm^3/s . Facilities include five ultrahigh vacuum systems; two low-range flowmeters; high-accuracy mercury manometers; pressure and vacuum control systems; and vacuum electronic, data acquisition, and data analysis equipment.

These facilities and measurement capabilities enable 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.

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RESEARCH FACILITIES

WATER FLOW MEASUREMENT FACILITY

The NIST water flow measurement facilities are used to establish, maintain, and disseminate flow-rate measurements, standards, and data for the wide range of conditions needed by U.S. industry. Industry requests include flowmeter calibrations, round-robin testing programs to establish realistic traceability chains in the form of flow measurement assurance programs, data-generation programs for industrial groups and trade associations, and testbeds for carrying out industrial research programs focused on flow measurement topics.

CAPABILITIES

Water flow facilities enable flow rates up to 1,000 liters/min in pipe sizes that range up to 500 mm in diameter. Maximum operating pressure is 1 MPa. Flow rate determination schemes use static and dynamic gravimetric systems.

APPLICATION

These facilities are used to establish and maintain the national bases for the liquid flow-rate measurement systems. The end result is orderliness in the marketplace, both domestically and internationally, for U.S. industries involved in the custody transfer and/or process control of valuable fluid sources and products. Potential users include the National Aeronautics and Space Administration, the Department of Defense, the oil and gas industries, the chemical and related industries, and the power and energy-generation industries.

AVAILABILITY

The facilities are available upon request to U.S. industry, other government agencies, and academia for collaborative research projects and calibrations.

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FLUID METERING RESEARCH FACILITY

The NIST Fluid Metering Research Facility combines primary calibration techniques with the capability to conduct detailed surveys of fluid velocity profiles in temperature-controlled water flows using laser Doppler velocimetry (LDV).

LDV is a non-intrusive technique for determining the fluid velocity at a particular location in the flow. It enables pipeflows to be surveyed for a wide range of piping configurations in pipe sizes up to 20 cm in diameter. Temperature control enables stable fluid and flow conditions to be established and maintained for extended test periods. The primary calibration technique uses dynamic gravimetric methods to determine accurately the bulk liquid flow rate.

CAPABILITIES

Water flow rates up to 240 liters/min in a range of pipe sizes up to 20 cm in diameter can be produced. Maximum operating pressure is 0.5 MPa, and temperature can be stabilized in the range from 16 °C to 30 °C.

APPLICATIONS

This facility is used to conduct calibrations, special fluid measurement tests, or selected research programs on flow topics. An industry-government consortium currently supports a research program on flowmeter installation effects, and the U.S. Navy is

sponsoring a series of tests to assess the performance of selected flow transfer standards in a range of non-ideal installation conditions.

The facility is used to generate critical databases used to initiate or update the national standards on generic fluid-metering topics. These standards are used for accurate custody transfer of fluid resources or products in the domestic and international marketplace or for process control in chemical manufacturing processes. Among the potential users of the facility are the Department of Defense, the National Aeronautics and Space Administration, the oil and gas industries, the engine manufacturing and testing industries, and the energy-generation industries.

AVAILABILITY

These facilities are available upon request to U.S. industry, other government agencies, and academia for collaborative research projects or calibrations.

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NITROGEN FLOW MEASUREMENT FACILITY

The nitrogen flow measurement facility is a mass-based reference system capable of both liquid and gas flow measurement. Well instrumented for temperature and pressure, the facility is adaptable and capable of a variety of piping arrangements. Located completely indoors, it is not subject to environmental changes.

CAPABILITIES

When configured for gas flow measurements, the facility has a flow-rate range of 0.5 kg/s to 2.4 kg/s. In this mode, the nitrogen gas is at pressures of approximately 4 MPa and temperatures of approximately 288 K. The facility has a flow-rate range of 0.05 kg/s to 10 kg/s when set up for liquid flow measurements. Liquid nitrogen can be at pressures up to 0.7 MPa and temperatures between 80 K and 90 K in this configuration. This continuous-flow facility permits dynamic mass flow measurements. For volume flow measurements, density is determined by making pressure and temperature measurements and calculating density from an equation of state.

APPLICATIONS

The nitrogen flow facility can be used for testing a variety of flow measurement instrumentation, including flowmeters, temperature sensors, pressure sensors, and densimeters. The ability to operate the facility at stable conditions for long periods of time permits testing of instrumentation stability. The ability to vary system parameters permits testing of instrument sensitivity.

AVAILABILITY

Collaborative or independent programs for this test facility can be arranged. The facility must be operated by NIST staff.

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NEUTRON DEPTH-PROFILING FACILITY

NIST operates two world-class neutron depth-profiling (NDP) instruments for the non-destructive evaluation of elemental depth distributions in materials. Working with the Institute's 20-megawatt nuclear reactor, researchers use the technique to provide concentration profiles for characterizing the near-surface regime of semiconductors, metals, glasses, and polymers to depths of several micrometers.

The first of the two instruments began operation in 1983. It uses a thermal neutron beam line, sapphire filters, and collimators to produce a high-quality beam with good thermal neutron intensity and minimal contamination with fast neutrons and gamma rays. The second instrument, which began operation in 1991, is part of the Cold Neutron Research Facility at NIST. (See page 88 under Materials Science and Engineering Laboratory.) Taking advantage of a liquid hydrogen moderated neutron beam, it has the highest reaction rate of any similar analytical neutron facility in the world. In both cases, an evacuated target chamber is used to analyze sample sizes from 1- to 200-mm diameter or greater. This means, for example, that entire silicon wafers are analyzed without the need to sacrifice them. A full array of electronic components is available for sample positioning, data acquisition, and analysis.

CAPABILITIES

Using the neutron beam provided by the reactor, depth profiling can be carried out with detection limits approaching 10^{10} atoms/cm². A single analysis produces a profile typically 1 μ m to 20 μ m deep with a resolution of better than 20 nm. Analysis of the sample can take from minutes to

hours depending on the information requested. Once calibrated with the appropriate elemental standard, the concentration scale is fixed independently of the sample composition, unlike most destructive analytical techniques. Elements that do not produce charged particles under neutron irradiation contribute no interference to the profile.

APPLICATIONS

Applications of NDP include range measurements for boron implanted in Si, GaAs, and other semiconductor materials; observation of the near-surface boron distribution in glasses; lithium concentration profiles in lithium niobates, tantalates, and aluminum alloys; measurement of high-dose nitrogen implants in steels; dopant and thickness determination of diamond films; and, most recently, profiles of oxygen-17 in a variety of materials. NDP is used to produce reference materials used in industry and at other analytical facilities.

AVAILABILITY

The facility is available to all qualified researchers on an independent or collaborative basis with NIST staff.

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PHYSICS LABORATORY

Attending to the long-term needs of many U.S. high-technology industries, NIST's Physics Laboratory conducts basic research in the areas of quantum, electron, optical, atomic, molecular, and radiation physics. This research is complemented by work in quantum metrology and efforts to improve the accuracy and precision of time and frequency standards.

Much of the laboratory's research is devoted to overcoming the barriers to the next technological revolution, in which individual atoms and molecules will serve as the fundamental building blocks of electronic and optical devices. To develop the necessary measurement capabilities for these new products, laboratory scientists are using highly specialized equipment, such as polarized electron microscopes, scanning tunneling microscopes, and a synchrotron radiation source, to study and manipulate individual atoms and molecules.

In support of industries ranging from photography to aerospace to lighting, the laboratory is working to improve optical measurement techniques used in remote sensing, advanced color graphics systems, and optically pumped atomic clocks. Research also is focused toward advancements in the measurement and dosimetry of ionizing radiation used in medicine and industry, and supports the development of emerging technologies, such as X-ray lithography, digital X-ray imaging, and electron beam processing.

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COOPERATIVE RESEARCH OPPORTUNITIES

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UV OPTICS TESTBED

The emerging field of high reflectance, normal incidence, soft X-ray/extreme ultraviolet (xuv) optics has a wide range of applications. The ability to produce high-quality images at wavelengths below 40 nm has allowed construction of xuv solar telescopes with unprecedented resolution, xuv microscopes able to study living biological samples with submicron resolution, and xuv photolithographic systems that will produce the next generation of integrated circuits.

NIST has initiated an xuv multilayer characterization facility at the SURF II electron storage ring, which is available to all researchers on a cooperative basis. The present facility is capable of measuring the reflectance or transmission of xuv optics (such as mirrors, filters, and gratings) as a function of wavelength, angle of incidence, and position on the optic from 8 nm to 60 nm. NIST is constructing a new facility that will extend measurement capabilities to shorter wavelengths, larger substrates, and more highly curved optics and, at the same time, increase resolution and accuracy. An optical testbed is also being constructed to measure the imaging properties

of individual optics and entire optical systems. The first element of this testbed will be a quasi-real-time imaging device with a resolution goal of 25 nm.

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VACUUM ULTRAVIOLET PHOTODIODES FOR RADIOMETRY

Highly stable photodiode detectors with uniform spatial sensitivity are developed, calibrated, and distributed as transfer standard detectors for radiometry in the wavelength region of 5 nm to 250 nm. Presently available detectors at NIST include Al_2O_3 photocathode windowless photodiodes for the region 5 nm to 120 nm, CsTe photocathode windowed (evacuated) photodiodes for the region 115 nm to 250 nm, and silicon photodiodes, developed in collaboration with industry, for the region 5 nm to 49 nm. Some other types of detectors can be calibrated by special arrangement. Broadband photometers have also been developed in collaboration with outside users and calibrated in this spectral region, e.g., combinations of silicon photodiodes with thin-film filters for plasma diagnostics and vacuum ultraviolet solar radiometry.

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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.

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CHARACTERIZATION OF LOW-TEMPERATURE PLASMAS

The properties of low-temperature plasma 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, Raman scattering, and optogalvanic methods. Modeling of the plasma is also an integral part of this characterization. Discharge sources include low-pressure rf plasmas, pulsed 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 ($<0.1 \text{ cm}^{-1}$) dye lasers; Ar ion-pumped dye and ring dye lasers; a Fizeau wavemeter; a high-throughput ($f/4$), high-resolution (0.01 nm) spectrometer with an auto-tuned intensified diode array detector; an 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 ion-atom equilibrium phenomena.

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NIST FACILITY FOR RESEARCH ON HIGHLY IONIZED ATOMS

NIST's new electron beam ion trap (EBIT) source provides many opportunities for precise measurements aimed at a basic understanding of plasma processes and atomic structure. In addition, possibilities for using the new source for nanofabrication and ion lithography currently are being considered. Ions can be generated

over a wide range of species and charge states (ultimately up to fully stripped uranium). Ions are trapped radially and probed with a mono-energetic electron beam. Electrostatic end caps confine the ions axially. A large magnetic field is applied by a superconducting magnet to pinch the electron beam to high density and provide additional radial trapping. The carefully controlled conditions in EBIT allow scientists to unravel complex collision processes and measure spectra with very high accuracy. Highly charged ions can be produced at low temperatures and observed in fluorescence with adequate brightness. The ion temperature can be further lowered by evaporative cooling techniques. A variety of instruments are available to characterize and probe the trapped ions, including X-ray spectrometers and a new laser system. Plans are under way to build an extraction system for directing beams of highly charged ions onto surfaces.

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LASER COOLING AND TRAPPING

Thermal motion of atoms often adversely affects measurements. Using the radiation pressure from near-resonant laser beams, NIST scientists can cool a gas of atoms to within a few microdegrees of absolute zero. These cold atoms can be trapped by laser beams or other electromagnetic fields. Facilities for cooling and trapping atoms include cw dye, solid-state, and semiconductor lasers. Atoms are trapped in laser traps, magneto-optical traps, and microwave traps. Sodium, rubidium, cesium, and xenon atoms are cooled, trapped, and used in such diverse applications as atomic-fountain frequency standards and studies of

laser-modified chemical reactions. Control of atomic motion by lasers is also being applied to problems such as atom interferometry and laser-directed deposition of atoms on surfaces.

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HIGH-PRECISION LASER SPECTROSCOPY

Highly stabilized tunable lasers permit the investigation of atoms and molecules with a level of detail and precision that cannot be obtained with conventional spectroscopic techniques. NIST work in this area ranges from observations of laser ionization of diatomic molecules in dense vapors to highly precise wavelength measurements that test the most advanced atomic theories for simple atoms. The high resolution provided by laser scanning permits study of spectral line profiles, including pressure broadening, isotope shifts, and hyperfine structure. Sensitive detection techniques, including FM and optogalvanic spectroscopy and use of thermionic diode detectors, permit observation of low concentration species in discharges and vapor cells. Typical applications of these data include wavelength standards, detection of trace elements in samples, and laser isotope separation. Facilities include stabilized lasers that are tunable from the near ultraviolet to near infrared and a unique Fabry-Perot wavemeter that is capable of real-time laser wavelength measurements with an accuracy of a few parts in a billion.

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MOLECULAR PHYSICS

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HIGH-RESOLUTION MOLECULAR SPECTROSCOPY

The NIST high-resolution spectroscopy group employs advanced spectroscopic methods using state-of-the-art lasers and microwave frequency sources in conjunction with molecular beam techniques to elucidate the details of chemical reactions that are important in a wide variety of industrial processes, including catalysis, combustion, chemical vapor deposition, and drug design. These benchmark studies provide means for real-time optimization of chemical processes and on-line monitoring for pollution control.

The group also carries out spectral studies of species important in atmospheric processes with particular emphasis on the reaction chemistry of ozone. The work provides spectral data for these species, which are used by scientists modeling the chemistry of the upper atmosphere. A recent thrust of the group centers around the determination of physical and electrical properties of numerous new chemical compounds that are being investigated by industry for use as alternative refrigerants.

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MOLECULAR DYNAMICS

The NIST molecular dynamics group employs sophisticated laser techniques and pulsed molecular beam nozzles to investigate the dynamics of chemical reaction mechanisms on picosecond and femtosecond time scales providing new insights into the details of reaction mechanisms with extremely high time resolution. The reactions being studied include those important in combustion processes, upper atmospheric chemistry, and catalysis.

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MOLECULAR THEORY

The NIST molecular theory group is developing new algorithms and theoretical methods in time-dependent quantum dynamics. These methods are being applied to describe collisional phenomena currently being observed in ultracold neutral atom traps, which ultimately will lead to the next generation of atomic clocks. Describing these novel collisions requires development of methods that can describe the quantum evolution of a system while it is interacting and exchanging energy with its environment. In laser cooling phenomena, the energy exchange is due to the dissipative process of spontaneous decay of excited states. The new theoretical methods are expected to find widespread applicability to many areas of chemistry and physics, such as reactions in condensed media or electron transport in nanoscale devices. Implementing these new methods will greatly benefit from the development of state-of-the-art massively parallel processing computers.

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RADIOMETRIC PHYSICS

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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 light emission 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. 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 include various laser and lamp sources, the NIST reference spectrofluorimeter, and a low-light-level spectroradiometer now under construction.

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PHOTOMETRY

Photometry is the application of radiometric measurement to human vision. NIST researchers recently have improved the accuracy of the SI base unit for photometry, the candela, by realizing the scale based on absolute detectors. The candela is a unit of measure of the apparent brightness of a light source as observed by the human eye. Research continues in the application of the detector-based candela to improving other photometric scales, such as luminous flux and luminance. Additionally, NIST researchers are applying photometry to new measurement problems, such as the colorimetry and perceived quality of flat-panel displays. Cooperative research opportunities exist in aspects of photometric measurements, as well as psychophysical and related human-factor issues as might apply to product designs and improvements.

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CRYOGENIC RADIOMETRY

Measurement of optical power by electrical substitution is improved at cryogenic temperatures. A cryogenic radiometer designed for high accuracy forms a basis for NIST optical scales, with a measurement uncertainty of 0.01 percent. Other cryogenic radiometers are employed to measure lower fluxes and faster flux changes. Ongoing efforts to further develop this measurement technique include studies into new methods for cryogenic thermometry, such as the thermoelectric inductance bolometer, and better analytic modeling of radiometer designs.

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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 involve the development of large-area blackbodies, use of Pt-Si as detector standards, and the characterization of thermal imaging cameras. Equipment available includes several heat-pipe blackbodies, a Pt-Si camera, and an infrared radiometer.

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UV RADIOMETRY

The measurement of terrestrial solar irradiance in the uv-b spectral region is being investigated by NIST researchers to provide improved techniques and standards in this region. This 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.

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SPECTRAL RADIOMETRY

Research and development programs at NIST span many activities associated with the measurement of optical radiation, covering the spectrum from 200 nm in the ultraviolet to the far infrared. Included are spectral radiance and irradiance measurements for many varied applications, such as manufacturing process control, remote sensing of the Earth's environment, and defense needs. Researchers at NIST take demanding problems, such as the spectrophotometric measurement of dense optical media, and develop the detector metrology to perform the measurements and relate them to the stable, U.S. radiometric measurement base. Emphasis is placed on solid-state photodiode metrology and its application to all areas of radiometry, especially calibration services.

