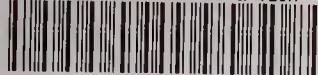


NAT'L INST. OF STAND & TECH



A11106 194823

NIST
PUBLICATIONS

2002 PHYSICS LABORATORY

SUPPORTING U.S. INDUSTRY,
GOVERNMENT, AND THE SCIENTIFIC
COMMUNITY BY PROVIDING MEASUREMENT
SERVICES AND RESEARCH FOR ELECTRONIC,
OPTICAL, AND RADIATION TECHNOLOGY.

NIST

National Institute of
Standards and Technology
Technology Administration
U.S. Department of Commerce

QC
100
-457
no. 994
2003
C.2

| | |
|---|----|
| <i>Physics Laboratory at a Glance</i> | 1 |
| <i>Director's Message</i> | 2 |
| <i>Electron and Optical Physics Division</i> | 4 |
| <i>Atomic Physics Division</i> | 12 |
| <i>Optical Technology Division</i> | 20 |
| <i>Ionizing Radiation Division</i> | 28 |
| <i>Time and Frequency Division</i> | 36 |
| <i>Quantum Physics Division</i> | 44 |
| <i>Office of Electronic Commerce in Scientific and Engineering Data</i> | 52 |
| <i>Honors and Awards</i> | 54 |
| <i>Physics Laboratory Resources</i> | 63 |
| <i>Organizational Chart</i> | 64 |

PHYSICS LABORATORY AT A GLANCE

PL VISION

Preeminent performance in measurement science, technology, and services.

PL MISSION

The mission of the NIST Physics Laboratory is to support U.S. industry, government, and the scientific community by providing measurement services and research for electronic, optical, and radiation technology. The Laboratory provides the foundation for metrology of optical and ionizing radiation, time and frequency, and fundamental quantum processes.

PL GOALS

Physics Laboratory develops goals within its mission and focus areas. These include health care quality assurance, nanoscale measurements and data, and measurements and standards that support homeland security. In addition to these overarching focus areas, which are shared by other NIST Laboratories, PL has substantial programmatic interest in time and frequency, optical and photonic, and environmental and energy metrology and applications.

Electron and Optical Physics Division: to support emerging electronic, optical, and nanoscale technologies.

Atomic Physics Division: to determine atomic properties and explore their applications.

Optical Technology Division: to provide the foundation of optical radiation measurements for our Nation.

Ionizing Radiation Division: to provide the foundation of ionizing radiation measurements for our Nation

Time and Frequency Division: to provide the foundation of frequency measurements and civil timekeeping for our Nation.

Quantum Physics Division: to provide fundamental understandings of nano-, bio-, and quantum optical systems in partnership with the University of Colorado at JILA.

Office of Electronics Commerce in Scientific and Engineering Data: to coordinate and facilitate the electronic dissemination of information via the Internet.

PL RESOURCES

- **199 full-time staff (147 scientific) with expertise in:**
 - Atomic, molecular, and optical physics
 - Computational physics
 - Condensed matter physics
 - Health physics
 - Medical physics
 - Nuclear physics
 - Biophysics
 - Chemistry
 - Metrology and precision measurement
- **\$61 million annual budget**
- **Unique facilities, including:**
 - Controlled Background Radiometric Facility
 - Electron Beam Ion Trap (EBIT)
 - Electron Paramagnetic Resonance Facility
 - EUV Optics Fabrication and Characterization Facility
 - High-Resolution UV and Optical Spectroscopy Facility
 - Low-Background Infrared Radiation Facility
 - Magnetic Microstructure Measurement Facility
 - Medical-Industrial Radiation Facility (MIRF)
 - Nanoscale Physics Laboratory
 - Neutron Interferometer and Optics Facility (NIOF)
 - NIST Beowulf System
 - Radiopharmaceutical Standardization Laboratory

- Spectral Irradiance and Radiance Responsivity Calibrations Using Uniform Sources (SIRCUS) Facility
- Synchrotron Ultraviolet Radiation Facility (SURF III)
- W.M. Keck Optical Measurement Laboratory
- **Standard time dissemination services:**
 - Radio stations WWV, WWVH, and WWVB
 - Automated Computer Time Service (ACTS)
 - Internet Time Service (ITS)
- **Measurement and calibration services for:**
 - Color and color temperature
 - Dosimetry of x rays, gamma rays, and electrons
 - High-precision time
 - Neutron sources and neutron dosimetry
 - Optical wavelength
 - Oscillator frequency
 - Phase and amplitude noise
 - Photodiode spectral responsivity
 - Photometry (e.g., luminous intensity, luminous flux, illuminance)
 - Radiance temperature
 - Radioactivity sources
 - Spectral radiance and irradiance
 - Spectral transmittance and reflectance

PL WEB SITE

<http://physics.nist.gov/>



DIRECTOR'S MESSAGE

We hope this report conveys the excitement and the relevance of the programs within the NIST Physics Laboratory. First and foremost, we support U.S. industry by providing measurement services and research for optical, electronic, and radiation technologies. Our great strength—and what distinguishes us from an academic or industrial laboratory—is that we are vertically integrated. Our world-class measurement services are backed by state-of-the-art engineering efforts to develop new measurement standards, which are in turn supported by frontier, mission-oriented research that anticipates the Nation's future measurement needs.

Thus the Laboratory addresses the fundamental triad of standards, measurements, and data in a climate of vigorous and competitive research. We believe that the quality of our service stems in large measure from the breadth, vigor, and excellence of our research programs and that our contributions gain credibility because they are based on the best technical judgment available.

For example, our Time and Frequency Division is delivering seven different kinds of time and frequency services while also developing optical-frequency atomic clocks, chip-scale atomic clocks, and a futuristic atomic clock for space flight.

While our Internet Time Service provides official U.S. time in a billion daily transactions, we are also pursuing research on trapped ions for the next generation of frequency standards—and quantum-logic devices. Similarly, our Ionizing Radiation Division is developing highly sensitive neutron detectors for homeland security while also using ultracold neutrons to investigate symmetries and parameters of the nuclear weak interaction.

We maintain the U.S. national standards for the Système International (SI) base units of time (the second), light (the candela), and non-contact thermometry (the kelvin, especially above 1200 K).

We provide the basis for such SI derived units as the hertz (frequency), the becquerel (radioactivity), and the optical watt and the lumen (light output). At the same time, scientists in the Physics Laboratory work with industry to develop new measurement technologies that can be applied to such fields as communications, microelectronics, nanomagnetism, photonics, industrial radiation processing, the environment, health care, transportation, space, energy, security, and defense.

Our partners are many and our outreach is extensive. For optical radiation measurements, we rely heavily on the Council for Optical Radiation Measurements (CORM), formed to help define pressing problems and projected national needs in radiometry and photometry. Its aim is to establish a consensus on industrial and academic requirements for physical standards, calibration services, and interlaboratory collaborative programs in the fields of ultraviolet, visible, and infrared measurements. Similarly, the Council on Ionization Radiation Measurements and Standards (CIRMS) helps to advance and disseminate the physical standards needed for the safe and effective application of ionization radiation, including vacuum ultraviolet, x ray, gamma ray, and energetic particle such as electron, proton, and neutron. When we can assist in an important area of measurement or research, we may form Cooperative Research and Development Agreements with industry groups or individual firms. Laboratory staff serve with distinction in standards-development committees, and readily give of their time to assist the public.

We have been recognized for the quality and excellence of our programs and staff many times over the years, by the American Physical Society, the Optical Society of America, and other leading scientific organizations. Members of our staff have been elected to fellowship in the National Academy of Science, the American Association for the Advancement of Science, the American Association of Physicists in Medicine, and other esteemed bodies. And twice since 1997, Laboratory staff members have won the Nobel Prize in Physics. Beginning on page 54 of this report, we highlight some of the awards and honors bestowed upon us in 2002.

Our talent is focused on meeting today's challenges—in health care, quantum technologies, and nanoscale metrology, to name but a few. For health care, the Physics Laboratory conducts research on standards to enable hospitals to use nuclear medicine more effectively. We develop ways to image single biomolecules and to use terahertz-frequency signals as diagnostic tools.

The Physics Laboratory is at the forefront of the nascent field of quantum information processing—computing and communications—challenging preconceived notions of computational complexity and communications security. Similarly, the Physics Laboratory has been a leading center for metrology at the nanoscale, since before “nanotechnology” gained prominence. We pioneered electron-spin microscopy, which images magnetic materials, and our unique EUV optics facility supports the electronic industry in its drive to develop advanced lithographic systems for producing ever smaller chips.

As you browse this summary of the Physics Laboratory, we expect you will want to learn more. We invite you to visit our web site, <http://physics.nist.gov/>, and we invite your inquiries and interest in measurement services and collaborations.

Katharine Gebbie

Katharine Gebbie
Director, Physics Laboratory

GOAL: TO SUPPORT
EMERGING ELECTRONIC,
OPTICAL, AND NANOSCALE
TECHNOLOGIES.

ELECTRON AND OPTICAL PHYSICS DIVISION

The strategy for meeting this goal is to improve measurement science and to develop the measurements and standards needed by emerging science and technology-intensive industries.

The first strategic focus is to develop techniques for fabricating nanostructures and measuring their electronic and magnetic properties.

Nanoscale Electronics and Magnetism

INTENDED OUTCOME AND BACKGROUND

The intended outcome of this work is the continuous improvement of techniques for fabricating and characterizing nanometer-scale electronic and magnetic structures, as required to meet current and future needs of the semiconductor and data-storage industries.

Our main tools for pursuing this program are scanning electron microscopy with polarization analysis (SEMPA) and scanning tunneling microscopy (STM). The Electron Physics Group in the Division has been a leading innovator in both of these techniques, which are outgrowths of work begun at NIST in the 1970s.

SEMPA enables us to use conventional scanning electron microscopy (SEM) to image nanometer-scale magnetic structure, through spin-polarization analysis of secondary electrons ejected from the sample. It has several unique capabilities that distinguish it from other magnetic imaging techniques: it is a surface-sensitive technique, and so is especially well suited for *in situ* studies of thin-film and surface magnetization; it provides a direct measurement of the magnetization of a material region, rather than of a magnetic field; it has the high spatial resolution (about 10 nm), long working distance, and large depth-of-field characteristic of SEM; and it facilitates simultaneous measurements of the magnetization and the topography. SEMPA studies have led to a number of breakthroughs in understanding the basic mechanisms of magnetism on the microscopic scale, and have also addressed

near-term measurement issues faced by the magnetic data-storage industry.

Our STM program is focused on understanding the mechanisms of growth of nanostructures on surfaces and determining their electronic properties. In recent years the STM program has been particularly concerned with the magnetic multilayer materials that have been investigated by SEMPA. The complementarity of SEMPA and STM measurements has elucidated many connections between conditions of layer growth and magnetic-device performance.

The main current direction of the STM program is the course of research made possible by the recently-completed Nanoscale Physics Laboratory. The laboratory was designed with the goal of measuring quantum-electronic structures with atomic-scale imaging resolution and high electron-energy resolution. Samples can be grown *in situ* and probed with magnetic fields of up to 10 T at temperatures down to 2.5 K.

ACCOMPLISHMENTS

Nanometer-Scale Measurements of the Vortex Lattice in a Type-II Superconductor

We have made the first real-space measurements of the hexagonal-to-square symmetry transition in the vortex lattice of V_3Si , a type-II superconductor. The mixed state in a type-II superconductor is characterized by the properties of the vortex or flux lattice that forms in the presence of an applied magnetic field. Vortices are formed at points where the magnetic field penetrates the superconductor in a flux tube through the sample. The flux penetrates the superconductor in quantized units of the flux quantum ($\Phi_0 = h/2e$), with the region near the core of the vortex acting as a normal metal. As the density of vortices in the material increases, a vortex lattice is formed by the interactions between the flux tubes or vortices.