Several well-equipped laboratories for optical measurements in the uv, visible, and infrared spectral regions are available for use, and new facilities are under development to enable scientists and engineers to conduct research on detector improvements, detector applications, and optical properties of materials.

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INFRARED SPECTRAL RADIOMETRY

Researchers at NIST are developing devices and techniques for high-precision measurements of radiant power in the 2 μm to 30 μm spectral region to enable characterization of spectral sources, optical components, and detectors. Novel experiments are being planned to investigate physical and

chemical processes in materials and molecular structures. State-of-the-art radiometers, a cryogenic blackbody with multiple apertures, lead salt lasers, spectral instrumentation, and solid-state infrared detectors are being acquired. A unique facility called the Low Background Infrared Radiation Facility is dedicated to this research and development effort. An Infrared Detector Comparator Facility, equipped with a prism-grating monochromator and an FTIR spectrometer for characterizing detectors at ambient background, is nearing completion.

Related research projects are investigating methods for measuring the optical density of filters using laser heterodyne technology and determining the spatial uniformity and linearity in the response of infrared detectors. Collaborative research opportunities exist in measuring the optical properties of materials and fundamental molecular structures and in developing novel detectors.

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BIDIRECTIONAL SCATTERING METROLOGY

The bidirectional characterization of optical scatter from surfaces is a useful diagnostic in evaluating elements contained within large optical systems that require the minimization of scattered light. This information is needed for the development of ring-laser gyroscopes, telescopes, and super-polished mirrors. It is used also for the characterization of materials for use in stray light reduction in thermal control and inspection processes in optical manufacturing settings. NIST research projects involve the development of a multiangle scattering reference instrument and the development of

measurement methodologies and Standard Reference Materials for the spectral range from the ultraviolet to the infrared region.

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QUANTUM METROLOGY

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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 (NSLS) at Brookhaven National Laboratory in New York, providing the highest flux, intensity, and energy-resolving power of any existing beamline in the X-ray energy range from 500 eV to 5000 eV. NIST equipment complements the synchrotron radiation instrumentation. X-ray absorption spectroscopy techniques, such as X-ray absorption near-edge structure and extended X-ray absorption fine structure, 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.

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 with 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, 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.

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HIGH-ENERGY X-RAY SPECTROSCOPY

NIST researchers have developed highly accurate spectroscopic instrumentation for measurements from the keV region to several MeV. This measurement system is connected to the basic SI units of frequency and length by means of X-ray interferometry and a precise lattice comparator. Main applications include accurate secondary standards in the X-ray and gamma-ray region and spectroscopic measurement of high voltage.

wide variety of instrumentation is available, and collaborative applications of these capabilities to technically significant problems are welcomed.

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PRODUCTION AND CHARACTERIZATION OF SYNTHETIC MULTILAYERS

In response to the need for short-wavelength characterization of multilayer structures for larger wavelength X-ray optics, NIST researchers have established a high-performance multi-axis diffractometer. This system provides highly collimated and monochromatic X-ray beams, which, after reflection from the structure under study, can be examined for both specular and non-specular reflection characterization. The normal operating wavelength is 0.154 nm, and the on-scale reflectivity covers a range of six decades.

In association with this program, the researchers have established a thin-film production facility capable of handling a wide variety of materials in the range of thicknesses from near one monolayer to a micrometer. The production process uses a beam sputtering with simultaneous gas-assisted neutral beam milling to produce thin layers of exceptional uniformity.

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PRE-FLIGHT AND POST-FLIGHT CALIBRATION

Significant numbers of X-ray instrumented satellites have been placed in Earth orbit, and more are planned. The flexible laboratory-based capabilities established in this division have been made available to support several missions. In addition to earlier work on the Solar Maximum Mission and P78-1, NIST researchers have made important contributions to currently orbiting observatories, including the Japanese satellites Yohkoh and ASTRO-D. They recently completed detector characterization for the Broadband X-ray Telescope and are currently focusing on the bolometer detector for the Advanced X-ray Astronomy Facility.

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IONIZING RADIATION

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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, amino acids, metalloporphyrins, and organic or inorganic radiochromic and luminescent 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 optical waveguide analysis, microcalorimetry, pulse radiolysis, laser-induced photochemistry, and conductivity measurements.

Various X-ray and gamma-ray sources and electron accelerators with energies in the 0.1-MeV 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 also are available.

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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 who are aware of this are creating components that facilitate such non-destructive testing. Research is underway 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.

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.

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MEASUREMENT QUALITY ASSURANCE

Credibility of ionizing radiation measurements has been a critical issue for the U.S. radiation medical diagnostics and therapy, occupational safety, industrial, energy, defense, and environmental communities. To this end, NIST scientists disseminate the standards and technology required for reliable measurement of ionizing radiation to federal, state, and local radiation control programs as well as to the medical, industrial, and defense communities. In addition, NIST researchers monitor and evaluate radiation measurements needs; participate in radiation research, metrology development, and quality control activities; and develop methods for improving the accuracy of field measurements through a national system of secondary standards laboratories.

NIST has a strong influence on the design and implementation of measurement quality assurance programs that are accredited under the National Voluntary Laboratory Accreditation Program (secondary calibration laboratories for ionizing radiation and

personnel dosimetry programs), the Conference of Radiation Control Program Directors (diagnostic X-radiation), Health Physics Society (private-sector calibration laboratories), and American Association of Physicists in Medicine (therapeutic radiation). Programs currently being developed will address MQA needs in sectors that include industrial processing, radio-bioassay, and radioanalyses for environmental remediation and waste management.

In support of the accreditation programs, NIST provides technical expertise for laboratory technical document review and evaluation, traceability to the national physical standards through performance evaluation testing, and on-site assessments. The major research thrust is the development of a wide variety of appropriate transfer standard instruments and materials.

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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 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.

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TIME, FREQUENCY, AND LASERS

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HIGH-PERFORMANCE DIODE LASERS

Diode lasers are now widely used in many applications where spectral and spatial purity is not critical, but they could be used in a variety of other applications if these properties were improved substantially. Such applications include analytical chemistry and sensing of trace impurities or pollutants as well as narrow-line sources for length standards and optical manipulation of atoms and molecules. Recognizing the broad range of measurement applications for high-performance diode lasers, NIST has started a program aimed at developing methods for controlling the output characteristics of these versatile and inexpensive lasers. The program selects specific practical applications and works on the system designs needed to provide solutions. Current projects include a calcium-stabilized laser

or use as a length reference, methods for synthesizing signals in the optical region, and laser-enhanced ionization as a means for detecting trace impurities.

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TIME TRANSFER AND NETWORK SYNCHRONIZATION

NIST has broad expertise in time transfer, particularly using satellite methods, which can be applied to synchronization of widely distributed network nodes. Telecommunications and electrical power networks are examples of systems requiring such synchronization. A NIST-developed, common-view method using GPS satellites provides time transfer accuracy of better than 10 nanoseconds, and two-way exchange of signals through telecommunications satellites offers even higher performance. NIST owns and operates a number of specialized GPS receivers and satellite Earth stations needed for such work, and the NIST time scale provides unsurpassed stability as a reference for remote synchronization.

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PHASE NOISE IN ELECTRONIC AND OPTICAL SYSTEMS

NIST has developed systems for making phase-noise measurements over a broad dynamic range of carrier frequency (into the millimeter range) and Fourier frequency (up to 10 percent of the carrier frequency). The accuracy of measurement is typically 1 dB or better depending on the frequency range. These systems provide the basis for specifications now arising in communication, radar, and other aerospace equipment. Signals at higher millimeter and optical frequencies also can be characterized by beating them against a stable optical reference. A wide range of noise measurement equipment and systems for analyzing the output data are available.

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STATISTICAL ANALYSIS OF TIME-SERIES DATA

Noise processes in high-performance clocks and oscillators are often not white (frequency independent), so the usual variance does not converge. The two-sample variances developed to handle such noise have become standards widely used in the specification of noise in systems demanding high spectral purity. These measures also have been applied with some success to other measurement data. NIST researchers have developed software for the efficient calcula-

tion of these measures. Outputs can be represented in both the frequency and time domains.

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FAR-INFRARED SPECTROSCOPY

NIST has unique capabilities for high-resolution studies of the spectra of atoms and molecules in the far-infrared region. The methods of tunable far-infrared spectroscopy and laser magnetic resonance (LMR) were developed by NIST, and several of each of these spectrometers currently are providing high-resolution measurements on spectra important in both space studies and studies of the chemistry of the upper atmosphere. Pressure-broadening studies at high resolution also have been performed providing the basis for locating (in altitude) important air pollutants. Recent improvements in the NIST LMR systems have dramatically improved their sensitivity, making them especially useful in searches for difficult-to-detect molecular species, such as free radicals and molecular ions.

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LASER STUDIES OF SEMICONDUCTOR MATERIALS

Laser probing of the gas-phase species involved in the molecular beam epitaxial (MBE) growth of III-V semiconductor materials is an area of high potential relevance for standards and technology. Work under way has demonstrated sensitive, direct-laser detection methods for study of all species during III-V growth, and it will be extended to II-VI species. With the incorporation of non-invasive single-photon laser ionization probes into advanced generations of MBE machines, NIST researchers will be able to carry out in-situ diagnostics to quantify and characterize the growth process, to provide optical feedback for adjustment of species concentrations, and to determine the purities of materials used during semiconductor fabrication.

In related experimentation, laser vaporization of thin films is used to produce sources of translationally energetic species for etching and deposition studies. Thermal chlorine molecules produce little or no etching of silicon materials, whereas etch rates increase dramatically with increasing kinetic energy, with an apparent threshold. New research will also explore the kinetic energy dependence of film growth by using

velocity selected beams of refractory materials and insulators.

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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. Exciting new possibilities arise from locking stable lasers to sharp quantum resonances, provided, for example, by atoms in an "atomic fountain."

Several laser-locking and scanning systems have been developed. One powerful NIST laser-stabilization system works entirely externally to a continuous-wave laser to suppress the output laser frequency and intensity noise. A precise scanning method is based on optical sideband production by broadband microwave phase modulation of the laser, allowing scans over a GHz range, with inaccuracy below 10 kHz. Another scan technique utilizes a novel interferometer/phase-locked rf system that effectively maps optical frequency change into the corresponding phase change of an rf signal suitable for control, stabilization, and scanning. In a final method, a doubly passed acousto-optic wideband modulator allows scanning the laser relative to a stable reference interferometer.

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SILICON THIN FILMS

Thin films of amorphous silicon are used in photosensitive devices, displays, and in photovoltaic cells. Scientists are examining physical and chemical mechanisms involved in discharge and thermal chemical vapor deposition (CVD) production of such films. A scanning tunneling microscope is used to examine in situ the morphology and chemical character of as-deposited films. A electronics, vacuum, and gas-handling apparatus necessary for producing and diagnosing discharge and thermal CVD films under controlled conditions are available.

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VISITING FELLOWSHIP PROGRAM

Since its founding in 1962, JILA has provided an opportunity for established scientists working in various fields of interest to JILA and NIST to spend 6 months to a year as "Visiting Fellows" working with members of the Institute's scientific staff. Approximately 10 of these awards are given each year. They provide a stipend to the awardee for partial salary, travel, and laboratory and/or computational expenses. JILA's broad range of research interests—including atomic, molecular, and chemical physics, non-linear optics, stabilized lasers, semiconductors, and precision measurement (relating to spectroscopy, gravitational physics, and geophysics)—encompasses work of interest to both academic and industrial scientists.

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* The Joint Institute of Laboratory Astrophysics (JILA) is a cooperative research venture of NIST and the University of Colorado.

RESEARCH FACILITIES

SYNCHROTRON ULTRAVIOLET RADIATION FACILITY II

The heart of the NIST Synchrotron Ultraviolet Radiation Facility II (SURF II) is a 300-MeV electron storage ring. The synchrotron radiation emitted is highly collimated, nearly linearly polarized, and of calculable intensity. Seven beamlines are available, and a users' program is in operation. SURF II is well suited for studies in radiometry; atomic, molecular, biomolecular, and solid-state physics; surface and materials science; electro-optics; and surface chemistry and radiation effects on matter. Special facilities are available for developing and testing soft X-ray optics and optical devices.

CAPABILITIES

The typical storage ring electron beam current is 200 mA at 284 MeV. The photon intensity in the region 60 nm to 120 nm is about 3×10^{12} photons per second per milliradian of orbit for an instrumental resolution of 0.1 nm. Experiments can be conducted conveniently throughout the wavelength range 4 nm to 1000 nm, from the soft X-ray region to the infrared. One normal incidence, two grazing incidence, and several toroidal grating monochromators are available to disperse the radiation. A large, ultrahigh vacuum spectrometer calibration chamber, 1.2 m \times 1.2 m \times 2.5 m and accessible through a clean room, is available for radiometric applications in a clean, vacuum environment. A 6.65-m

normal-incidence vacuum spectrometer, with resolving power of about 100,000, is available on a beamline dedicated to high-resolution vacuum ultraviolet radiation research.

APPLICATIONS

The continuous radiation from SURF II is used as a national standard of spectral irradiance for radiometric applications and for fundamental research in the following areas:

- atomic and molecular absorption spectroscopy;
- optical properties of materials;
- electron density of states in solids;
- surface characterization;
- photoelectron spectroscopy;
- molecular kinetics and excitation and ionization dynamics; and
- radiation interactions with matter (such as lithography, radiation damage, dosimetry, photobiology).

AVAILABILITY

Beam time on SURF II is available to any qualified scientist if beamline vacuum requirements are met and scheduling arrangements can be made. Proposals should be submitted for NIST review before use of the facility is desired. Informal contact also is encouraged.

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HIGH-RESOLUTION UV AND OPTICAL SPECTROSCOPY FACILITY

Accurate atomic data for neutral atoms and ions are required in support of high-technology products and manufacturing processes as well as advanced scientific applications. The primary source of such data is high-resolution optical spectroscopy. Spectrographs produced in NIST's High-Resolution UV and Optical Spectroscopy Facility are the most powerful in the world for observations of emission and absorption spectra in the soft X-ray to near infrared regions. The 10.7-m grazing-incidence and normal-incidence vacuum spectrographs permit observations from 3 nm to 600 nm with resolving powers of 70,000 to 400,000 and wavelength uncertainties as low as 0.0002 nm. In the visible and near-infrared region, an echelle spectrograph provides resolving powers exceeding 1,000,000. A variety of discharge sources are used to excite spectra of neutral atoms and ions stripped of up to 20 electrons. Species up to 40 times ionized are observed in plasmas created by ablating samples with a high-power laser.

Current NIST research includes development of wavelength standards used for calibration of the high-resolution spectrograph on the Hubble Space Telescope, observations of transitions in highly ionized atoms for plasma diagnostics in tokamaks, development of a promising new scheme for an extreme uv laser, and precise isotope shifts of mercury wavelengths needed to interpret uv spectra of stars.

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LOW-BACKGROUND INFRARED RADIATION FACILITY

In the NIST Low-Background Infrared Radiation Facility, radiant background noise levels less than a few nanowatts are attained in a large (60-cm-diameter \times 152-cm-long) vacuum chamber by cooling internal cryoshields to temperatures less than 20 K using a closed-cycle helium refrigerator system. An absolute cryogenic radiometer (ACR) of the electrical substitution type that operates at 2 K to 4 K is housed in the chamber.

CAPABILITIES

The ACR is a broadband detector with a flat response from the visible to the long wavelength infrared spectral region. It can measure power levels of 20 nW to 100 mW at its 3-cm-diameter aperture within an uncertainty of less than 1 percent. The ACR has a resolution of 1 nW, and its time constant is about 20 s.

APPLICATIONS

This unique facility can be used to measure total radiant power from sources such as cryogenic blackbodies. Ongoing improvements will allow measurement of the spectral distribution of radiation from sources and characterization of infrared detectors and optical components.

AVAILABILITY

The facility is operated by NIST staff in support of user infrared calibrations. It is available for collaborative research by NIST and outside scientists in areas of mutual interest.

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ELECTRON PARAMAGNETIC RESONANCE FACILITY

NIST is leading a national and international effort in electron paramagnetic resonance (EPR) dosimetry for measuring ionizing radiation. Paramagnetic centers (molecules/atoms with unpaired electrons) are produced by the action of radiation on materials. In the EPR measurement, irradiated materials are placed in a magnetic field and electron spin transitions are induced by an electromagnetic field of the appropriate frequency (typically GHz). EPR is used as a non-destructive probe of the structure and concentration of paramagnetic centers. The centers created by ionizing radiation are proportional to the absorbed dose and provide a sensitive and versatile measurement method.

CAPABILITIES

The EPR dosimetry facility is supported by a state-of-the-art X-band EPR spectrometer capable of measuring radiation effects on a wide range of materials from inorganic semiconductors to biological tissues. The recently upgraded data acquisition system provides full computer control of all spectrometer functions, including real-time spectral display and rapid acquisition scan to analyze rapidly decaying signals. The data acquisition system is interfaced with an advanced data analysis station for data manipulation and is capable of simulating and deconvoluting multicomponent spectra.