Many of the important applications of superconductors rely on the formation and stabilization of the vortex lattice at

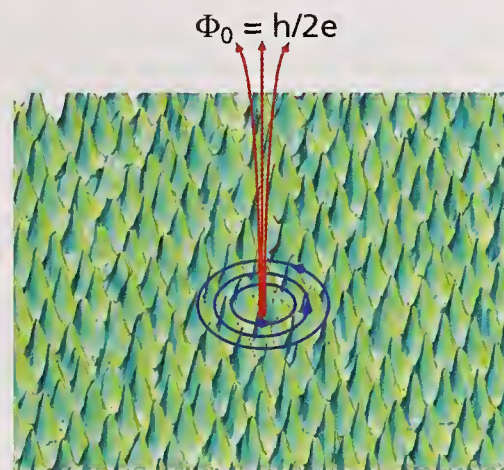


Figure 1. Vortex flux lattice in V_3Si observed in STM Fermi-level conductance image at $H=3$ T and $T=2.3$ K. The peaks indicate the location of vortices with a single flux quantum of magnetic flux.

high values of applied field. For example, the optimization of vortex pinning in high- T_c materials controls flux creep and is responsible for the high critical currents needed for the operation of superconducting magnets. Probing the underlying physics of the vortex lattice is not only of technological importance, it is also the key to understanding more complex interactions, such as the coexistence of superconductivity and magnetism.

Real-space measurements of vortex lattices are difficult because the length scale of the vortex unit cell is in the nanometer range for field strengths on the order of 1 T. Such measurements are now possible using cryogenic scanning tunneling microscopy, which probes the electronic structure of the superconductor on the atomic scale.

Measurements of the symmetry transition in V_3Si were made by recording spatial maps of the local density of states (LDOS) of the superconductor as a function of magnetic field, using the low-temperature scanning tunneling microscope of the Nanoscale Physics Laboratory in the Electron Physics Group. At the location of the vortex, the superconductor is a normal metal and has a much higher density of states for energies inside the superconducting gap. Thus, spatial maps of the LDOS show a bright spot at the location of the vortex.

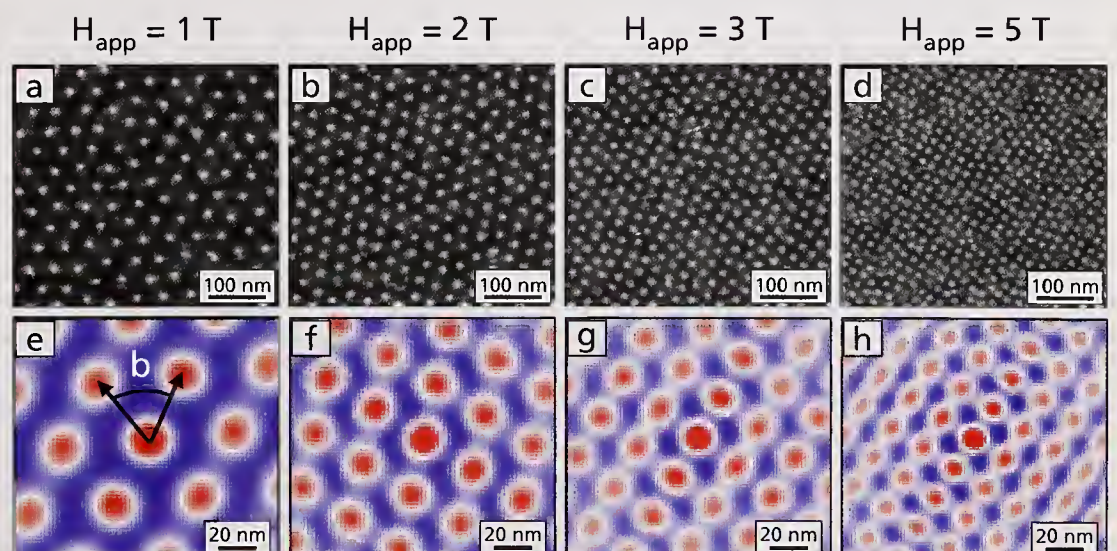


Figure 2. (a-d) STM Fermi-level conductance images of the vortex lattice of V_3Si as a function of applied magnetic field at 2.3 K. (e-h) Corresponding auto-correlation images showing the unit cell of the vortex lattice undergoing the hexagonal-to-square symmetry transition.

Measuring the vortex lattice as a function of magnetic field shows that vortex-vortex interactions are important in determining the symmetry of the vortex lattice. Moreover, the measurements reveal that symmetries in the electronic structure of the superconductor play an important role, as they directly link the symmetry of the vortex lattice to the underlying crystal structure.

CONTACT: Dr. Joseph A. Stroscio
(301) 975-3716
joseph.stroscio@nist.gov

Magnetic Nanostructures in Patterned Ferromagnetic Rings

Small, patterned, magnetic, thin-film structures are a critical part of emerging magneto-electronic technologies, which range from non-volatile magnetic random-access memories to magnetic biosensor arrays. To be useful in devices, the magnetic structure of these rings must assume only a few well-defined magnetic states, and the switching between states must be reproducible.

In collaboration with the Naval Research Lab and the University of Cambridge Thin-Film Magnetism Group, we have used the NIST Scanning Electron Microscopy with Polarization Analysis (SEMPA) facility to non-intrusively image the magnetic nanostructure of a promising subclass of these structures: microscopic magnetic rings. The SEMPA images provided a first direct look at these magnetic states.

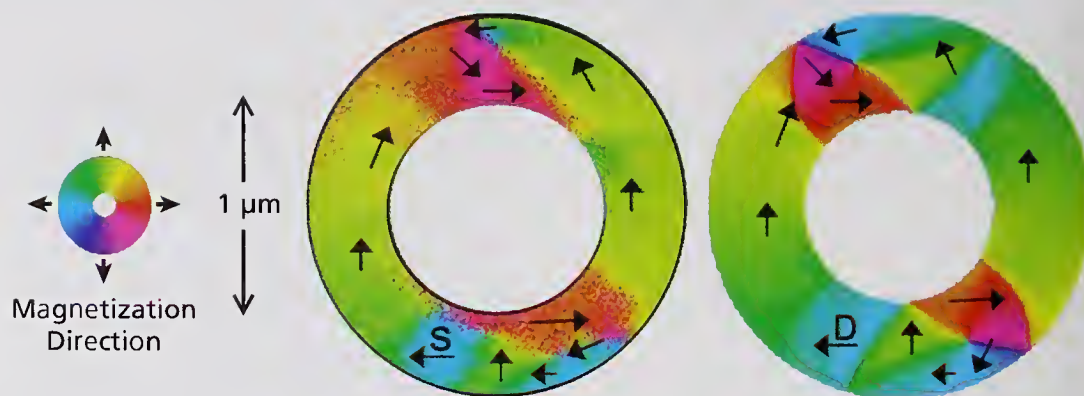


Figure 3. SEMPA image of a magnetic Co ring (center) along with a micromagnetic simulation (right).

By comparing different sized thin-film elements grown under various conditions, the SEMPA images revealed that the interplay between shape and crystalline anisotropy can lead to unexpected magnetic configurations. In particular, undesirable magnetic vortices can be induced in thick-walled rings during switching. The SEMPA images were also used as a quantitative test of micromagnetic models that, in turn, can explore regions of the switching behavior not accessible to static SEMPA measurements.

CONTACT: Dr. John Unguris
(301) 975-3712
john.unguris@nist.gov

Switching Nanomagnets

A current passing through two ferromagnets separated by a non-magnetic spacer layer exerts a torque on each magnetization whenever the two magnetization directions are not parallel. In the appropriate configuration, a large enough current passing through such a multilayer can switch the relative alignment of the mag-

netizations of the layers between parallel and antiparallel. In other configurations, it appears that the magnetization of one layer rapidly precesses around that of the other layer.

These effects, which were observed starting in 1999, are being studied for two device applications. If the size of the current necessary to reverse magnetic bits can be reduced sufficiently, spin-transfer torques could provide a way to switch bits in magnetic random-access memory (MRAM). Alternatively, if the interpretation of recent experiments as precession is correct, it should be possible to make controllable-frequency oscillators.

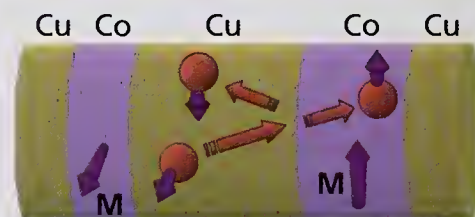


Figure 4. Electron spin scattering from a ferromagnetic interface. The change in spin due to scattering rotates the magnetization.

We have developed quantitative models for spin-transfer torques to help enable the development of devices based on this effect. These models require three types of calculations. We have carried out quantum-mechanical calculations to determine the fate of an electron that scatters from an interface with a ferromagnet. These calculations show that the transverse component of the incident spin current is absorbed close to the interface.

We use this result as a boundary condition in the second type of calculation, semiclassical transport. These calculations determine the polarization, both magnitude and direction, of the current throughout the structure. With the input from the first-principles calculations, our semiclassical calculations reproduce both the transport properties of the structures and the current-induced torques.

Analyzing the calculations in detail highlights the important physical processes, which are difficult to access experimentally. The calculated torques can be used as input to the third type of calculation, classical simulations of the magnetization dynamics.

CONTACT: Dr. Mark D. Stiles
(301) 975-3745
mark.stiles@nist.gov

Linking the Micro and Nano Worlds with Nanolines

As technologies ranging from electronics and data storage to biotechnology become more and more miniaturized, there is an increasing need for ways to make measurements that bridge the domains of the micrometer and the nanometer.

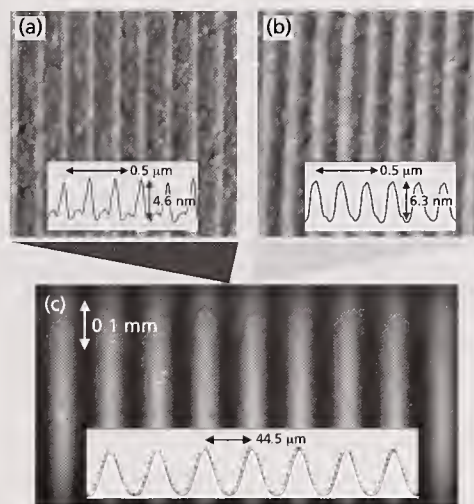


Figure 5. Beating of nanolines: the superposition of two nanoscale patterns with slightly different periodicities results in an optically visible beating on the microscale.

We have collaborated with scientists from the University of Nijmegen to make an artifact that facilitates this connection. It relies on a technology first demonstrated in the Electron Physics Group in 1993, called laser-focused atomic deposition. In its original form, an optical standing wave focused chromium atoms onto a surface, creating an array of lines with a highly precise spacing of 212.78 nm. In the new process, two arrays of lines with slightly different spacing are superimposed, creating a beating, or Moiré, pattern with periodicity of 44.46 μm. When viewed through crossed polarizers, this pattern is clearly visible with an optical microscope.

The result of this process is that nanometer-scale and micrometer-scale patterns are created on a single substrate in coherent registration with each other. Ongoing investigations indicate that because of the resonant nature of the laser-focused atomic-deposition process, the dimensions

of the patterns may be accurately traced to an atomic frequency, so that the patterns can be used as absolute length standards on the nano- and micro-scale.

CONTACT: Dr. Jabez J. McClelland
(301) 975-3721
jabez.mcclelland@nist.gov

Electron Beam Induced Magnetic Switching

Understanding and controlling the magnetic properties of ferromagnetic thin films grown on semiconductor substrates is a critical element in developing hybrid magnetic/semiconductor magneto-electronic devices. We use the exquisite surface sensitivity provided by SEMPA to systematically explore the properties of various ferromagnet/semiconductor combinations. As part of this work, we discovered that electron beams can be used to induce changes in the magnetization direction in ferromagnetic thin films.