APPLICATIONS

EPR dosimetry is operable over several orders of magnitude in absorbed dose (10^{-2} Gy to 10^5 Gy) and impacts many facets of society and industry. Areas of application include:

- Radiation Protection/Accident Dosimetry. Using biological tissues (bone, tooth enamel) or inanimate materials (clothing, retrospective dose assessment and mapping can be accomplished.
- Clinical Radiology. Ionizing radiation doses administered in cancer therapy can be measured for external beam therapy using dosimeters of crystalline alanine (an amino acid) or validated for internally delivered bone-seeking radiopharmaceuticals using bone biopsies.
- Industrial Radiation Processing. Routine and transfer dosimetry for industrial radiation facilities can be performed using alanine dosimeters, as well as post-irradiation monitoring of radiation-processed meats, shellfish, and fruits using bone, shell, or seed.

The EPR facility also serves as a fully functional materials research facility for analyzing radiation effects on semiconductors, optical fibers, functional polymers, and composites.

AVAILABILITY

The EPR facility is available for collaborative research by researchers from industry, academia, and other government agencies under the supervision of NIST staff.

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RADIOPHARMACEUTICAL STANDARDIZATION LABORATORY

Radioactivity measurements for diagnostic and therapeutic nuclear medicine in the United States are based on measurements at NIST. Activity measurements for the gamma-ray-emitting radionuclides are made using the NIST "4 π " γ ionization chamber. The calibration process also includes identification of radionuclidic impurities by germanium spectrometry. Recent development work has focused on therapeutic nuclides for nuclear medicine, radioimmunotherapy, and bone palliation.

CAPABILITIES

The radiopharmaceutical standardization laboratory provides calibration services for the gamma-ray-emitting radionuclides and is available for technical users who must make measurements consistent with national standards or who require higher accuracy calibrations than are available with commercial standards.

NIST also undertakes basic research to develop new methods of standardizing radionuclides for diagnostic and therapeutic applications. These studies include measurements of decay-scheme parameters, such as half lives and gamma-ray emission probabilities, and identification of radionuclidic impurities.

AVAILABILITY

The customer has no direct use of the facility. NIST staff can provide calibration services for the gamma-ray-emitting radionuclides that comply with the specifications as stated in NIST Special Publication 250-10.

Working at NIST, research associates of the United States Council for Energy Awareness produce standards that are certified by NIST as Standard Reference Materials for distribution to the nuclear power and radio pharmaceutical communities.

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MAGNETIC MICROSTRUCTURE MEASUREMENT FACILITY

The magnetic microstructure of materials can be measured with very high spatial resolution by a technique called scanning electron microscopy with polarization analysis (SEMPA). An ultrahigh-vacuum electron microscope has been modified so secondary electrons from the sample can be analyzed for their electron spin polarization. This allows for a measurement of the surface magnetism with moments both in the plane and perpendicular to the plane of the sample.

CAPABILITIES

SEMPA allows the simultaneous observation of surface microstructure and surface magnetic domains at a resolution of 0.05 μm .

APPLICATIONS

This unique measurement facility can be used for research in magnetic thin films, high-coercivity magnetic materials, high-density magnetic storage media, and other advanced magnetic materials.

AVAILABILITY

These facilities are available for collaborative research by NIST and outside scientists in areas of mutual interest on a time-available basis.

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MATERIALS SCIENCE AND ENGINEERING LABORATORY

Materials science and engineering programs at NIST cover the full range of materials issues from design to processing to performance. A unifying aim is to acquire the knowledge and tools needed for intelligent manufacturing methods with real-time automated process controls.

Separate research initiatives address ceramics, metals, polymers, composites, and superconductors. This research supports efforts by U.S. industry to develop reliable, low-cost manufacturing methods for producing tailor-made materials and products with superior properties.

Through laboratory-organized consortia and one-to-one collaborations, NIST's materials scientists and engineers work closely with industrial researchers. Examples include work on improved processing of rapidly solidified metal powders, polymer composites, ceramic machining, aerospace alloys, and non-destructive evaluation sensors for aluminum and steel manufacturing. The laboratory is also strengthening its relationships with manufacturers of high-technology products, the major users of advanced materials.

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COOPERATIVE RESEARCH OPPORTUNITIES

INTELLIGENT PROCESSING OF MATERIALS

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INTELLIGENT SENSORS, CONTROLS, AND PROCESS MODELS

Advanced materials are capable of providing outstanding properties, but they generally require unusual processing operations and tend to be expensive. Intelligent processing offers the potential to design and produce materials with substantially improved quality, reduced lead time, and increased flexibility in production.

Intelligent processing incorporates four principal elements, including materials processors, non-destructive evaluation sensors that can measure physical and mechanical characteristics of materials in real time during processing, rigorous models to describe the materials production process, and expert systems to control the production process in real time through integration of sensors and process models.

Research sponsored by the Office of Intelligent Processing of Materials is directed to process models, sensors, and intelligent control systems. Research topics at NIST include processing modeling, sensing and control of the production of metal powders by high-pressure gas atomization, magnetic methods for measuring mechanical properties during steel processing, process modeling for thermomechanical processing of

steel sheet, process modeling of gas metal arc welding, ultrasonic measurement of interfaces, powder-particle-size sensing, process modeling for producing polymer blends, fluorescence spectroscopy in polymers processing, magnetic resonance imaging and ESA for ceramic processing, eddy-current sensing in metals and composites, and laser ultrasonic methods.

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CERAMICS

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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. 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 microstructures and properties.

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SURFACE PROPERTIES OF CERAMICS

The surface properties of ceramics are crucial for the control of wear, proper lubrication, and efficient machining, all of which are important technological issues. Research conducted at NIST has uncovered basic wear mechanisms of ceramics under concentrated sliding conditions. Subsurface damage in the form of dislocations, microcracks, and intergranular fractures often controls the initiation of the transition to severe wear. Microstructural design through innovative sintering aids, processing, and colloidal chemistry can change the damage process significantly. Current research efforts emphasize the identification of critical microstructural features and the development of microstructures that can release strain from contact stresses without significantly affecting the strength and fracture toughness of silicon nitrides.

Lubrication prolongs the life of ceramic components in engine applications. Researchers at NIST have explored various chemistries to uncover new technologies capable of forming a lubricating film on ceramic surfaces under boundary lubrication conditions. Several new chemistries have been discovered that are capable of

controlling friction and wear of ceramic contacts. This information on surface reactivity of ceramics with various functional groups also may prove to be useful in bearing, gear, and engine component design.

Machining can account for about 50 to 90 percent of the cost of finished ceramic components. Utilization of chemical compounds to form soft layers under the heat and stresses of the machining process not only can reduce the mechanical stresses the work piece is subjected to but also can improve the surface finish of the work piece. Initial experiments at NIST have demonstrated the feasibility of the concept; by using chemical compounds, cutting rates on Si_3N_4 have been increased by 60 percent with concomitant reduction in surface roughness.

Industrial partnerships to jointly develop technologies in the above areas are solicited.

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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 the development of optical switches and modulators.

NIST researchers are investigating crystal perfection at a unique, monochromatic X-ray topography facility at the NIST beamlines on the high-energy ring at Brookhaven National Laboratory's National

Synchrotron Light Source in New York. Conducted jointly with growers of high-quality crystals, current studies are expected to improve substantially the quality, and hence the performance, of these crystals.

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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.

One program involves the use of an indentation strength procedure to determine the fracture toughness behavior of monolithic ceramics and to relate the toughness to the specific microstructure of the material. In-situ microscopic observations of crack growth demonstrate the presence of grain bridging and frictional sliding in the crack wake as a significant source of material toughening.

A program in composites is aimed at determining the effects of the fiber/matrix interface on fracture behavior of these materials. 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 Si_3N_4 have been investigated and their behavior related to differences in microstructure, particularly grain size.

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 $\pm 1 \mu\text{m}$ at 1500 °C.

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CERAMIC PHASE EQUILIBRIA

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

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ULTRASONIC CHARACTERIZATION OF MATERIALS

To evaluate the quality of advanced materials, NIST researchers are developing the theoretical basis and the measurement technology for ultrasonic characterization of material properties. Research is under way in modeling wave propagation, improving transduction techniques, developing signal processing methods, and understanding the nature of acoustic wave interactions with materials.

In modeling, a wavelet formulation has been developed that enables the computationally efficient modeling of acoustic wave propagation in composite materials. The results are used to optimize measurement methods and to interpret waveform perturbations.

Recent advances in transduction include non-contact, gas-coupled transducers and very sensitive, high-fidelity sensors for acoustic emission. A high-pressure, gas-coupled, transmission, acoustic microscope has been developed for high-resolution ultrasonic inspection of electronic packages without the need for immersion in a liquid.

New signal processing methods include a waveform-based interpretation of ultrasonic signals generated and received by point-contact, broadband transducers, and an

adaptive algorithm for an ultrasonic sensor array used to image defects in thick composite materials.

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MICROSTRUCTURAL ENGINEERING

NIST researchers are developing process models and sensors to link the properties of hot rolled steels to composition and thermomechanical processing parameters. Microstructure determines properties, and thus, the key to property control is understanding the thermal and microstructural states of the steel at each processing stage.

Analytical models of plastic deformation during hot rolling, continuous cooling transformation kinetics, and structure property relations are used to predict mechanical properties for a given temperature/deformation schedule. The results are experimentally verified in a thermomechanical processing simulator developed by NIST. The simulator is used to subject specimens to prescribed deformations and to measure the in-process metallurgical changes that occur such as deformation resistance, recrystallization, and phase transformations.

Recently, a program on sensors for microstructural engineering was initiated. The first task is to develop ultrasonic sensors for on-line measurement of grain size during hot rolling. The idea is to relate attenuation

measurements to grain size. Facilities are being developed to measure attenuation in steel samples at temperatures up to 1200 °C.

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MICROMECHANICAL MEASUREMENTS

The mechanical behavior of materials within electronic interconnect structures controls the reliability of advanced electronic devices. NIST has developed experimental techniques to measure thin-film mechanical properties, to map strain fields around interfaces between materials, and to study thermal stresses and map the associated temperature distributions.

Mechanical properties of thin films are measured in an electronic probing station equipped with a loading stage with a resolution of 0.5 mN in load and 2.5 nm in displacement. Thin films are prepared using electronic microfabrication techniques to deposit the film and to etch away the substrate in the test section. A picture-frame concept is used to facilitate handling of the specimens.

Electron-beam moiré is a novel technique to map displacement fields with five times the resolution of optical moiré. Electron beam lithography is used to create arrays of lines with pitches down to 100 nm. The specimens are stressed mechanically or thermally inside a scanning electron microscope (SEM). The SEM raster scan serves as the reference grid permitting strain measurements at a magnification of 2000 over gage lengths of 10 µm to 30 µm.

Differential thermal expansion is the primary cause of stress in electronic devices. NIST researchers use an infrared microscope to measure temperature fields with a resolution of 30 μm . These measurements can verify the stress analysis used for device design.

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INTELLIGENT WELDING

To improve the reliability of welded joints, NIST researchers are developing sensing and control systems to replace the eyes, ears, and know-how of a skilled welder. Through-arc sensing and signal processing techniques detect changes in the electrical characteristics of the arc. A laser vision system is used to relate these changes to the welding process, i.e., the metal transfer from the electrode to the weld puddle. Process models are being developed to predict the arc behavior and metal transfer characteristics. The goal is to combine the sensors and process models into an automatic control system.

NIST researchers have developed automated systems for gas metal arc and flux cored arc welding that can detect contact tube wear, degradation of gas shielding, and mode and stability of droplet transfer. Through-arc sensing relies on simple measurements of voltage and current, and thus the welding torch is free of extra devices.

A typical system consists of electrical sensors, a digital-to-analog converter, signal conditioners, software, and a personal computer.

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POLYMERS

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PROCESSING SCIENCE FOR POLYMER COMPOSITES

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.

NIST researchers are developing new measurement tools to characterize the starting materials for composite processing and to study in the laboratory the chemical and physical changes that occur during processing. The scientific understanding that can be generated with these tools will facilitate both advances in processing methods and implementation of on-line control and automation.

The infiltration of a resin into a fiber preform during processing is the critical step in composite fabrication by liquid molding. Test methods to characterize the resistance of the preform to resin infiltration have been developed. NIST is working with several companies, including the Automotive

Composites Consortium (Ford, General Motors, and Chrysler), Grumman Corp., and Boeing, to characterize this resistance in a variety of materials and use the results in computer simulation models to optimize the liquid molding process.

In addition, NIST is developing measurement techniques to monitor the chemical, morphological, and molecular changes that occur during processing. The program currently has 10 different spectroscopic, dielectric, thermal, and mechanical techniques available for process monitoring, and others are under development. This diversity of tools provides a unique capability for evaluating and calibrating new measurement methods, for developing process models, and for analyzing model resin systems.

For example, through cooperative projects with NIST, several industries have selected and developed monitoring methods for their particular problems.

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POLYMER MECHANICS AND 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 semi-crystalline 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-nm 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.

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 (SAXS) techniques, which include the use of position-sensitive detectors, also are used in these investigations.

NIST scientists use both positron annihilation spectroscopy (PAS) and SAXS to study the microstructure of amorphous polymers. SAXS and PAS studies complement macroscopic measurements of samples using conventional mechanical testing, as well as a unique torsional dilatometer.

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DENTAL AND MEDICAL MATERIALS

Modern dental and medical materials have dramatically improved the delivery of health care to the American public. As good as these materials are, significant problems remain to be solved.

NIST has a program aimed at helping to solve those problems. This program is developing basic science and engineering that can be used to formulate new materials and includes transferring that science and technology to industry, in particular, but not exclusively, to the dental industry.

The program has the active participation of researchers from the American Dental Association, the National Institute of Dental Research, dental industries, and universities.

Researchers are working in a number of areas. For example, a strong effort exists on understanding the mechanisms of and improving adhesion of dental biomaterials to tissues. Also, biodegradable materials are being developed for hard tissue repair and are being evaluated clinically. Improved resins that have higher resistance to degradation by oral fluids and that reduce polymerization shrinkage are being developed. An in-mouth radiation shield, to protect cancer patients from secondary radiation emitted from metallic restorations during radiation therapy, is in clinical trials with industrial sponsorship. The interfaces between fillers and resins of resin-based composite restoratives are being investigated with the goal of improving interfacial strength and durability of composite restorations. Work is in progress with the NIST Metallurgy Division to develop a metallic, mercury-free restorative that can be used like dental amalgam.

Test methods are being investigated for their relevance to clinical failures. Finite-element analyses (FEA) and fractographic analysis of ceramic dental fixed partial dentures, subjected to an in-vitro test, have implicated the interface between dissimilar materials as the source for failures, in concert with clinical experience. Weibull statistical analysis, coupled with FEA, is being employed for identifying improvements in material systems via risk-of-rupture analyses.

Weibull analysis also is being applied to statistical analysis of censored clinical data on failure of ceramic-metal restorations, to test the hypothesis that this can be a more facile and informative method of analysis than either Kaplan-Meier or Cox Proportional Hazard analyses of survivability.

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ELECTRICAL AND OPTICAL 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, monitoring the curing of microelectronic packaging materials, thermal expansion and thermal conductivity of electronic packaging materials, measurement of space charge distribution within polymer films, and electro-optic properties of polymers.

Scientists have developed instrumentation and data analysis techniques to measure the dielectric constant and loss of polymer films over a frequency range from 10^{-3} Hz 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 scientists also have designed instrumentation and data analysis techniques to measure the charge or polarization distribution across the thickness of a 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 non-uniform electric fields in the poling of piezoelectric polymers and to investigate the sign, magnitude, and distribution of charge injection when polymers are subjected to high electric fields.

The facility is referred to as the thermal pulse facility, and it is available for proprietary research.

Organic molecules with highly delocalized π -conjugated electrons offer great potential in the field of non-linear optics due to their relatively large second-order susceptibilities and their picosecond response times. The orientation and stability of orientation of polar groups in polymers containing these groups are being investigated by measurements of uv-visible spectroscopy, dielectric relaxation, and space charge or polarization distribution.

Techniques to monitor the degree of cure of thin polymer films used in microelectronic packaging are being investigated to correlate with their mechanical and electrical properties. Photoacoustic, fluorescence, and dielectric spectroscopies are among the methods employed. Instrumentation for measuring thermal expansion coefficients of thin-film microelectronic packaging materials is being developed.

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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 that control phase separation kinetics and morphology.

Shear cells for neutron scattering and light scattering measurements also have been developed and used for in-situ structure characterization and melt processing of shear mixed polymer blends and alloys.

Researchers currently are testing kinetic theories of phase separation and late-stage coarsening and 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.

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FLUORESCENCE MONITORING

NIST researchers are using fluorescence spectroscopy to characterize structural and dynamic properties of polymers and to monitor the behavior of polymer flows during processing.

Fluorescence quenching is employed, for example, to monitor the uniformity of mixing in polymer blends and in particle-filled polymer melts. Excimer fluorescence is used to monitor the cure of thermoset resins, to detect crystallization and glass transition temperatures, and to measure the temperature of polymers during processing. Fluorescence anisotropy is used to measure molecular orientation and to monitor the non-Newtonian flows of polymer solutions and melts.