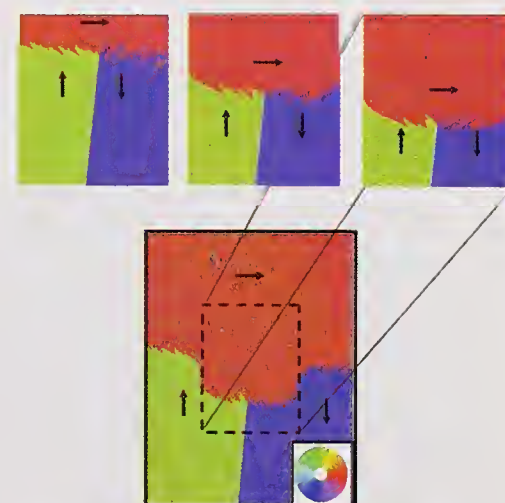


Figure 6. A series of SEMPA images from Fe/GaAs(110) showing the electron-beam-induced magnetization reorientation.

When Fe films are grown epitaxially on the (110) crystal surface of GaAs, the magnetization can be trapped in a metastable state, oriented along the [-110] direction. Irradiating the sample with an electron beam causes the magnetization to locally rotate by 90° into the stable [100] direction.

In addition to providing information regarding domain-wall dynamics in Fe/GaAs, this phenomenon may also provide a means of locally writing magnetic information or patterns in Fe films with electron-beam precision. Work is underway to understand the electron-beam/sample interaction that drives the reorientation, and to investigate its potential for electron-beam writing of magnetic information.

CONTACT: Dr. John Unguris
(301) 975-3712
john.unguris@nist.gov

Figure 7. NIST Synchrotron Ultraviolet Radiation Facility (SURF III) and Beamlines 1-5, with principal users and staff.



The second strategic focus is the development of metrology for extreme-ultraviolet (EUV) optics, the maintenance of national primary standards for radiometry in the EUV and adjoining spectral regions, and the operation of national user facilities for EUV science and applications.

Extreme Ultraviolet Radiation Metrology

INTENDED OUTCOME AND BACKGROUND

The intended outcomes of this program are: maintenance and continuous improvement of the national primary measurement standards for extreme-ultraviolet radiation (EUV: wavelengths between 2 nm and 200 nm, from soft x rays to vacuum ultraviolet), development of techniques for fabricating and characterizing EUV optical systems, and the development of a synchrotron-based, national primary standard for source-based optical radiometry.

The Division has longstanding responsibility for the primary national radiometric standards in the EUV region. EUV radiation

is an important tool for determining the electronic structure of materials, diagnosing plasmas, measuring dynamics of the upper atmosphere, and probing the structure and dynamics of astrophysical objects. One of the key candidates for next-generation semiconductor lithography is an EUV light source, since its short wavelength (13 nm vs. 193 nm for present ultraviolet production lithography) enables diffraction-limited imaging of features with smaller critical dimensions. We are working actively with the semiconductor industry to develop "optical bench" capabilities for characterizing EUV imaging systems.

The Division's key tool for EUV optical metrology is the NIST Synchrotron Ultraviolet Radiation Facility (SURF III). SURF III, the successor to the world's first dedicated source of synchrotron radiation, is a low energy (< 400 MeV), high beam current (up to 1 A), perfectly circular electron storage ring. Its operational characteristics are ideal for EUV metrology, since it does not produce the hard x-ray radiation of higher-energy sources and can be operated over a wide range of beam energies to match the spectral response of systems of interest. As a calculable source of radiation from the far infrared through EUV spectral regions, SURF is also used as a primary standard for source-based radiometry throughout the optical spectrum.

ACCOMPLISHMENTS

Metrology for Extreme-Ultraviolet Lithography

New semiconductor industry requirements for highly accurate EUV reflectivity measurements have provided the impetus for an international comparison of results of measurements at four different EUV facilities: the Advanced Light Source at Lawrence Berkeley National Laboratory (CXRO), the PTB instrument at the BESSY storage ring in Berlin, the ASET instrument in Japan, and SURF III at NIST.

Each lab provided at least one multilayer mirror, which they measured before and after the entire set had been measured at the other facilities. (This was to account for the aging of the mirrors.) For each mirror, the object was to determine the wavelength of peak reflectivity, and the reflectivity at that wavelength.

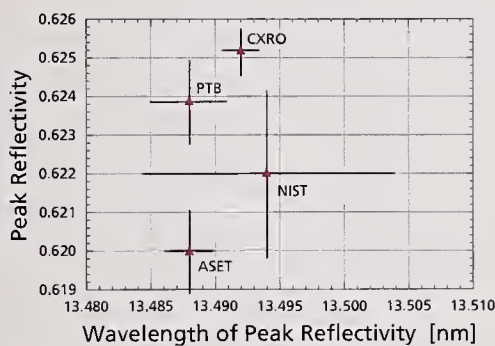


Figure 8. Results of the international comparison of reflectivity and wavelength of maximum reflectivity of a test EUV multilayer mirror, from the Center for X-Ray Optics, (Berkeley, CA), the Physikalisch-Technische Bundesanstalt (Berlin), the Association of Super-Advanced Electronics Technologies (Japan), and NIST.



Figure 9. White light from SURF III (right) is reflected by diffraction grating (foreground), to display spectrum on screen.

Figure 8 shows the results for one sample that is typical of the set. From these results we are confident that the NIST-quoted uncertainty of 0.3 % is a reliable estimate. This uncertainty represents a factor-of-ten improvement over earlier instrument performance, before a comprehensive set of improvements were made in response to more stringent industry demands.

CONTACT: Dr. Charles S. Tarrío
(301) 975-3737
charles.tarrío@nist.gov

Absolute Radiometry at SURF III

The NIST Synchrotron Ultraviolet Radiation Facility (SURF III) serves as the Nation's primary standard for absolute source-based optical radiometry from the visible through the extreme-ultraviolet (EUV) spectral regions. It supports a variety of scientific and measurement missions, primarily in the EUV.

One of SURF's main customers is NASA, which calibrates virtually all its spaceborne EUV spectrometers at the spectrometer calibration facility on SURF Beamline 2. Recent calibrations include instruments flown on the Thermosphere Ionosphere Mesosphere Energetics and Dynamics (TIMED) mission, the EOS SORCE SOLSTICE A and B missions (Earth Observing System, Solar Radiation Climate Experiment, Solar Stellar Irradiance Comparison Experiment), and the SETI/UCSB (VUV Stimulated Mid-IR Experiment) mission.

We have completed an upgrade of the accelerator to improve the radiometric performance, both in accuracy and spectral range. Absolute flux uncertainties are better than 1 % from 2 nm to beyond 400 nm. The storage ring now operates typically at an electron energy of 380 MeV, rather than the 284 MeV energy of SURF II. This results in a significant increase in the flux at soft x-ray wavelengths. Testing of the magnet system has shown the capability of operating from 73 MeV to 417 MeV.

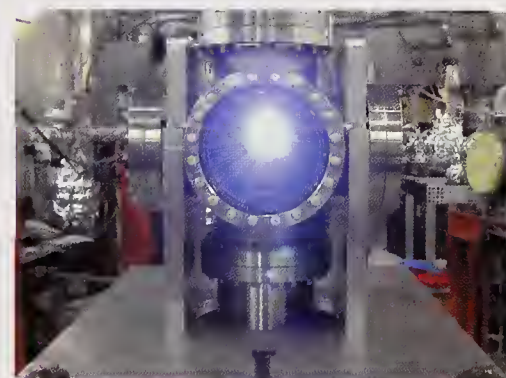


Figure 10. The new white-light radiometry endstation on Beamline 3.

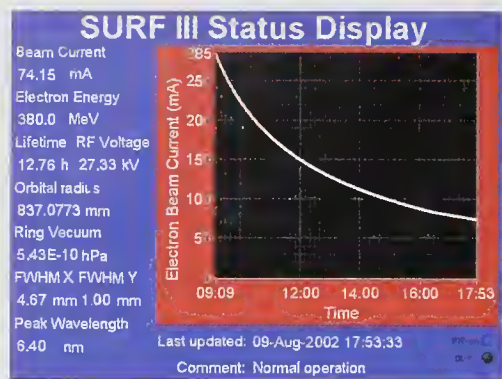


Figure 11. SURF operations at high current for EUV optics characterization.

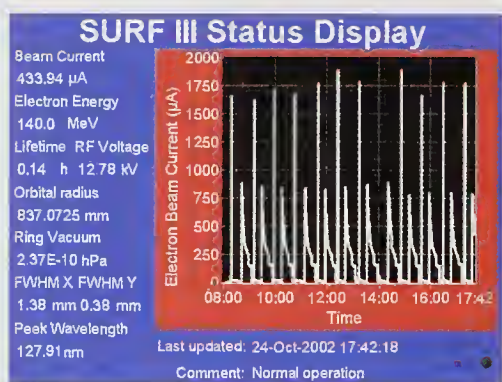


Figure 12. SURF at low current for EUV spectrometer calibration.

SURF can be run under a wide variety of operating conditions according to the needs of different users. Figures 11 and 12 show the quite different conditions required for EUV optics metrology and satellite spectrometer calibration.

CONTACT: Dr. Mitchell L. Furst
(301) 975-6378
mitchell.furst@nist.gov

The third strategic focus is metrology for coherent matter-wave and quantum information processing devices.

Coherent Matter-Wave and Quantum Information Processing Metrology

INTENDED OUTCOME AND BACKGROUND

The intended outcome of this program is to provide measurements and data needed for the development of ultracold atom technology, in particular the use of coherent matter waves in sensors, atom interferometers, and quantum information processing devices.

The Division maintains two efforts in this area, one theoretical and one experimental. The theoretical program is focused on quantitative modeling of degenerate quantum gases, with particular attention to the dynamics of Bose-Einstein condensates subject to external forces, e.g., manipulation of condensates confined in an optical lattice. This program is an outgrowth of extensive collaborations with experimental groups at NIST, JILA, and elsewhere, begun in the mid-1990s.

The primary goal of the experimental program is the development of deterministic atom-delivery systems, i.e. devices that can deliver one and only one atom to a predetermined location, on demand. In addition, the Division is a partner in a

project to develop a testbed for quantum-communication systems, together with the Atomic Physics Division and the Information Technology Laboratory.

ACCOMPLISHMENTS

Coherent Matter-Wave Device Physics

The development of coherent matter-wave sources, based on Bose-Einstein condensates of dilute atomic gases, has opened up a new frontier of precision measurement. There are long-range prospects for the use of such sources for sensitive gravitational and inertial sensors, direct-write atomic lithography, and quantum information processing. In collaboration with experimental programs in Gaithersburg and Boulder, we work on quantitative studies of the dynamics of coherent matter-wave systems, with a particular focus on first-principles modeling and simulation of their dynamics.

One subject of current interest is the dynamics of ultracold atoms in optical lattices, a candidate system for quantum information processing. Optical lattices are defect-free crystal potentials. Solid-state crystal structures tend to favor certain types of lattices and their actual potentials are very complex. Optical lattices, in contrast, are completely controllable, with the potentials being perfectly sinusoidal; or, in general, a sum of sinusoidal potentials.

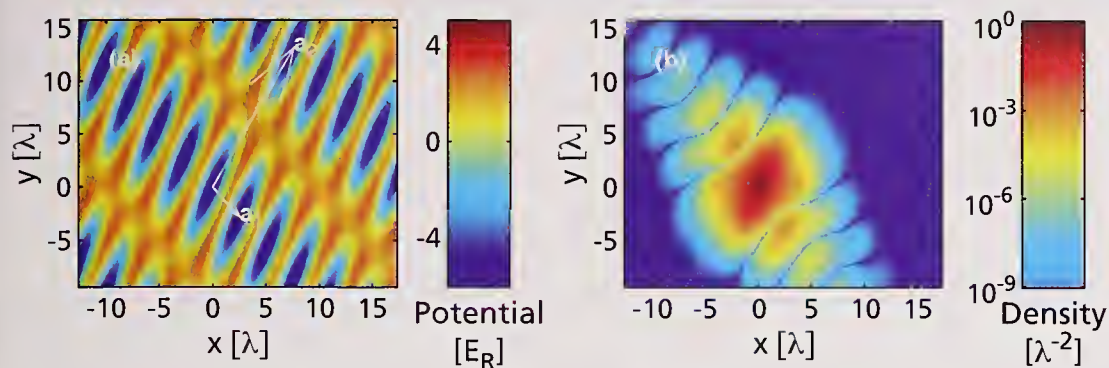


Figure 13. Two-dimensional optical lattice potential (left), and its associated lowest Wannier state (right). Potential and density distributions are shown.