For polymer processing and composites monitoring, optical fibers are used to transmit fluorescence and excitation light energy between the processed polymer and light

source and detection equipment. Well-equipped laboratories containing laser light sources, spectrofluorimeters and a nanosecond spectrofluorimeter are available for carrying out this research.

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METALLURGY

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METALLURGICAL PROCESS CONTROL SENSORS

Special facilities at NIST enable researchers to develop advanced measurement methods and standards for application in process modeling and control for intelligent processing of materials. Measurement methods available include ultrasound, eddy current and acoustic emission. In particular, non-contact ultrasonic facilities featuring high intensity pulsed lasers and electromagnetic acoustic transducers have been designed.

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.

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CORROSION DATA PROGRAM

Corrosion reduces manufacturing efficiency, employee safety, consumer safety, and consumer confidence or perception of quality. To help U.S. industries avoid the negative impact of corrosion, NIST and the National Association of Corrosion Engineers (NACE) joined together to form the NACE-NIST Corrosion Data Program. The objective of this program is to use the latest advances in information science and technology to provide industry with convenient and reliable information on materials performance and corrosion control. Working with experts from industry, NACE-NIST knowledge engineers work to develop expert systems, databases, and modeling programs that are distributed to industry to help avoid corrosion failures.

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CORROSION MEASUREMENTS AND MONITORING

The corrosion of metals in natural and man-made environments is very costly to industry and government. Researchers at NIST are working to develop improved laboratory and field techniques for measuring and monitoring the chemical reactions that degrade the performance of materials in service. NIST researchers were instrumental in the development of transient and static electrochemical techniques for assessing corrosion reactions such as potentiodynamic polarization, electrochemical noise, ac impedance, and in-situ ellipsometry. Also, NIST researchers have developed methods for measuring the corrosion of metals in field

conditions, such as steel in soil and seawater, electric utility lines in soil, and of steel in concrete. Currently, NIST researchers are working on in-situ monitoring of electrochemical conditions and using the information obtained from electrochemical measurements to predict the performance of materials in service.

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MICROSTRUCTURE AND DEFECTS IN CAST ALLOYS

Recent advances in the modeling of metal solidification are making possible a quantitative understanding of the development of microstructure and the origin of defects in cast metal parts. NIST researchers are investigating the ways in which knowledge of thermodynamic phase equilibria and of the dynamics of phase transformations can be used to improve the modeling of complex alloys. Thermophysical properties of these alloys at elevated temperatures are being measured to provide a basis for the modeling studies.

Working in collaboration with a consortium of industries and universities established under the auspices of the Office of Intelligent Processing of Materials, NIST workers are analyzing samples produced in their own laboratories or in the foundries of their collaborators. Such samples are used to test and refine the models so that they can be used more effectively to shorten the design stage of industrial casting processes.

In addition, advanced sensors are being developed to monitor the solidification process.

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PERFORMANCE OF ADVANCED MATERIALS IN SERVICE

The performance of materials in service frequently deviates from that observed in the research laboratory. This discrepancy is due primarily to chemical reactions that occur between the service environment and the material. For new advanced materials, the lack of service experience makes critical materials selection and design decisions difficult and inhibits the acceptance of these materials by industry. NIST scientists are working to assist the development of advanced materials by studying the mechanisms by which service environments influence the performance of these materials. Ultimately, the goal is to develop methods for measuring, quantifying, and predicting the performance of any new material in any application.

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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. Nanocomposites, composition-modulated alloys, high-temperature superconductors, metallic glasses, and icosahedral crystals are among the materials being investigated. Hysteresis, Barkhausen effect, and other magnetic properties of materials are being investigated through computer modeling. Magnetic properties are characterized by ac and dc (vector VSM and SQUID), magnetic susceptibility measurements, magnetocaloric properties, Barkhausen effect, magneto-optic Kerr effect, flux distribution imaging, ferro-

magnetic resonance, and Mössbauer effect observations. Magnetic standards are being developed. Applications include magnetic refrigeration, intelligent processing of materials, information storage, and non-destructive evaluation.

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VAPOR-DEPOSITED THIN FILMS

Obtaining new fundamental understanding of the detailed physics and chemistry of thin-film formation from high-temperature vapor sources is an objective of NIST researchers. This effort is currently developing a laser-produced vapor deposition facility, with measurement access for a variety of existing vapor diagnostics facilities.

These in-situ facilities include high-pressure sampling molecular beam mass spectrometry, optical multichannel emission spectroscopy, laser-induced fluorescence spectroscopy, and optogalvanic effect spectroscopy. These diagnostic techniques provide time-resolved, species-specific gas-phase compositions during the gas transport process.

In addition, film characterization facilities, including magneto-optical Kerr effect, SEM and TEM-based X-ray analysis, and Auger/ESCA are available. Current plans are to extend measurements on film-producing environments to conventional sputtering conditions as well. Films of current interest include electronic, magnetic, and high T_c materials.

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MECHANICAL PROPERTIES OF ADVANCED MATERIALS

Reliable databases of the mechanical properties of advanced materials, such as intermetallics and metal-matrix composites, are needed to facilitate their exploitation in industrial applications. Materials scientists and engineers at NIST are developing the specialized mechanical test methods and measurement techniques needed to evaluate the properties of these materials, which often exhibit anisotropy, inhomogeneity, very low ductility, or other characteristics that negate the use of conventional test methods.

Extensive facilities are available for this work. These include a wide range of testing equipment with associated instrumentation for tensile, compressive, and torsional tests, and also for combined load and fracture tests under a variety of simulated service environments. In addition, separate laboratories are devoted to fatigue, creep, impact, and hardness testing. The staff has extensive experience in all of these areas as well as in related fields such as failure analysis, analytical fracture mechanics, stress analysis, and the modeling of mechanical processes.

Examples of recent and current activities in these areas include mechanical property measurements from the microscale (e.g., electronic solder connections) to multi-million pound-force scales (e.g., fracture toughness of heavy section steels) and studies of the fatigue properties of metal-matrix composites and the residual stresses in welds.

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REACTOR RADIATION

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NEUTRON NON-DESTRUCTIVE EVALUATION

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

NIST and Department of Defense (DOD) scientists are continuing a cooperative project to develop and apply neutron diffraction to texture and residual stress characterization. Texture studies have centered on copper, tantalum, and uranium-alloy components for a variety of DOD end items; recent work has included ceramic superconductors. Neutron residual stress studies have focused on components made of the above metals, ceramics, fiber-reinforced ceramic composites, and steel—including weldments.

NIST scientists are collaborating with scientists from the Smithsonian Institution to continue the examination of art works by

neutron autoradiography. The technique also has been applied to industry-related problems, and efforts are being made to extend its capabilities to cold neutron autoradiography.

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NEUTRON SPECTROSCOPY

The vibrational dynamics and diffusion of hydrogen in metals and molecular species in heterogeneous catalysts, clays, and other layered materials are studied at NIST with inelastic and quasi-elastic neutron scattering. The results of this research reveal the bonding states and atomic-scale interactions and diffusion paths in such materials. 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 that affect 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. Collaborations with researchers from outside laboratories also include studies of the dynamics of atoms and molecules in fullerenes and other molecular solids, alloys, and zeolites.

For the above research, the 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} s to 10^{-14} s. Controlled

temperature (0.3 K to 1300 K) and pressure devices are available for changing sample environments.

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SMALL-ANGLE NEUTRON SCATTERING

Small-angle neutron scattering (SANS) is used to characterize submicron structural and magnetic properties of materials in the size regime from 1 nm to 500 nm. The SANS diffraction patterns produced by structural features in this size regime—for example, by small precipitates or cavities in metal alloys, by micropores or cracks in ceramics, by colloidal suspensions and micro-emulsions, or by polymers and biological macromolecules—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. This detailed microstructure information is often a key to the prediction or understanding of the performance or failure modes of structural materials and materials processing conditions.

A number of scientists from the chemical, communications, advanced materials, and aerospace industries already are engaged in SANS research at NIST.

Three SANS instruments are available in the NIST Cold Neutron Research Facility, which is described on page 88.

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NEUTRON DIFFRACTION

Precise information on crystal structures 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, for example, fullerenes, ceramics, catalysts, and rapidly solidified alloys, often can be obtained only in powdered form. In addition to single-crystal diffraction, state-of-the-art capabilities are available at NIST for measuring and analyzing the crystal and magnetic structure of polycrystalline materials by neutron diffraction. Both single-crystal and multidetector, high-resolution powder diffractometers are available.

NIST researchers continue to develop improved methods for accurate structure refinement. A major effort is under way in relating atomic arrangement, including defects, to 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.

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NEUTRON REFLECTOMETRY

The importance of thin films, layer structures, and interfaces has grown significantly in the last few years in a number of applications areas. Analogous to electromagnetic radiation, neutrons can undergo specular reflection at surfaces. Because neutrons can distinguish between different isotopes of the same element (such as hydrogen and deuterium), can penetrate to focus on sub-surface interfaces, and are sensitive to magnetic properties of materials, they provide an important complement to other surface probes.

Thermal neutron reflectometry and grazing-angle diffraction are currently available at the NIST reactor. For the former, reflectivities as low as 2×10^{-7} have been measured, which is competitive with any neutron reflectometer in the world. An even more sensitive instrument is now operational in the NIST Cold Neutron Research Facility. Reflectometry studies at NIST and elsewhere include superconducting and magnetic layers, magnetic multilayers, polymer interfaces, and solid-liquid interfaces.

Neutron grazing-angle diffraction—first demonstrated at NIST—is a very new technique. With this approach, lattice spacings of planes with normals parallel to the sample surface are determined to depths of ~ 10 nm.

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RESEARCH FACILITIES

NIST RESEARCH REACTOR

The NIST research reactor is a national center for the application of reactor radiation to a variety of problems of national concern. A wide variety of internal and external programs have benefited from the broad range of capabilities available to researchers from industry, universities, and government laboratories.

CAPABILITIES

The NIST reactor is an enriched-uranium, D₂O cooled and moderated reactor, with a peak thermal core flux of 4×10^{14} neutrons/cm²-s. The core comprises 30 fuel elements of a unique, split-core design, in which nine radial beam tubes look at a 17-cm gap between fuel-element halves. A large-volume cold source, two tangential and one vertical beam tube, a thermal column, several vertical thimbles, and four "rabbit" tubes complete the configuration. The reactor operates continuously, 24 hours a day on monthly cycles, followed by approximately a week of shutdown for refueling and maintenance.

The reactor utilizes the flux available in a very efficient manner through relatively short core-to-instrument distances and large-diameter beam tubes. As a result, the flux on the sample for certain instruments is comparable to that at other major research reactors of higher power and peak core flux.

The experimental facilities in the reactor hall are used for neutron scattering and diffraction, neutron radiography, trace analysis and depth profiling, neutron dosimetry and standards development, irradiations, and isotope production.

Sample environments for low and high temperature, low and high pressure, and high magnetic fields are routinely available. On-line graphics, plotting, and data fitting are available via personal computers, Macintoshes, Micro-VAXs, and a DEC 5810.

- Elastic Scattering. Three beam ports are dedicated to elastic scattering studies. A new high-resolution powder diffractometer is installed at beam tube 1 (BT-1). It is a 32-detector instrument that provides three monochromator positions, each set at 0.154-nm wavelength but at different take-off angles to allow maximum flexibility in selecting the optimal resolution function for a given measurement. Collimations down to 7'-20'-7' are available.

A triple-axis spectrometer with a four-circle goniometer is installed at BT-6 and is used primarily for residual stress and texture measurements, although inelastic scattering experiments also can be performed. This spectrometer is typically operated in the elastic scattering mode without an analyzer for texture studies and with the analyzer for residual stress measurements. Incident energies are continuously variable with $2\theta_M$'s from 20' to 75' available. Beam sizes up to 30×50 mm² and down to 2×2 mm² (for residual stress studies) are utilized. Single-crystal structure determinations are performed on this instrument while a new residual stress/texture/single-crystal diffractometer is being completed on BT-8.

A new thermal-neutron reflectometer, in which the incident beam can be polarized and the spin state of the reflected beam analyzed, is operational on BT-7. In this reflectometer, a pyrolytic graphite (PG) filtered beam is incident on the vertically focusing PG monochromator set for a principal wavelength of 0.235 nm. For collimations of

~1' preceding and 1' following the monochromator, respectively, the wavelength resolution $\delta\lambda/\lambda \sim 0.01$, and the actual flux on the sample is $\sim 5 \times 10^5$ neutrons/cm²-s. Two ³He detectors are incorporated: one for reflectivity measurements; the other for grazing-angle-diffraction experiments.

Polarization of the incident beam is accomplished in transmission by one or more polarizing Fe-Si supermirrors deposited on single-crystal Si substrates. Reflectivities down to about 2×10^{-7} with a signal-to-noise ratio of about 1 have been measured.

- **Inelastic Scattering.** Three triple-axis inelastic scattering spectrometers are operational. The BT-4 instrument employs two remotely selectable, vertical-focusing monochromator crystals (pyrolytic graphite and Cu), which provide incident energies from 3 meV to 300 meV continuously. It is capable of elastic-peak resolution down to 0.04 meV and also can be used in the inverted-filter mode for energy-loss spectroscopy of vibrations in the 15-meV to 280-meV range. The BT-9 spectrometer offers variable incident energy in the 5-meV to 50-meV range and collimations down to 10'-12'-12'-16'.

The BT-2 instrument has both triple-axis and polarized-beam (up to 96 percent) capabilities. Either a pyrolytic graphite or a Heusler-alloy monochromator, each vertically focused, are available, with remotely insertable cold beryllium or pyrolytic graphite filters. Built-in guide fields and spin rotators and collimation as low as 10'-5'-5'-20' are available.

- **Elemental Analysis.** Neutron activation analysis is performed utilizing the clean room for sample preparation, the reactor irradiation facilities, semi-hot and warm radiochemistry labs, and state-of-the-art radiation-counting labs. Development of methodology has aimed at accuracies and sensitivities over concentrations of 10^{-10} percent to 100 percent.

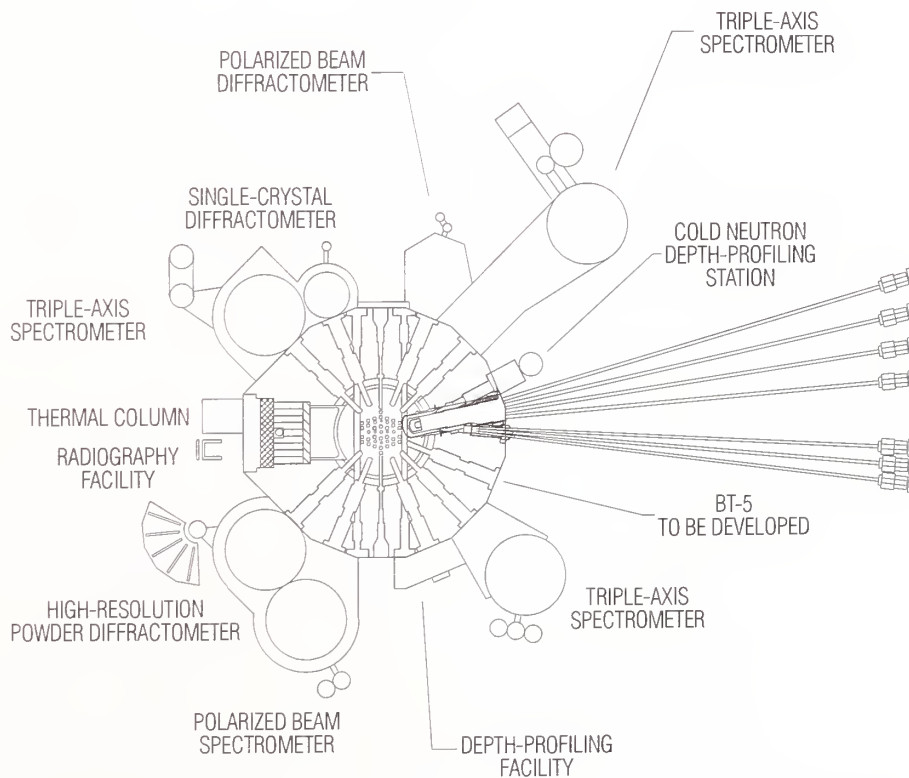
Radiochemical separations for specific elements and multielement analysis at the ultratrace level are available. A thermal neutron-capture prompt-gamma activation analysis facility is operational, with a neutron fluence of 5×10^8 n/cm²-s in a 2-cm-diameter beam.

A thermal neutron-depth-profiling facility is installed on BT-3 for non-destructive determination of near-surface elemental depth distributions in a variety of materials. Sensitivities approaching 10^{13} atoms/cm² with a spatial resolution of better than 30 nm for depths of 5 mm to 20 mm are achievable.

- **Neutron Standards and Dosimetry.** A number of neutron fields for standards and dosimetry are available. These include a Cf fission source, a ²³⁵U cavity fission source, the thermal column beam, an intermediate energy standard neutron field, and 2-, 24.5-, and 144-keV filtered beams.

- **Irradiation Facilities.** Four pneumatic tubes for 40-cm³ rabbits with fluence ranges of 3×10^{11} to 2×10^{14} n/cm²-s for irradiations of seconds up to hours are available. The cadmium ratio range for these facilities is 4 to 3000 (Au). For long irradiations 6-cm- and 9-cm-diameter in-core thimbles are used. These are D₂O filled with fluences of $2-4 \times 10^{14}$ n/cm²-s.

- **Neutron Radiography.** Radiography facilities are available at a highly thermalized beam of the thermal column. Fluences range from 10^5 to 10^7 n/cm²-s, depending on resolution, with a Cd ratio of 500:1 and an L/D ratio adjustable from 20:1 to 500:1. The beam is 25 cm in diameter at the image plane 2 m from the reactor face. Facilities for autoradiography also have been developed.



APPLICATIONS

Many of the principal applications have been described elsewhere in this report. Others include:

- Structural and Spectroscopic Studies of Magnetic Materials. Recent efforts have focused on rare-earth compounds, amorphous magnets and spin glasses, superconductors, magnetic bilayers, and hydrogen in metals.
- Elemental Analysis Programs. Examples include studies in environmental chemistry, nutrition, biomedicine, energy and electronic devices—with emphasis on Standard Reference Materials for these applications.
- Neutron Dosimetry Studies. Specific projects include neutron fluence standards for power reactor pressure vessel irradiation surveillance, ultralight mass assay for commercial track recorder detectors, absolute fission-rate measurements, and development of thermal neutron beam monitors.

AVAILABILITY

There are 25 thermal neutron facilities at the reactor, which provide about 125,000 instrument hours per year. In 1992, over 700 researchers from 14 NIST divisions, 28 other government organizations, 114 U.S. industrial and university laboratories, and 65 foreign laboratories utilized the facilities, either collaboratively with NIST staff or independently.

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COLD NEUTRON RESEARCH FACILITY

The NIST Cold Neutron Research Facility (CNRF) is the first in the United States devoted exclusively to cold neutron research. The facility provides U.S. researchers prime access to a key tool of modern materials science. When fully complete in 1994, the \$30 million project will provide 15 new experimental stations for use by U.S. researchers, with capabilities currently unavailable in this country.

The facility is focused on the cold source, a block of D₂O ice (with 8 percent H₂O added) cooled to ~40 K by recirculating helium gas. The cold source is viewed by one port inside the reactor hall and seven neutron guide tubes. The guide hall and associated office and laboratory space has more than tripled the workspace available at NIST for neutron beam researchers.

CAPABILITIES

Instruments currently in operation include:

- Small-Angle Neutron Scattering (SANS). The NIST/Exxon/University of Minnesota and the NSF/NIST Center for High Resolution Neutron Scattering (CHRNS) 30-meter SANS instruments combine long flight paths and variable collimation to provide flexibility, angular resolution, and beam intensities that compare favorably with any SANS instruments in the world. Large-area position-sensitive detectors provide exceptional sensitivity to materials structures ranging from roughly 1 nm to 500 nm. An 8-m SANS instrument also is available. Computer-automated equipment is available for maintaining samples at temperatures from 4 K 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. Polarized neutron capabilities are planned for both 30-m instruments.

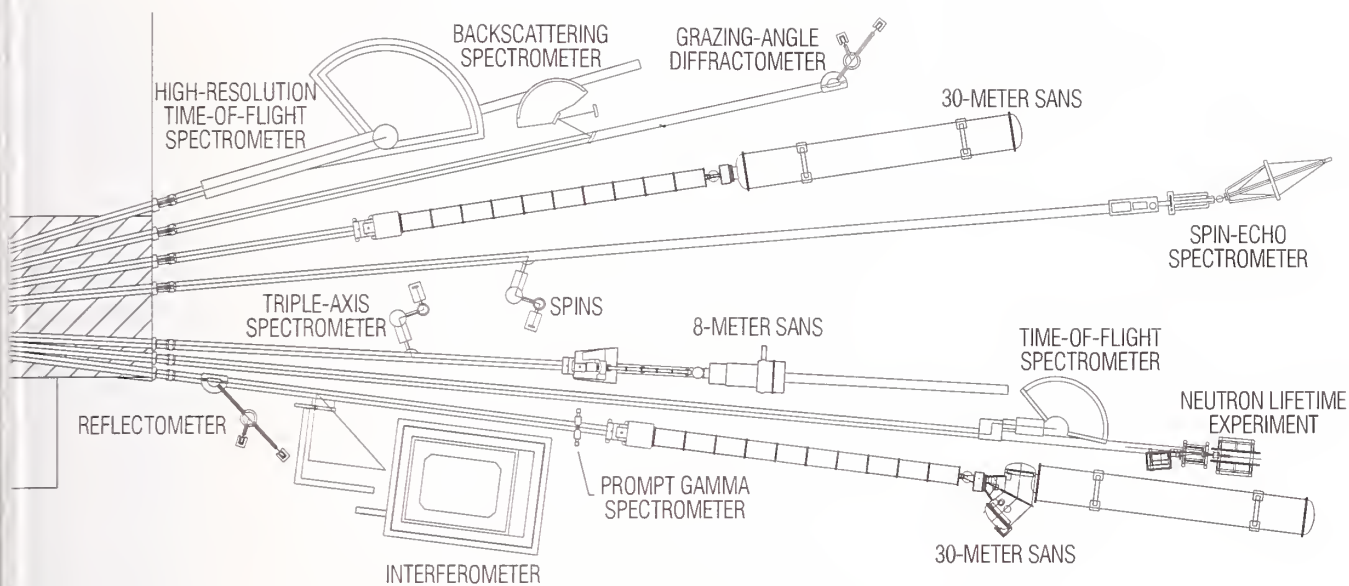
- Depth-Profiling Instrument. With a measured chemical sensitivity 20 times that of the existing NIST thermal-beam instrument, this station features automated sample handling, near real-time spectral processing, goniometer positioning of sample and detectors, and sample temperature control. Increased signal intensity will permit multidimensional imaging of elemental distributions and profiling of nuclides with absorption cross-sections for charged particle emission of less than 1 barn.

- Prompt-Gamma-Ray Activation Analysis. Providing much greater sensitivity for this method than any existing thermal-beam instrument in the world, this equipment provides unique measurements of chemical elements, such as hydrogen (detection limit $\leq 2 \mu\text{g}$), that are difficult to detect by other means.

- Medium Resolution Time-of-Flight Spectrometer. The energy resolution of this instrument, 40 to 600 μeV , is suitable for a broad range of studies of diffusional motions and magnetic and vibrational excitations. A combination of double-crystal monochromator and Fermi chopper, with a detector array covering a large range of scattering angles, allows incident energies from 2.2 to 15.5 meV and (elastic) momentum transfers from 1.0 to 49 nm^{-1} .

- NIST/IBM/University of Minnesota Cold Neutron Reflectometer. This instrument is expected to exceed the sensitivity of the thermal instrument—already among the best in the world. In addition, the CNRF reflectometer incorporates vertical scattering-plane geometry and a horizontal sample plane that allows examination of liquid surfaces. Independent movement of sample and detector allows measurement of off-specular scattering. A grazing-angle diffraction capability will be added in the future.

- Fundamental Physics Station. Available for use only in collaboration with the NIST fundamental physics research group, an end guide position physics station currently is instrumented for a new measurement of the



lifetime of the neutron. A second fundamental neutron physics station, a neutron interferometer, is also operational.

- A neutron optical bench is available for testing and calibrating neutron devices such as focusing capillary tubes.
- A cold neutron triple-axis spectrometer is operational.

Instruments planned for completion by the end of 1994 include a spin-polarized inelastic neutron spectrometer, a high-resolution time-of-flight spectrometer, a back-reflection spectrometer, and a spin-echo spectrometer.

APPLICATIONS

The unusual sensitivity and range of measurements possible at the NIST CNRF provide applications in materials structures, materials dynamics, chemical analysis, and neutron physics. Currently operational instruments are used to study microstructures in metals, ceramics, and colloidal mixtures; thin films, layered structures, and interfacial properties; magnetic properties and shear-induced phenomena; molecular geometry of polymer and biological macromolecules; chemical composition of

semiconductors, high-tech materials, air-pollution filters, and other samples; and neutron decay rates.

AVAILABILITY

The CNRF operates as a national facility open to all qualified researchers. NIST develops experimental stations for use by the general U.S. research community. Two-thirds of the available time on these stations (three-fourths on CHRNS instruments) will be allocated by a Program Advisory Committee (PAC) on the basis of scientific merit of written proposals. The second mode involves Participating Research Teams (PRTs), which are developing the remaining stations. The PRTs are responsible for design, construction, and maintenance of the facilities in return for three-fourths of the available time. The remaining time will be allocated by the PAC. For all instrumental stations, instrument-responsible scientists will be designated to assist users in performing their experiments.

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METALS PROCESSING LABORATORY

The metals processing laboratory at NIST contains special facilities for the production of rapidly solidified alloys, including equipment for gas atomization and electrohydrodynamic atomization to produce rapidly solidified alloy powders, melt spinning to produce rapidly solidified alloy ribbons, and electron beam surface melting to produce rapidly solidified surface layers. Hot isostatic pressing equipment is available for consolidating alloy powders.

CAPABILITIES

- **Gas Atomization.** The gas atomization system can be used to produce up to 25 kg of rapidly solidified alloy powder per batch while maintaining a controlled atmosphere throughout the atomizing and powder handling process. High-energy gas (Ar or N) impinging on a liquid metal stream breaks up the liquid into small droplets, which solidify rapidly. Cooling rates are up to 10^5 K/s. The atomized powder, entrained in the gas flow, is collected in removable, vacuum-tight canisters. This facility can be used for proprietary research.

- **Electrohydrodynamic Atomization.** In the electrohydrodynamic atomization system, a liquid metal stream is injected into a strong electric field. The field causes the stream to disintegrate into droplets, which solidify rapidly to produce extremely fine ($<1\ \mu\text{m}$ diameter) alloy powder. Powder produced by this process is well-suited for studying solidification dynamics. As the system is presently configured, small quantities for microscopic examination can be produced from alloys with melting points up to $900\ ^\circ\text{C}$.

- **Melt Spinning.** Melt-spinning techniques can be used to produce rapidly solidified alloys in ribbon form. Because of the high cooling rates (up to $10^6\ \text{K/s}$) with this method, amorphous alloys as well as crystalline alloys can be produced. Ribbons up to 3-mm wide and 0.05-mm thick can be produced in quantities of several grams per batch. Materials with a wide range of melting points, from aluminum alloys to superalloys, have been produced.

- **Electron-Beam Surface Melting.** An electron-beam system, which provides surface melting and subsequent rapid resolidification of surface layers, can be operated in either a pulsed or continuous mode. The electron beam can be focused to a spot less than 1 mm in diameter and deflected at frequencies up to 5 kHz.

- **Hot Isostatic Press.** A hot isostatic press (HIP) with microprocessor control of the temperature-pressure-time cycle is available for consolidation of powder or compacted powder shapes. The HIP has a cylindrical working volume 15 cm in diameter and 30-cm high. The maximum working pressure is 207 MPa. The molybdenum furnace has a maximum heating rate of 35 K/min and is capable of maintaining $1500\ ^\circ\text{C}$.

AVAILABILITY

These facilities are designed to produce alloy research samples that otherwise are difficult for users to obtain. Typically, industrial companies or universities send workers to NIST to participate in preparing alloys of special industrial and scientific interest for further analyses in their home laboratories and to collaborate with NIST scientists in investigations of generic relationships between processing conditions and resulting alloy microstructures and properties.

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POLYMER COMPOSITE FABRICATION FACILITY

The composite fabrication facility permits the preparation of well-controlled polymer composite samples for scientific studies and the evaluation of results from NIST's processing science program in a realistic fabrication environment.

CAPABILITIES

The facility involves five major components and associated support equipment: a prepregger to prepare sheets (up to $180\ \text{cm} \times 30\ \text{cm}$) of unidirectional fiber coated with resin; a fully computerized autoclave capable of temperatures up to $430\ ^\circ\text{C}$ and pressures up to 2.1 MPa; an automated hydraulic press (temperatures up to $535\ ^\circ\text{C}$) with water-cooled platens for rapid, controlled cooling; a unidirectional flow facility for characterizing the permeability of fiber preforms in all three directions; and a specially designed two-component pumping system for fabrication of samples by resin transfer molding and for conducting flow visualization experiments.

APPLICATIONS

The facility can be used to study a variety of questions, such as the details of resin flow and void formation during processing and the influence of processing conditions, fiber orientation, and fiber-surface treatments on performance.

AVAILABILITY

Used by NIST staff in an active research program on polymer composites, the facility is available for collaborative studies with industry, academic institutions, and other government agencies.

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POWDER CHARACTERIZATION AND PROCESSING LABORATORY

Advanced ceramics are manufactured by the consolidation of fine powders. Researchers at NIST are working to develop the scientific foundation needed for improving reproducibility and reducing the cost of producing ceramic components. The powder characterization facility offers specialized instrumentation for measuring physical properties, phase composition, and surface chemical properties. In addition, facilities exist for processing and synthesizing ultrapure powders.

CAPABILITIES

- **Physical Properties Measurement.** Particle-size distribution, specific surface area, specific gravity, and porosity are some of the major physical properties for which instrumentation is available. Powder-size distribution can be determined by gravity sedimentation followed by X-ray absorptiometry, centrifugal sedimentation, light diffraction, and photon correlation spectroscopy.

The size range of these instruments covers 0.03 μm to 200 μm . Each instrument works in a specific range and provides the data in the form of a discrete size range. The particles are examined directly by the application of scanning and transmission electron microscopy of particles as small as 0.001 μm .

- **Surface and Interface Chemistry Measurements.** The surface and interface characterization of powders contributes to the knowledge base of the surface interactions of particles in contact with solvents. As the particles become smaller, their surface characteristics become more significant. MicroRaman and Fourier transform infrared spectroscopy are used to study surface composition, and electrophoretic mobility and acoustophoretic mobility are used to study modification to the powder surface as a result of an interaction with a solvent.

- **Phase Composition.** Since most of the ceramic powders undergo phase transformation during densification, understanding the phase changes in specific densification environments is an active part of NIST research. The Siemens high-temperature X-ray diffractometer has a temperature range from room temperature to 3000 K and a position sensitive detector. In addition, sintering can be carried out in oxygen-free argon or nitrogen environments.

- **Solid-State Imaging.** The solid-state nuclear magnetic resonance (NMR) spectrometer/imager carries out measurements in chemical shift, nuclear spin density, relaxation times, and imaging of NMR active nuclear distribution. Ceramic powder slurries, green bodies, and dense ceramics can be analyzed for identification of impurities, chemical state, and composition distribution by non-destructive evaluation. In addition, the NMR can determine amorphous phase content of the powders.

- **Powder Synthesis.** The ability to synthesize powders of controlled characteristics is necessary for development of a powder-processing knowledge base. The fine-powder synthesis facility consists of a chemical flow reactor for controlled synthesis and inert atmosphere chambers. A solution atomizer is available to generate polydisperse aerosols in the range 0.01 μm to 1.0 μm , as is a spray dryer to form monodisperse agglomerates in the range 0.5 μm to 100 μm .

- **Colloidal Suspensions Preparation.** Colloidal processing of ceramic powders has emerged as an attractive technology for producing defect-free ceramics. However, some major issues still remain to be addressed, including the lack of characterization techniques for slurries that contain high concentrations of solids and scientific understanding of limitations in the preparation of such slurries. The powder processing laboratory consists of an acoustophoresis instrument, a rheometer, a high-energy agitation ball mill, and slurry consolidation equipment. These techniques are used to study interface chemistry, flow behavior, size reduction, morphology modification, and densification of polydisperse particles and similar processes resulting from interactions between the particles and their environment.

AVAILABILITY

These facilities are used primarily to support NIST research programs using ceramic powders. They are available for collaborative or independent work by qualified government, industry, or university personnel with preference given to projects related to ceramics research.

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A256 Materials Building

CRYOGENIC MATERIALS LABORATORY

NIST has the nation's leading facilities for the evaluation of the mechanical, physical, and thermal properties of materials at low temperatures, particularly for liquid helium (4 K) and liquid oxygen (90 K). These facilities are used routinely by industry and other government agencies to characterize materials for superconducting magnets, aerospace propulsion systems, and energy storage and transportation equipment.

CAPABILITIES

A wide range of mechanical properties can be measured at cryogenic temperatures, including tension, compression, torsion, shear, fatigue, creep, and fracture toughness. Eight test machines with maximum load capacities ranging from 4 kN to 5000 kN are equipped with cryostats and fixtures for the various tests.

Elastic constants and related physical properties are measured over the temperature range 295 K to 4 K. Thermodynamics links elastic constants with specific heat, thermal expansivity, atomic volume, and the Debye temperature. Related studies are conducted in an X-ray diffraction unit equipped with a cryogenic stage. Other physical property measurement capabilities include magnetic susceptibility and thermal properties.