We have calculated the band structure for 2D and 3D optical lattices for parameter regimes appropriate to the experiments at NIST. The energy eigenstates determined by these calculations, known as Bloch states, are useful for calibrating lattice properties (e.g., beam orientation and depth).

As a case study, we investigated the types of lattices that can be prepared for a 2D system made by three light fields in the plane. We showed that, for this simple arrangement, all five types of 2D lattices can be made (square, rectangular, centered rectangular, oblique, and hexagonal).

CONTACT: Dr. Charles W. Clark
(301) 975-3709
charles.clark@nist.gov

Atoms on Demand

Nanotechnology deals with understanding and manipulating matter on the nanometer scale—that is, on the scale of a few tens of atoms to a few hundred atoms. As we gain skill and knowledge in this regime, the natural question arises, can we go further? Can tools be developed that work controllably with single atoms individually, and, if so, what new science and applications will become available?

With these questions in mind, we have recently developed a way to reliably isolate one—and only one—atom, essentially “on demand.” Using laser cooling and trapping techniques, we have isolated single, cold chromium atoms in a magneto-optical trap, and used feedback control over the loading and loss processes to eliminate nearly all the random fluctuations in trap occupation number that would ordinarily plague such a trap.

The result is a source in which single atoms can be extracted and replenished reliably at rates ranging from several tens of atoms per second in the current configuration to several hundred per second or more in the theoretical limit. Applications for these deterministically produced atoms range from fundamental studies of quantum coherence, which take advantage of the purely quantum nature of isolated atoms, to structured doping of nanostructures, in which a small, countable number of dopant atoms is required in nanostructures to tailor their electronic, magnetic, or optical properties.

CONTACT: Dr. Jabez J. McClelland
(301) 975-3721
jabez.mcclelland@nist.gov

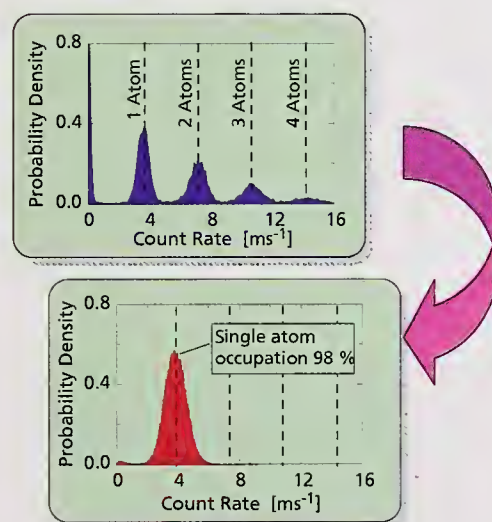


Figure 14. Atoms on demand; the chance of having exactly one atom goes from the random-walk value of 37 % to a value near 100 % by the application of feedback.

GOAL: TO DETERMINE
ATOMIC PROPERTIES
AND EXPLORE THEIR
APPLICATIONS.

ATOMIC PHYSICS DIVISION

The strategy of the Atomic Physics Division is to develop and apply atomic-physics research methods to achieve fundamental advances in measurement science relevant to industry and the technical community, and to produce and critically compile physical reference data.

The first strategic element is to advance the physics of electromagnetic-matter interactions and to explore new applications for laser cooled and trapped atoms.

Light-Matter Interactions and Atom Optics

INTENDED OUTCOME AND BACKGROUND

This strategic element focuses on the physics of laser cooling and electromagnetic trapping of neutral particles, the manipulation of Bose-Einstein condensates (BECs), and the use of optical dipole forces as a new tool for analyzing of microscopic objects in biochemistry. It includes both fundamental and applied studies, such as developing measurement techniques for biomolecular systems and developing a quantum information processor. A strong theoretical-experimental collaboration is aimed at interpreting experimental results and providing guidance for new experiments.

The development of laser cooling and trapping techniques allows exquisite control over the motion of atoms. Such control has been exploited to build more precise atomic clocks and gravity gradiometers. These techniques also enable the study and manipulation of atoms and molecules under conditions in which their quantum or wave behavior dominates. This research has revolutionized the field of matter-wave optics.

Our research includes theoretical and experimental projects that contribute to the understanding and exploitation of Bose-Einstein condensation of neutral atoms, matter-wave optics, optical and magnetic control of trapped-atom collisions, advanced laser cooling and collision studies for atomic clocks, ultracold plasmas and Rydberg atoms, the study of the superfluid to Mott-insulator quantum phase transition, quantum information processing, quantum-computing architectures,

and optical characterization and manipulation of single molecules, biomolecules, and biomembranes.

ACCOMPLISHMENTS

From an Atomic BEC to Mott-Insulator to a Molecular BEC

Recent theoretical calculations show how to obtain a quantum phase transition that takes the superfluid state appropriate to a BEC in a shallow, three-dimensional, optical lattice and transforms it to a Mott-Insulator state appropriate to a deep optical lattice. In the superfluid state all the atoms are identical, whereas in the deep lattice, Mott-Insulator state the atoms are distinct since they are individually labeled by their lattice position.

We have shown that if we start with an average of two atoms per optical lattice site and increase the lattice depth to obtain a Mott-Insulator state with exactly two atoms per well site, we can then convert the atom pairs into ground state molecules using laser light. Finally, after molecular formation, the Mott-Insulator

can be “melted” to yield a molecular BEC. Specific calculations have been done for the homonuclear species $^{87}\text{Rb}_2$ and the heteronuclear species KRB.

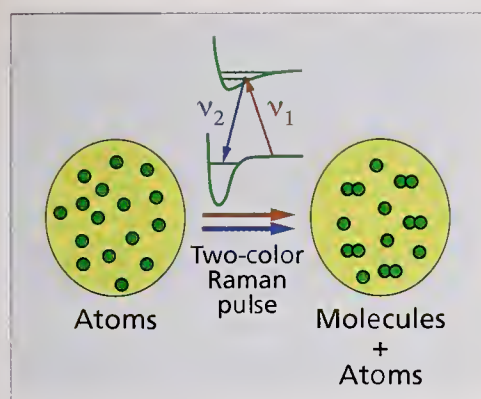


Figure 1. Schematic showing two-color formation of molecules in their ground electronic state by Raman Photoassociation. In a BEC this process is initially coherent and leads to a wavefunction that is both atoms and molecules.