Thermal property measurement capabilities include thermal expansion and thermal conductivity. For insulating materials, thermal conductivity is measured in guarded hot plate (GHP) apparatus; the laboratory has four GHPs with measurement capabilities ranging from 4 K to 1200 K. A fixed-point compression probe is used for conducting materials such as metals.

Several unique facilities are available for oxygen compatibility studies. Friction and wear studies are conducted on bearing materials for liquid oxygen pumps in a ball-on-disk tribometer capable of operating in liquid and gaseous oxygen environments. A high-pressure/high-temperature differential

thermal analysis apparatus is used to study the oxidation of metals in liquid-oxygen propulsion systems.

AVAILABILITY

These facilities are available to guest researchers for collaborative programs. NIST routinely performs research and measurement services for outside sponsors.

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SMALL-ANGLE X-RAY SCATTERING FACILITY

Small-angle X-ray scattering (SAXS) is a technique in which a highly collimated beam of X-rays (wavelength range 0.07 nm to 0.3 nm) is used to probe the structure of materials on the size scale of 0.1 nm to 100 nm.

Materials exhibiting structure in this size range include polymers, biological macromolecules, ceramics, metals, and alloys. The small-angle scattering patterns can be analyzed to characterize the size and shape of the scattering centers as well as their spatial distribution and surface area. Data obtained from these experiments are complementary to data obtained from other diffraction studies and from morphological studies using electron microscopy.

CAPABILITIES

The NIST 10-m SAXS camera uses a 12-kW rotating anode X-ray generator as a source of X-rays. The target is usually copper $\lambda(K\alpha) = 1.54$, but additional wavelengths are available. The collimation path is defined so as to permit a 10^{-2} nm^{-1} resolution in reciprocal space at the surface of a two-dimensional position-sensitive proportional detector. The collimation path and the scattered beam path are evacuated, and all elements of vacuum operation, X-ray optical configuration, sample selection, and

calibration are computer controlled. Image data are collected by a minicomputer, and a complete collection of software is available for displaying, analyzing, and modeling the results.

Sample chambers are available for measurements at high temperatures and to deform specimens during measurement.

APPLICATIONS

The SAXS technique is used to study molecular conformation, microphase domain structures, crystallization phenomena, network formation, craze initiation, void distribution, and similar phenomena resulting from fluctuations in electron density within a material. Such studies are currently of broad interest in all areas of materials science.

AVAILABILITY

This facility is operated by members of the NIST staff in support of their active research program in polymeric materials. It is available for use by researchers from industry, academia, and other government agencies on either a collaborative or independent basis.

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MATERIALS SCIENCE X-RAY BEAMLINES

NIST operates two beamstations on the X23A port at the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory in New York. The light source provides an intense continuous-spectrum beam of collimated and polarized X-rays many orders of magnitude brighter than the beams provided by conventional laboratory sources. These two beam stations offer access to dedicated instrumentation for small-angle X-ray scattering, X-ray diffraction imaging (topography) and extended X-ray absorption fine structure.

CAPABILITIES

Small-angle X-ray scattering can be carried out in the photon energy range from 5 keV to 11 keV. The minimum wavevector is $4 \times 10^{-3} \text{ nm}^{-1}$ and the wavelength resolution is $\Delta\lambda/\lambda = 10^{-4}$, enabling anomalous small-angle scattering with excellent resolution. Diffraction imaging of single crystals and powders is carried out with monochromatic photons between 5 keV and 30 keV. An energy-tunable X-ray image magnifier enables imaging of microstructure down to less than 1 mm. The energy-scanning experiments, primarily EXAFS, also are performed over an energy range from 5 keV to 30 keV.

APPLICATIONS

Small-angle scattering measurements on ceramic and metallurgical materials are used to characterize the microstructure in the 2-nm to 1- μm size range as a function of starting chemistry and processing parameters. Scattering from a particular entity can be separated from other scatterers in a complex material using anomalous small-angle X-ray scattering. Diffraction imaging is used to study imperfections and strains in single crystals and powder compacts. The structure of strained semiconductor interfaces and metal multilayers can be studied using EXAFS. A combination of EXAFS and diffraction will provide a capability for site-specific local structure determination in crystals.

AVAILABILITY

Beam time is available to qualified scientists provided safety requirements are met and scheduling arrangements can be made. Proposals for collaborative use of the facility are reviewed at NIST; proposals for independent use of the facility should be submitted to the NSLS.

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BUILDING AND FIRE RESEARCH LABORATORY

Major goals of the NIST Building and Fire Research Laboratory are to improve the productivity of the U.S. construction industry, which now faces stiff competition from overseas firms, and to reduce the human and economic losses resulting from fires, earthquakes, winds, and other hazards. Through performance prediction and measurement technologies, as well as technical advances, the laboratory works to improve the life-cycle quality of constructed facilities.

The laboratory studies fire science and fire safety engineering; building materials; computer-integrated construction practices; and structural, mechanical, and environmental engineering. Products of the laboratory's research include measurements and test methods, performance criteria, and technical data that are incorporated into building and fire standards and codes. Staff members are involved in more than 100 activities to develop voluntary standards.

The laboratory conducts investigations at the scene of major fires as well as structural failures due to earthquakes, hurricanes, or other causes. The knowledge gained from these investigations guides research and is applied to recommendations for design and construction practices to reduce hazards.

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B216 Building Research Building

COOPERATIVE RESEARCH OPPORTUNITIES

Structures

- 93 Structural, Earthquake, and Wind Engineering

Building Materials

- 94 Cement and Concrete
94 Organic Building Materials

Building Environment

- 95 Lighting
95 Indoor Air Quality
95 Refrigeration Machinery
95 Thermal Insulation
96 Building Controls
96 Computer-Integrated Construction

Fire Safety Engineering

- 96 Fire Protection Applications
97 Fire Modeling
97 Hazard Analysis
97 Large Fires

Fire Science

- 97 Advanced Fire Sensing
98 Smoke and Toxic Gas Prediction
98 Polymer Combustion Research

RESEARCH FACILITIES

- 98 Large-Scale Structures Testing Facility
99 Tri-Directional Test Facility
99 Large Environmental Chamber
100 Calibrated Hot Box
100 Line Heat-Source Guarded Hot Plate
100 Fire Research Facilities

COOPERATIVE RESEARCH OPPORTUNITIES

STRUCTURES

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B168 Building Research Building

STRUCTURAL, EARTHQUAKE, AND WIND ENGINEERING

Under the National Earthquake Hazards Reduction Program, NIST performs research and development work used in standards for the seismic safety of structures. Experimental and analytical research under way at NIST helps to develop knowledge for design and construction standards for new and existing buildings and lifeline structures. The work involves identifying mechanisms of failure and establishing criteria to ensure structural safety.

Research is coordinated with researchers and practitioners from industry, academia, and federal and state governments. The results provide designers and constructors with improved methods to predict and assess the resistance of buildings and structures to seismic loads, guidelines for strengthening new and existing structures, and technologies to revise civil engineering related standards and codes.

Current research addresses:

- a rational procedure to determine the ultimate shear strength of partially reinforced masonry walls;
- strength and ductility of connections in precast concrete structures;

- drift control criteria for flexible frames;
- evaluation criteria for base-isolation systems and test procedures for evaluating the response of structures subjected to seismic loading;
- strengthening methodologies for concrete frame structures; and
- effects of subsurface conditions on ground motion.

Other structural research includes:

- studies of structural performance for developing standards and test methods for high-performance concrete in major construction applications;
- response of low-rise structures and cladding to extreme wind loads;
- techniques and instrumentation for assessing the properties of existing structures and for developing technical criteria and methodologies for strengthening and repairing existing structural members and systems; and
- analytical and experimental methods for identification of dynamic response characteristics of flexible members and structural networks.

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BUILDING MATERIALS

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CEMENT AND CONCRETE

NIST researchers are undertaking research to develop a fundamental understanding of the relationship between chemistry, microstructure, performance, and service life of conventional and high-performance concrete and other inorganic building materials. Their goal is to develop tools for predicting 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 the concrete.

Models are being developed to consider service conditions, including the chemistry 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.

This work will help the U.S. construction industry be competitive in advanced concrete materials and construction. The research is being coordinated with industry and voluntary standards organizations and trade associations, the National Science Foundation's Center for Advanced Cement-Based Materials, and federal and state government agencies.

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B348 Building Research Building

ORGANIC BUILDING MATERIALS

NIST is conducting basic and applied research to develop methods for predicting the performance and service life of organic building materials, such as protective coatings for steel, roofing materials, and asphalt. Researchers at the Institute are investigating degradation mechanisms, improving characterization methods, and developing mathematical models of the degradation processes. Stochastic models, which are based in reliability theory and life-testing analysis, are included in the modeling efforts for coatings and roofing materials.

To help in understanding the mechanisms of degradation and provide data for models, materials are characterized in many ways, including Fourier transform infrared spectroscopy, thermal analysis, scanning electron microscopy/energy dispersive X-ray, and visual and infrared imaging. Researchers also are developing improved ways to characterize atmospheric environments to which these materials are exposed. Characterization of environmental parameters that cause degradation is needed to link material properties with service life.

The NIST work provides a strong scientific and technical basis for standards used by industry. The research is coordinated with voluntary standards organizations and trade associations, industry, and other federal agencies.

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BUILDING ENVIRONMENT

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B306 Building Research Building

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 systems. NIST researchers are working to develop improved evaluation methods and design tools for design and operation of efficient lighting systems; test and rating methods to determine energy performance of lighting fixtures and systems; and lighting quality metrics sensitive to changes in obstruction, reflections, and different lighting configurations. Their research is performed in collaboration with industry organizations, including professional societies, trade associations, academia, and federal and state governments.

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 will 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.

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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. The results of this work produce improved methods to predict and perform ventilation measurements for use by researchers and practitioners to predict and design room environments, including air distribution, air quality, design ventilation systems, and ventilation performance of existing systems.

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

The first phase of the research is complete. 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.

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REFRIGERATION MACHINERY

NIST researchers are exploring refrigerant mixtures to improve the efficiency of refrigeration cycles and replace harmful fluorocarbon refrigerants that are believed to be damaging the ozone layer of the upper atmosphere. Working with industry, they help improve capabilities in determining the performance of refrigeration mixtures and help refrigeration equipment manufacturers in designing refrigeration systems.

The researchers evaluate a wide variety 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. This is 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 and equipment built and evaluated. A mini-breadboard that uses a very small charge also has been built so that rare refrigerants of limited production can be studied. Research findings are incorporated into appropriate standards and codes.

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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), and refining a dynamic test procedure for building components.

A 1-m guarded hot plate is used to develop SRMs; 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.

This work provides the national "meter-bar" for the thermal insulation industry. All advertised thermal insulation product performance is traceable to measurements made in this program.

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B320 Building Research Building

BUILDING CONTROLS

NIST research is fostering the development of more intelligent, integrated, and optimized building mechanical systems. A dynamic building/heating, ventilating, and air-conditioning 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. NIST technologies serve as a basis for ASHRAE standards to assist the control system manufacturers to develop interoperable systems and methods for testing conformance to the standard.

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 is under way to develop an HVAC/building emulator/EMCS tester, which will provide a method for evaluating application algorithms.

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COMPUTER-INTEGRATED CONSTRUCTION

NIST researchers are developing rational techniques for defining and testing computer representations of information needed throughout the building process, from the conception of a building to its demolition. The goal of the program is to develop validated neutral data representations for use in standards for accessing, exchanging, and archiving information. As a corollary, the program seeks to develop testing methods that assure consistency, completeness, and correctness of information. The research draws on evolving information technologies, including knowledge engineering and semantic modeling. Subject areas for research include standards and codes, engineering drawings, and product data.

Past research has resulted in methodologies for representing, analyzing, and expressing standards, and for interfacing standards to computer-aided design systems. Recent results are being applied in the development and validation of national and international standards for product data. This work led to the improved 3D Piping IGES Appli-

cation Protocol (AP) to meet a high-priority data exchange requirement of industry and government. It also has produced a prototype AP framework to provide a structure to classify APs and to plan DOD Computer-Aided Acquisition and Logistics Support Program APs and the work of the International Organization for Standardization's project on developing the Standard for the Exchange of Product Model Data.

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FIRE PROTECTION APPLICATIONS

The expedient transfer of scientifically based technology from NIST to the professional user community and the creation of a link between NIST computer-based activities and others doing similar or complementary work will enhance fire safety and reduce its costs. Over the past decade, NIST researchers have developed many computer models of various aspects of fire. Researchers develop engineering systems for design application and fire investigation, collect supporting data and programs, and operate training programs and user workshops.

This work has resulted in advanced methods to solve fire safety problems, which are then implemented through improved designs and regulations.

In addition, NIST maintains the Fire Research Information Service (FRIS) consisting of national and international fire research literature and FIREDOC, the automated database of fire research literature. FRIS is the only comprehensive national library resource for the fire community.

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FIRE MODELING

Predictive fire models need accurate representations of burning objects. The most important of these for residences are upholstered furniture and wall coverings. NIST researchers are using both laboratory experiments and computer modeling to understand the processes that govern these types of combustion. Algorithms are being developed and validated for use in hazard analysis. This research results in improved prediction methods of the rate and extent of fire spread on interior room surfaces and furniture and the movement of fire products around buildings.

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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 that

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 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.

The results of this research help manufacturers, purchasers, designers, code officials, fire investigators, and practitioners evaluate the fire hazard implications of the products and fire protection strategies they use.

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LARGE FIRES

Large fires result from industrial or transportation accidents, natural disasters, arson, or when fire protection systems in constructed facilities fail to perform adequately. While these fires present a hazard to building occupants, firefighters, and the surrounding area, little is known about their characteristics, their growth and control, and methods of mitigating their impact. NIST is performing research and developing techniques to measure, predict the behavior of, and better control large fires. Large building fires involve the interaction of strongly buoyant gas flows and thermal radiation with complex structures. In some cases, sudden releases of fire gases erupt into uninvolved spaces through failures of barriers or control systems. Experiments to evaluate the use of helium and

SF₆ mixtures to measure the flow of strongly buoyant fire gases in building structures will provide a tool to reduce vulnerability to large fires.

NIST also is measuring smoke plumes from large, open-air fires to help develop computer models that can predict their size and movement. Further fire dynamics research and advanced computational fluid dynamics will lead to methods capable of assessing the local impact of large fires. These methods can be used by industry in preplanning analysis for potential accidents or as technical support for emergency response.

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FIRE SCIENCE

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ADVANCED FIRE SENSING

Fires that are detected and suppressed quickly do little damage. NIST researchers are studying new "fire signatures" that would enable the development of a new generation of detectors. The signals from these detectors would be electronically analyzed to alert occupants or suppression devices, perhaps even before flames exist. The research also is intended to understand and provide technology for avoiding the high false alarm rate of current detectors. Advanced concepts for fire suppression chemicals, reduced explosion potential, and

minimizing collateral damage from the application of the suppressant also are being explored.

The results demonstrate the response of discriminating detection systems to early fire events and the performance of alternative suppressants that are consistent with regulatory and economic constraints of the fire protection systems manufacturers and the industries and agencies that they serve.

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SMOKE AND TOXIC GAS PREDICTION

Most people who perish in fires die from smoke inhalation. Many are exposed to this smoke for longer periods because the blackness of the smoke impedes their escape from the burning building. NIST research is developing the scientific base and the predictive methods for the yields of carbon monoxide (the predominant toxicant) and soot. These require improved knowledge of the chemical and physical processes in flames, combined with the fluid mechanical processes that dominate air entrainment into fire plumes and the flow fields within a compartment.

The results of this research have been used to formulate a global model of soot formation and oxidation processes, improve strategies for incorporating chemistry into turbulent flow fields, and extend optical investigations into flames where the effects of chemistry-turbulence interactions can be probed effectively.

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POLYMER COMBUSTION RESEARCH

The materials industry is seeking products that are both low in flammability and will not pose environmental hazards over their life cycle. NIST is working on several key research areas needed to produce natural and synthetic polymers and composite materials that can meet these goals. One area is the measurement of flammability properties by bench-scale methods, directly relevant to real fires, and the development of mathematical models that use the measured flammability properties as inputs to predict fire performance of materials in the conditions of actual use.

Another research area concerns approaches to environmentally acceptable, char-forming flame retardant treatments for flaming and smoldering combustion. This effort includes studying the physical and chemical nature of char and how its properties can be enhanced. The experimental work is complemented by theoretical modeling using molecular dynamics and quantum mechanics to develop a technical basis for the design of a new generation of fire resistant materials, which, while retaining their intended-use properties, will be low in combustion toxicity and safe for the environment.

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RESEARCH FACILITIES

LARGE-SCALE STRUCTURES TESTING FACILITY

The NIST large-scale structures testing facility consists of a universal testing machine (UTM) that may be used with a 13.7-m-high reaction buttress equipped with a horizontal hydraulic ram of 4.5-MN capacity. A combination of horizontal and vertical forces may be applied to large-scale specimens.

CAPABILITIES

The UTM portion of the facility is a hydraulically operated machine of 53.4-MN capacity and is one of the largest in the world. It tests large structural components and applies the forces needed to calibrate very large capacity force-measuring devices. It can apply compression forces to column sections or fabricated members up to 18 m in height. The reaction buttress will resist horizontal forces to 4.5 MN from floor level to 12.2 m high. Flexure and tension specimens may be subjected to forces up to 18 MN and 26 MN, respectively. Two-m-thick test floors east and west of the machine may be used to tie specimens in place.

A servo system has been added to the original manual controls of the UTM. It may be programmed by function generator or computer to create any desired loading function using force, strain, or displacement as the variable.

Loads may be applied to a specimen by both the UTM and horizontal ram. A four-rail track system equipped with low-friction rollers has been used for concrete column tests. An "A" frame was used to resist horizontal reaction forces generated by the ram and was attached to the buttress at the desired height.

APPLICATIONS

A testing program was conducted to evaluate the performance of concrete columns 1.5 m in diameter and up to 9.1 m high. Another test series evaluated fracture propagation in steel plates 1 m wide and 0.1 m and 0.15 m thick. A third experiment used the servo-control system programming repeated loads applied to composite specimens.

Low-cycle fatigue tests, destructive or ultimate loads, earthquake simulation in two dimensions, and complex loading of components may all be accomplished in this facility. Servo operation of this machine creates a unique potential for precisely controlled very large forces applying to test components.

AVAILABILITY

This facility, which must be operated by NIST staff, is available for cooperative or independent research. Tests should be arranged as far in advance as possible as special hardware may be needed for attaching specimens.

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B168 Building Research Building

TRI-DIRECTIONAL TEST FACILITY

The tri-directional test facility at NIST is a computer-controlled apparatus capable of applying cyclic loads simultaneously in three directions. It is used to examine the strength of structural components or assemblies under the application of a variety of loading phenomena, such as an earthquake or wind. This is one of the largest such facilities in the world, both in terms of its high load capacity and its capability to handle large, full-scale specimens.

CAPABILITIES

The facility can apply forces and/or displacements in six directions at one end of a specimen. The other end of the specimen is fixed. Specimens up to 3.3 m high \times 3 m in length or width may be tested. The six degrees of freedom are translations and rotations in and about three orthogonal axes. The forces are applied by six closed-loop, servo-controlled hydraulic actuators that receive instructions from a computer. Operating under computer control, the facility simultaneously maintains control of the load and/or displacements in each of the three orthogonal directions. Loads may be applied up to 2,000 kN in the vertical and about 890 kN in each of the two horizontal directions.

APPLICATIONS

The test facility is limited only by the size of the test specimen. Loads may be cyclic or unidirectional depending on the type of loading condition being simulated. The facility is used to study masonry shear walls subjected to reverse cyclic lateral loading and precast concrete connections also subjected to reversed cyclic lateral loading. This facility supports NIST's role in conducting research for seismic design and construction standards in the National Earthquake Hazards Reduction Program.

AVAILABILITY

The tri-directional test facility is used by NIST staff in a variety of NIST research projects and collaborative projects with other agencies. It also is available for independent research but must be operated by NIST staff.

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LARGE ENVIRONMENTAL CHAMBER

The large environmental chamber is 14.9 m \times 12.8 m \times 9.5 m high. It has an earth floor and may be excavated as needed for building construction. The chamber is one of the largest of its kind, capable of accommodating two-story houses under simulated environmental conditions. This chamber has been used for thermal performance, heating and cooling load measurements, and energy consumption studies of buildings of different kinds.

CAPABILITIES

The chamber is capable of automatically maintaining steady and/or dynamic temperature profiles from -45°C to 65°C and humidity from 50 percent relative humidity (rh) at 1.7°C up to 35 $^{\circ}\text{C}$ dewpoint at 49°C . A wider range of rh (15 percent to 80 percent) may be obtained manually. Air circulation maintains the temperature variation within the chamber to within $\pm 1^{\circ}\text{C}$. Damper-control return ducts in all four corners of the chamber permit good air distribution. Supply air is furnished by ceiling diffusers.

APPLICATIONS

The chamber is used to measure indoor temperature fluctuation, heat loss and heat gain through building envelopes, energy conservation and moisture condensation studies, and air infiltration under simulated and dynamically fluctuating outdoor temperature cycles. The chamber has been used to test a wide variety of conventional and special structures and equipment, including military hardware (such as inflatable life rafts, relocatable air-inflatable hospital units, and portable walk-in coolers) under extreme climatic conditions.

AVAILABILITY

This facility, along with several smaller chambers (including one designed for vehicles), has substantial potential for use by researchers in industry and universities. Collaborative programs and individual research can be arranged.

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CALIBRATED HOT BOX

The NIST calibrated hot box measures the heat transfer coefficient of full-scale building wall sections. Designed in accordance with ASTM Standard C976, it consists of two large, heavily insulated chambers—an environmental chamber and a climatic chamber—each with one open side. Indoor and outdoor conditions are simulated in the chambers. The open test section measures 3 m × 4.6 m. A well-insulated frame supports the wall specimen that is clamped between the open sides of the two chambers.

CAPABILITIES

This facility is the only one of its kind designed to perform simultaneous dynamic transfer measurements of air, moisture, and heat during simulated winter and summer conditions under steady-state and dynamic climatic conditions. While the environmental chamber temperature and humidity are maintained to simulate a relatively steady and narrow range of indoor conditions, the climatic chamber can attain temperatures ranging from -40 °C to 65 °C. The apparatus measures the performance of homogeneous or composite walls having a range of thermal resistance from 0.35 m² to 8.8 m² · C/W. It accommodates wall specimens up to 0.6 m thick and up to 700 kg/m² in weight per unit area.

APPLICATIONS

NIST researchers use the facility to develop standard test methods to evaluate dynamic thermal performance of full-scale walls under cyclic temperature conditions. The building industry and government agencies are seeking reliable evaluation techniques for wall thermal mass, especially to predict energy consumption of buildings with heavy mass effects in comparison to standard wood-frame buildings.

NIST has participated in round-robin test activities with domestic and overseas thermal insulation laboratories.

AVAILABILITY

The facility provides a unique opportunity to measure simultaneous transfer of air, moisture, and heat through wall and roof specimens with openings for windows and doors. While available for use by those outside NIST, this apparatus must be operated by NIST staff.

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LINE HEAT-SOURCE GUARDED HOT PLATE

The 1-m guarded hot-plate apparatus measures thermal conductivity of building insulation. NIST researchers use the hot plate to provide calibration specimens for guarded hot plates in other laboratories. The hot plate also is used to investigate edge heat loss from thick thermal insulation materials. This facility is the only one of its kind in the world that will permit low-density thick insulation to be measured with an uncertainty of less than 0.5 percent.

CAPABILITIES

This apparatus has a test temperature range of 80 °C for the hot plates and -20 °C for the cold plates. The apparatus permits measurement of vertical and horizontal heat flow to simulate heat transfer through ceilings and walls, respectively. This apparatus operates within its own carefully controlled temperature and humidity environment shielded by an insulated aluminum enclosure. This facility provides for absolute measurement of thermal resistance of thick and low-density test specimens used as transfer standards. These standards are used to calibrate or verify heat flowmeter (ASTM C508) or guarded hot-plate (ASTM C177) equipment.

AVAILABILITY

This apparatus is available for use by those outside NIST, but it must be operated by NIST staff. Collaborative programs may be arranged.

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FIRE RESEARCH FACILITIES

As the federal government's principal fire research laboratory, NIST maintains some of the country's best and most extensive fire testing facilities. A substantial portion of NIST's fire tests are performed in a specially equipped fire research building, which measures 27 m × 57 m and is designed for large-scale fire experiments. Smoke abatement equipment permits large fire tests to be conducted safely without polluting the environment.

In addition to several individual burn rooms, which are modified from time-to-time to accommodate special NIST testing requirements, the facility also houses several specially designed calorimeters for measuring the rate of heat release from materials and large samples, a room/corridor facility for studying smoke and toxic gas transport, pilot furnaces, and reduced-scale model enclosures. Also, a two-story "townhouse" is used to study fire spread from a burning room, smoke transport between levels, and sprinkler performance. The townhouse features a living room that is continuously weighed, allowing the burning rate of finish materials to be measured.

A new computer-based data acquisition system provides state-of-the-art data collection capabilities for all large-scale fire testing. Up to 300 instruments with scanning rates over 100 channels per second can be dedicated to a single test. During an experiment, real-time, full-color graphics present the data as collected, with automatic conversion to engineering units for gas analysis, rate of heat release, temperature, and other measurements.

CAPABILITIES

- **Heat-Release Rate Calorimeters.** NIST pioneered and developed the oxygen consumption methodology for measuring the rate of heat release and has used it longer and in more devices than any other laboratory. The major benefit of this technique is the independence of the apparatus in measuring enthalpy responses to changes in heat release rate.

NIST has two calorimeters available for measuring the rate of heat release of free-standing items, such as pieces of furniture. The smaller one has a capacity of $\frac{1}{2}$ MW; the larger, 7 MW. Provisions for measuring smoke production and gas species yield are available with both instruments.

- **Room/Corridor Facility.** NIST researchers have constructed and used a room/corridor facility to evaluate an analytical model that predicts the transport of smoke and toxic gases from the room of fire origin into the corridor and secondary target rooms. The design of this facility makes it possible to measure the hazards associated with the burning of wall linings or room furnishings by evaluating the rate of heat release, smoke production, and toxic gas generation. The facility is available in its present form or with design modifications for evaluating a variety of building contents and furnishings.

- **Burn Rooms.** A standard burn room built to ASTM specifications, 2.4 m \times 3.7 m \times 2.4 m high, adjoins a large overhead hood that collects the exhaust products from the room fires. The exhaust collection system is calibrated to measure the rate of heat release and the generation rates of smoke and other combustion products from the fire. The burn room is available for developmental and validation studies of mathematical models and for studies of fire performance of furnishings and interior finish materials.

The room fire environment can be characterized in terms of temperature and pressure gradients and the spatial distribution of thermal flux, gaseous combustion products, and smoke. Other measurements permit the calculation of thermal losses to the room boundaries and mass and energy flows from the room. Smaller burn rooms also are available.

- **Pilot Furnaces.** A pilot furnace for evaluating the fire endurance of wall assemblies or floor/ceiling assemblies is available. This furnace, capable of handling specimens 1 m \times 1 m, may be used for research purposes only and cannot be used for code acceptance testing. Typically, fire exposure similar to that specified by ASTM E119, under carefully controlled conditions of furnace pressure and oxygen concentration, can be carried out. Depending on the parameters required, a variety of other exposure conditions can be applied.

- **Reduced-Scale Models.** NIST facilities are available for reduced-scale modeling of full-scale fire configurations. Physical models offer an economical means of achieving sufficient variation of physical parameters for a generalized understanding of fire behavior. Based on the results of reduced-scale experiments, limited full-scale verification then can be performed.

AVAILABILITY

Industry, university, and government representatives are encouraged to use these fire testing facilities on a collaborative or independent basis, with certain restrictions. For safety reasons, NIST staff must closely supervise all use of the facilities.

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COMPUTER SYSTEMS LABORATORY

Both users and manufacturers of computer and telecommunications technology benefit from the work of the Computer Systems Laboratory (CSL). Its research and testing programs foster the orderly development of an "open systems" environment intended to make all forms of information technology compatible and interoperable. For manufacturers of hardware and software, industry-wide adoption of standards expands marketing opportunities, and users are freed of the constraints and frustrations of incompatible proprietary systems.

Much of CSL's work consists of advising and assisting industry in developing standards that satisfy user needs and yet accommodate innovations that differentiate the products of competing vendors.

To help protect information in federal computer systems, laboratory personnel advise and assist federal agencies in planning computer security programs, increasing awareness of the need for computer security, and carrying out computer security training.

The laboratory also has research programs on parallel processing, automated speech and image recognition, database and network management, software engineering, and other topics related to the effective use of information technology.

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COOPERATIVE RESEARCH OPPORTUNITIES

Information Systems Engineering

- 102 Database Testing
- 102 Geographic Information Systems
- 103 Computer Graphics Testing

Systems and Software Technology

- 103 Interfaces for Computer Environments
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Computer Security

- 104 Computer Systems Security
- 104 Security in ISDN and OSI Networks
- 104 Malicious Code and Related Threats
- 104 Data Encryption

Systems and Network Architecture

- 105 Network Management
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Advanced Systems

- 105 Integrated Services Digital Network
- 106 Performance of Modern-Architecture Computers
- 106 Optical Disk Tests
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RESEARCH FACILITIES

- 107 Information Systems Engineering Facility
- 107 Computer and Network Security Facility
- 108 ISDN and Distributed Systems Facility

COOPERATIVE RESEARCH OPPORTUNITIES

INFORMATION SYSTEMS ENGINEERING

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DATABASE TESTING

To aid the management of information resources, NIST researchers are developing test methods and techniques for evaluating implementations of the database Language SQL and Information Resource Dictionary System (IRDS) 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.

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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 interdisci-

plinary uses of GIS technology through studies integrating computer graphics standards, database management standards, expert systems technology, and Global Positioning Satellite technology to support GIS applications. This group's research is focused on providing GIS compatibility through standards and conformance testing for GIS standards, such as the Spatial Data Transfer Standard (FIPS PUB 173). Because the activities of many governmental and private organizations are land and/or location based, GIS technology will be important in integrating existing spatial data to administer, manage, and monitor people, money, and activities in accomplishing the objectives of these organizations.

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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), and the programmer's hierarchical interactive graphics system (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, is used in these efforts. Existing test suites are available that determine conformance of GKS-FORTRAN implementations, PHIGS-FORTRAN implementations, CGM files, and CGM generators. Future test suites

developed will concentrate on GKS-C implementations, PHIGS-C implementations, and CGM interpreters.

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INTERFACES FOR COMPUTER ENVIRONMENTS

For the past several years, NIST has collaborated with vendors, users, and voluntary standards organizations to advance the implementation and use of the POSIX family of standards. POSIX promotes the portability of computer applications at the source code level. NIST researchers continue to work with voluntary standards committees to develop additional standards needed for interfaces to operating systems, including commands and utilities, system administration, and operating system security. Research efforts focus on the large-scale, heterogeneous distributed systems aspects of NIST's Application Portability Profile for Open System Environments. These specifications integrate federal, national, and international standards to provide functionality needed for a broad range of government information technology applications.

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INTERACTIVE MEDIA

Portable multimedia courseware (computer-based interactive training software) provides a viable alternative to the current practice of distributing courseware with proprietary interfaces to system services. NIST and other federal agencies are working together to develop a strategy for multimedia courseware that would create an environment in which high-quality portable courseware is available as commercial, off-the-shelf products competitively supplied by vendors. Researchers are developing a computer-based interactive training applications profile that would identify needed standards in response to user needs.

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SOFTWARE QUALITY

Growing dependence on computers requires assurance that critical systems will operate reliably and exactly as intended without adverse effects, even when outside circumstances cause other systems to fail. NIST researchers are studying problems and potential solutions in building and operating high-integrity systems and are looking at life-cycle methodology, risk management, formal methods, object-oriented design, software reliability, clean-room techniques, and formal verification.

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COMPUTER SECURITY

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COMPUTER SYSTEMS SECURITY

Computer systems are vital elements of today's business and scientific environments. However, as sensitive and critical information is processed and stored on computer systems 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 cost analysis of such measures and the resulting reduction in losses. NIST researchers are investigating various technologies that can be used 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 often are 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.

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SECURITY IN ISDN AND OSI NETWORKS

NIST has initiated a laboratory-based 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 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.

Researchers plan 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. Specifications will be developed 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. 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.

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MALICIOUS CODE AND RELATED THREATS

Operators and users of computer systems and networks are experiencing an increased number of incidents of malicious code (such as computer viruses and "worms"),

unauthorized access ("hackers," for example), and similar threats. Protection from such threats requires a combination of management awareness, user involvement, and technical protection.

NIST researchers are actively involved in improving each of these areas. Their research involves an understanding of both the potential technical vulnerabilities of systems and of how systems are used and administered. Advanced methods of system protection, anomaly detection, system self-audit, and related techniques are being developed. In addition, methods of rapid reaction and response to computer security incidents are being developed and coordinated throughout the federal government.

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DATA ENCRYPTION

NIST researchers are working with industry and voluntary standards groups to advance technology and to develop standards in computer cryptography, a mathematical process that transforms information to an unintelligible form in a process called encryption and then back to an intelligible form, the process of decryption. Cryptography can be used to protect the secrecy of information, to generate codes that indicate whether any unauthorized changes have been made to a message while in transit on a network or stored in a computer, to authenticate users of systems, to control access to systems, and to electronically sign documents.

Research projects involve the development and evaluation of techniques for secret key and public key cryptography applications, and for validation systems that test equipment for conformance to cryptography standards. As new national networks are developed, cryptographic-based security serv-

ices will be needed to protect data and resources in distributed processing systems.

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NETWORK MANAGEMENT

NIST researchers are working with industry to establish standards for exchanging network management information between heterogeneous 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 for exchanging 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 areas include network management user displays, network management applications software development, and application of expert systems to network management.

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NETWORK PROTOCOL ENGINEERING

NIST researchers in the area of network protocols are promoting the standardization, convergence, and commercialization of networking technology. Research projects involving network applications are focused on promoting standardization of security services such as distribution and management of encryption keys and the design of a specialized protocol for the negotiation of a wide range of security services and their related parameters.

Research projects involving lower layer network applications include promoting the convergence of network addressing schemes used in OSI stacks and in the Internet environment. NIST researchers prototype convergent schemes to demonstrate viability and promote acceptance. Lower-layer research also includes promoting the standardization of multicast transport and routing algorithms. Additional work focuses on interoperability testing of dynamic network routing and frame relay products.

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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.

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ADVANCED SYSTEMS

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INTEGRATED SERVICES DIGITAL NETWORK

In cooperation with industrial and other users, NIST advances the development of standards for Integrated Services Digital Network (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. NIST researchers also are involved in the research and standardization of B-ISDN-based protocols as well as FDDI conformance tests.

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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; the other has 16 processors in a shared-memory configuration.

These NIST researchers also are involved in the development of instrumentation and related management techniques for gigabit networks used for visualization-based applications.

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OPTICAL DISK TESTS

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

with voluntary standards committees and interested federal agencies.

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DISTRIBUTED SYSTEMS

NIST researchers are developing application profiles that will promote integrated platforms for video, imagery, computer data, and voice, thus defining multimedia applications in a distributed processing environment. This research focuses on prototype development and demonstration using ISDN technology.

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SPOKEN LANGUAGE TECHNOLOGY

Recent advances in automatic speech recognition and understanding technology have resulted in computers able 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 the Defense Department's Advanced Research Projects Agency 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 spontaneous speech. Among the research facilities used are several Sun Microsystems workstations, speech-processing peripherals and software tools, and CD-ROM production tools. Areas of interest include characterization of the speech database materials (such as acoustic-phonetic locators and classifiers), artificial neural nets, performance measurement, and natural languages.

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IMAGE RECOGNITION

Image recognition research at NIST focuses on developing methods for evaluating image quality, compression efficiency, and image systems used in optical-character recognition. These evaluation methods 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.

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RESEARCH FACILITIES

INFORMATION SYSTEMS ENGINEERING FACILITY

The NIST information systems engineering facility consists of laboratories with the computer hardware and software needed for research and development of standards, guidance to federal agencies, and validation tests. The following areas are included: graphics; programming languages; database management systems; distributed database management systems; object database management systems; data dictionary systems; data administration, especially database design; data interchange; knowledge-based and expert systems; hypertext and hypermedia; and geographic information systems (GIS).

CAPABILITIES

The facility contains a variety of computers. Among them are a VAX 11/785, Symbolics 3650 LISP machine, 386 and 486 microcomputers, Macintosh II, Silicon Graphics IRIS workstation, and a SUN SPARC II workstation. Other computer systems, such as the NIST Cray Y-MP supercomputer, are accessible. Also available are a variety of hard-copy output devices, such as laser printers, camera output systems, and color thermal transfer printers.

Software used in the facility includes:

- graphical kernel system (GKS) and programmer's hierarchical interactive graphics system (PHIGS) implementations, which allow graphics programmers to design a wide variety of graphics programs, ranging from simple passive graphics to complex real-time systems;
- computer graphics metafile (CGM) implementations that permit transfer of graphical pictures among heterogeneous graphic devices;

- a variety of programming language processors and system software;
- database management systems for the VAX, workstations, and microcomputers supporting SQL and object technologies;
- a prototype implementation of the Information Resource Dictionary System (IRDS) standard;
- LISP and Prolog;
- microcomputer expert system shells; and
- GIS systems.

Validation suites are available for testing conformance to Federal Information Processing Standards (FIPS) for COBOL, FORTRAN, Pascal, C, MUMPS, Ada, GKS, CGM, and database language SQL. Testing services are provided for COBOL, FORTRAN, Pascal, C, MUMPS, Ada, GKS, CGM, and SQL.

APPLICATIONS

An active area of cooperative work is the development and evaluation of tests to validate the conformance of language processors and other system software to FIPS. Major programs under way are validation of the programming language processors COBOL, FORTRAN, Pascal, C, MUMPS, and Ada; validation of the GKS, PHIGS, and CGM graphics systems; validation of database language SQL; and validation of IRDS.

Possible future work includes the development of tests and procedures for validating additional programming language systems, such as VHSIC Hardware Description Language, LISP, and Prolog; for validating the computer graphics interface; and for validating the following data management and data interchange software: SQL2, SQL3, data description file for information interchange, and abstract syntax notation one (ASN.1).

AVAILABILITY

The facility, which must be used under the guidance of NIST staff, is available for collaborative projects in test development and application research.

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COMPUTER AND NETWORK SECURITY FACILITY

The NIST computer and network security facility is used to improve the current security posture of federal computer and telecommunication systems and to provide security for these systems as they migrate toward open system environments. Research performed in the facility is aimed at applying methods to protect the secrecy and integrity of information in computer systems and data networks; evaluating personal identification and authentication techniques to control access to information resources; and developing computer and network security architectures to determine proper implementation of controls for integrity and confidentiality of information and authentication of users.

CAPABILITIES

The facility is equipped with mini- and microcomputers, security devices, terminals, personal identification systems, and access to large mainframes and supercomputers through local area, national, and global networks. A variety of communications technologies and applications environments are available for research efforts, including Open Systems Interconnection and Integrated Services Digital Network for developing and testing security protocol standards.

Operational capabilities include a computer emergency response team to facilitate identification and response to acute computer and telecommunications security incidents involving self-replicating computer viruses. Test and evaluation capabilities range from specific functionality tests of cryptographic modules to test methodologies for network security protocols to the specific criteria used to evaluate the trustworthiness of systems that handle unclassified, but sensitive, data.

A risk management laboratory, utilizing a Dell System 325 (AT clone), is available for research in risk management techniques and methodologies and evaluation of risk management software to determine applicability to different agency environments. Three Sun computers support the development of advanced-computer access control systems based on smart-token technology. The virus laboratory uses two IBM PS/2 Model 60s, a Sun workstation for research in multiuser environments; and a Macintosh SE for research in the MacOS environment. A small systems security laboratory completes the computer and network security facility.

APPLICATIONS

The facility is used primarily to develop and test federal standards for computer and network security. Support is provided to other federal agencies and industry where the protection of unclassified data is required.

AVAILABILITY

Collaborative research programs can be arranged.

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ISDN AND DISTRIBUTED SYSTEMS FACILITY

The NIST Integrated Services Digital Network (ISDN) and distributed systems facility provides laboratories for research and development, standards, and conformance testing in distributed computer systems and advanced computer communications, including ISDN and the fiber distributed data interface. Significant research and development programs include open distributed systems, transaction processing, distributed multimedia, ISDN applications, ISDN conformance testing, and broadband ISDN.

CAPABILITIES

The facility is equipped with microcomputers, workstations, minicomputers, multimedia display units, ISDN and Ethernet communications, and laser printers. Access to mainframes and supercomputers is provided via local, national, and global networks. The laboratories have eight basic rate interface (BRI) ISDN lines, three Sequent computers (S27, S81), five Sun workstations, four 386-class microcomputers, four ISDN terminal adapters, four ISDN telephones, two ISDN protocol analyzer/emulators, and two Macintosh microcomputers. Researchers access primary rate interface ISDN as well as the BRI. The laboratories also feature software for compiling formal descriptions of distributed systems into implementations, tool kits for programming distributed systems, user interfaces, and advanced operating systems such as MACH.

APPLICATIONS

Facilities are used primarily for developing and testing federal, national, and international standards for advanced communications and distributed multimedia systems.

Research activities support the North American ISDN Users' Forum (NIUF), chaired by NIST. The forum was established by NIST with industry in 1988 to create a strong user

voice in the implementation of ISDN applications. Through the forum, users and manufacturers concur on ISDN applications, the selection of options from standards, and conformance tests. NIST works with the forum to develop tests that determine whether the agreed-to specifications will result in compatible products and services.

A principal focus is standards conformance test design for ISDN implementations based on recommendations of the International Telephone and Telegraph Consultative Committee. NIST has developed reference implementations for the Q.921 and Q.931 recommendations, conformance test suites for both recommendations, and a conformance test system based on these items. In addition, conformance research on broadband ISDN is conducted.

Also under development are application profiles for ISDN, research in distributed computing environments, and prototype distributed multimedia information systems based on ISDN and other communications media. Researchers have produced a distributed reference implementation for the International Standard Transaction Processing Protocol directly from a formal specification and are investigating how transactions support multimedia information access and cooperative processing.

AVAILABILITY

Collaborative research programs with government, industry, and academia can be arranged and are encouraged.

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COMPUTING AND APPLIED MATHEMATICS LABORATORY

The NIST Computing and Applied Mathematics Laboratory develops mathematical, statistical, and state-of-the-art scientific computing tools that help other NIST researchers and their collaborators accomplish their research objectives. NIST mathematicians and statisticians also support U.S. industry through computer-aided modeling of complex manufacturing processes and statistical methods for improving the quality of products and processes.

Other research programs focus on advanced computer graphics programs that produce two- and three-dimensional visualizations of complex problems; new methods for displaying, manipulating, analyzing, and transmitting large volumes of data; and software applications for harnessing the problem-solving power of parallel processors, an effort carried out in conjunction with the federal government's multiagency program on high-performance computing and communications.

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COOPERATIVE RESEARCH OPPORTUNITIES

Applied and Computational Mathematics

- 109 Scalable Parallel Algorithms
- 110 Non-Linear Mechanics
- 110 Mathematical Modeling
- 110 Optimization and Computational Geometry
- 110 Mathematical Software

Statistical Engineering

- 111 Industrial Experiments
- 111 Measurement Assurance

Scientific Computing Environments

- 111 Scientific Visualization

Continual Upgrades

COOPERATIVE RESEARCH OPPORTUNITIES

APPLIED AND COMPUTATIONAL MATHEMATICS

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SCALABLE PARALLEL ALGORITHMS

A major problem for users of massively parallel computers is the lack of libraries of commonly used subroutines. Algorithms and computer codes developed for single-processor machines rarely give massive speedups when transferred to massively parallel computers.

NIST researchers concentrating on algorithm research for massively parallel computations are making substantial progress in algorithms for important problems in computational geometry, such as triangulation in two and three dimensions. Additional research focuses on random processes, including Monte Carlo simulations and randomizing algorithms.

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NON-LINEAR MECHANICS

Mathematical analysis, used with symbolic computation, leads to efficient analytical approximations by computers. Perturbation algorithms applied to non-linear differential equations, especially in celestial mechanics, result in analytical developments where the complexity grows exponentially with the order of the approximation. Several avenues are being explored at NIST to simplify literal developments generated by perturbation algorithms applied to non-linear systems. These include identifying 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 creating natural intermediaries.

Problems being examined include 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.

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MATHEMATICAL MODELING

Mathematical and computational problems are becoming more elaborate as measurement techniques, physical understanding, and computational capability improve. Solving these problems requires innovative combinations of the methods of modern applied

and computational mathematics. With scientists and engineers, NIST mathematicians develop and analyze mathematical models of phenomena; design and analyze computational methods and experiments; transform these methods into efficient numerical algorithms for modern, high-performance computers; and implement them in high-quality mathematical software. Active areas of interest include crystal growth, fluid flow, electromagnetic waves, magnetic materials, molecular dynamics simulations, partial differential equations, and several kinds of inverse problems.

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OPTIMIZATION AND COMPUTATIONAL GEOMETRY

In many aspects of NIST's research, the need arises for computational procedures, such as curve fitting, parameter estimation, and maximum entropy calculations. These activities require solving various types of optimization problems. NIST researchers investigate many aspects of numerical optimization, including large-scale linear and quadratic programming problems by interior-point methods, and the extension of these procedures to general large-scale non-linear programming problems via sequential quadratic programming methods. Researchers also have developed procedures for non-linear least squares and orthogonal distance regression problems, and they produce software for these methods as needed.

Computational geometry is a rapidly emerging field with applications in robotics, statistical mechanics, cartography, computer graphics, materials science, and molecular dynamics. Researchers at NIST develop robust and efficient computational schemes to compute triangulations and shellings of point sets, Voronoi diagrams, and other geometrical calculations. Algorithms for two- and three-dimensional triangulation are implemented for sequential and parallel machines and are used at NIST and other scientific centers.

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MATHEMATICAL SOFTWARE

The increasing prevalence of computation in science and engineering has generated an acute need for accurate and robust computer software to solve frequently occurring mathematical and statistical problems. NIST mathematicians and computer scientists are actively involved in the development of algorithms for the solution of such problems on modern high-performance computers. These algorithms are then implemented in well-engineered software that is both reliable and easy to use. Problem areas addressed by recent efforts have ranged from the parallel evaluation of mathematical functions to the high-speed solution of partial differential equations on vector supercomputers.

This work engenders associated research in mathematical software methodology such as software parts design, graphical user interfaces, expert advisory systems, and automated distribution mechanisms. Recent

efforts have focused on the Guide to Available Mathematical Software, a network-based software repository system developed at NIST.

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INDUSTRIAL EXPERIMENTS

Most NIST/industry collaborative research projects involve conduct of experiments, generation of data, and analysis of the results. NIST statisticians participate in these collaborations by contributing strategies for experimentation, graphical and analytical data analysis, stochastic empirical modeling, estimation of uncertainty, computationally intensive methods, and fitting of reliability distributions. A Senior Research Fellowship Program funded by the National Science Foundation and managed by the American Statistical Association encourages formation of NIST collaborative research projects keyed to industrial needs.

Ongoing collaborative research projects include the following:

- development of a non-contact sensor for measuring the temperature of hot rolled aluminum;

- comparison of various methods to machine ceramic piece parts;
- determination of optical-fiber geometry by gray-scale analysis with robust regression;
- non-destructive evaluation of the concentration of impurities and dopants in high-technology materials through neutron depth profiling;
- optimization of parallel processing MIMD programs;
- modeling of the measurement errors in automated milling machines;
- sampling data points for the effective use of coordinate measuring machines;
- friction characterization of ultralow speed turning machines;
- evaluation of properties and processing of recycled concrete; and
- analysis of the failure laws for electro-migration and accelerated testing.

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MEASUREMENT ASSURANCE

Measurement is the backbone for advancing scientific research and creating new technologies. NIST statisticians collaborate with subject experts in developing techniques for tying measurement processes to accepted standards and assuring the quality of measurements. Expertise in the design of experiments, modeling, estimation of components of variance, reliability, and computer-intensive methods, coupled with a strong research focus, brings statisticians into contact with leading researchers in measurement science, both at NIST and abroad. It also provides opportunities for contributing to the measurement science base for emerging technologies.

In the initial phases of such programs, models for describing the error structure of the measurements are developed and validated by planned experimentation, and problem areas are identified through estimation of error components. The initial characterization, which may require several rounds of experimentation and produce refinements to the measurement process, is followed by the development of artifact standards for applying the technology to the area of interest.

For example, statisticians are currently working with NIST scientists in cooperation with the Federal Bureau of Investigation on developing standards to assure the quality of DNA measurements that are introduced as physical evidence in legal proceedings. This phase of the program follows an intense phase of experimentation and data analysis where sources and magnitudes of error in measuring DNA fragments were determined.

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SCIENTIFIC COMPUTING ENVIRONMENTS

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SCIENTIFIC VISUALIZATION

Researchers at NIST are developing and applying advanced methods for using state-of-the-art, computer-based scientific graphics for rendering complex experimental,

computational, and analytical results in physics and chemistry. Researchers use 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. Techniques also have been developed to manipulate dynamic objects in automated design and manufacturing systems; to display quasicrystal structures with icosahedral symmetries and scanning electron tunneling microscopy data with polarization analysis; and to study models of turbulent combustion showing the dependence of solutions on time and fuel-oxidizer mixture parameters.

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CONTINUAL UPGRADES

The laboratory maintains a central scientific computing environment for NIST staff at Gaithersburg and Boulder. It procures and operates computer and communications facilities and maintains them at state-of-the-art levels suited to the needs of a highly diverse scientific and engineering R&D community. The continuing program of upgrading responds to advances in hardware, software, and communications technologies, as well as to changes in the kinds of tools used in modern scientific research.

NIST specialists log and analyze the use of the components of the facilities—hardware, software, operating systems, and networks—to determine what changes or new equipment will be most useful. They take steps to acquire them where possible or to develop them internally. They design interfaces as needed for users to gain access to the resources best suited to their needs. This work proceeds within a broad view of the overall operation of the computing environment and its interactions with external environments, as well as detailed understanding of the progress of hardware and software capabilities and of the roles of visualization and networking in the design and execution of scientific computing projects.

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