Studies of atomic BEC systems have proven to be extraordinarily fruitful, with connections to a number of disciplines, including atomic, molecular, and optical physics, quantum optics, condensed-matter physics, solid-state physics, quantum field theory, and quantum information and computing. One of the primary purposes of the Mott-Insulator transition is the initialization of a neutral-atom quantum register for quantum computing. The production of molecular BECs will extend applications to molecular species. Experiments along some of these lines are being planned.

CONTACT: Dr. Carl Williams
(301) 975-3531
carl.williams@nist.gov

Photoassociation in a Bose-Einstein Condensate

We have investigated the photoassociation of atoms (two colliding atoms absorbing a photon, forming a molecule) in a trapped, sodium BEC. We measured a rate coefficient that exceeds the classical limit by more than four orders of magnitude. The measured rate coefficient is, however, in good agreement with results from a quantum-mechanical two-body scattering theory. Classically, atoms have to be next to each other to form a molecule, but quantum mechanically, the BEC has a single wavefunction for all the atoms extending over the entire trapped gas.

This is another example of how the quantum world can give remarkably different results than the classical world. Such studies are important for developing theories that describe the BEC. The theories can then be used to exploit the BEC as a source of atoms analogous to the source of photons from a laser for use in precision measuring devices, such as atom interferometers.

CONTACT: Dr. Paul Lett
(301) 975-6559
paul.lett@nist.gov

Real-Time Measurements of Antigen-Antibody Binding

Adhesion is an ubiquitous process in biological systems. We have developed a new technique to study the adhesion of biomolecules in real time under biologically relevant conditions, similar to the situation when two cells collide and adhere.

Using optical tweezers, we trap a pair of microspheres, one coated with an antigen and the other coated with the corresponding antibody, and bring them close enough to each other that they repeatedly collide due to thermally driven motion. By monitoring the position of the trapped, antigen-coated microsphere, we can observe single antigen-to-antibody binding events in real time. We also measure the single molecule, spontaneous dissociation rate and the average rate at which antigen-antibody pairs unbind due to thermal fluctuations. By varying the number of antigen-to-antibody bonds that can form in a collision, we can observe cooperativity in the binding. We observe not only positive cooperativity, but also negative cooperativity (which is rarer in nature) depending on how rigidly the antigen molecule is attached to the microsphere surface.

CONTACT: Dr. Kristian Helmerson
(301) 975-4266
kristian.helmerson@nist.gov

Patterned Loading of Atoms into an Optical Lattice

Quantum systems, such as individual atoms, can be used as bits of information. The processing of such information, governed by the rules of quantum mechanics, is called quantum computing. There is currently great interest in realizing a quantum computer, which is predicted to require exponentially less effort than a classical computer to solve certain large-scale problems, such as factoring large numbers.

We are developing a processor for quantum information, using neutral atoms trapped in an optical lattice as the quantum information register. In an optical lattice, atoms are trapped in the periodic intensity pattern formed from the interference of intersecting laser beams.

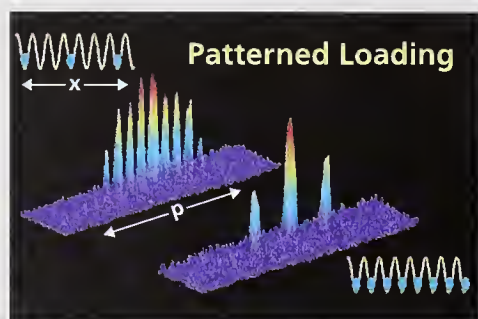


Figure 2. Diffraction pattern showing the contrast between atoms coherently loading into every third lattice site, versus every lattice site.

In order to achieve the best performance for quantum information processing, we would like atoms tightly confined, which can be achieved with a short-period optical lattice. However, to initialize and read out the quantum register, we would like atoms in sites spaced more than an optical wavelength apart. We have taken a major step towards achieving this goal by loading every third site of a one-dimensional, short-period optical lattice with atoms from a rubidium Bose-Einstein condensate.

CONTACT: Dr. James (Trey) Porto
(301) 975-3238
trey.porto@nist.gov

The second strategic element is to develop advanced optical and x-ray measurement techniques for applications involving laboratory and space plasmas, thin-film structures, and nanoscale devices.

Plasma and X-Ray Measurement Methods

INTENDED OUTCOME AND BACKGROUND

This strategic element focuses on the use of atomic radiation as an efficient, non-interfering probe of plasmas and industrially important materials. Our research includes sizable plasmas used for etching semiconductor wafers, small-scale plasmas confined in electromagnetic traps, and nanoscale plasmas induced on surfaces by individual, highly charged ions. Information is obtained by measuring the emitted photons and massive particles using a variety of instruments, including visible, ultraviolet, and x-ray spectrometers, microcalorimeters, mass spectrometers, submillimeter wave detectors, and spatial imaging systems. In addition, surface effects are analyzed at the atomic level using a scanning tunneling microscope and an atomic-force microscope.

Our plasma diagnostic research includes collaborations with industry, university, and government partners. For example, Intel and International SEMATECH have requested that the NIST electron-beam ion trap be utilized to assist in the development of EUV lithography light sources.

We work with x rays since their weak interactions make them a nearly ideal penetrating probe. The primary goals of this research are the development and application of high-resolution x-ray scattering techniques, the production of reference samples of thin-film and multilayer structures, and the understanding of the microstructure of thin-film and multilayer structures appropriate to the semiconductor industry.

Following on our experience fielding a high-energy, curved crystal spectrometer at the OMEGA laser facility at the University of Rochester, we are presently producing a more ambitious, broadband, multichannel x-ray spectrometer system for the National Ignition Facility (NIF). These types of instruments will serve the plasma-diagnostic community by providing information about such things as the hot-electron energy distribution and the plasma temperature.

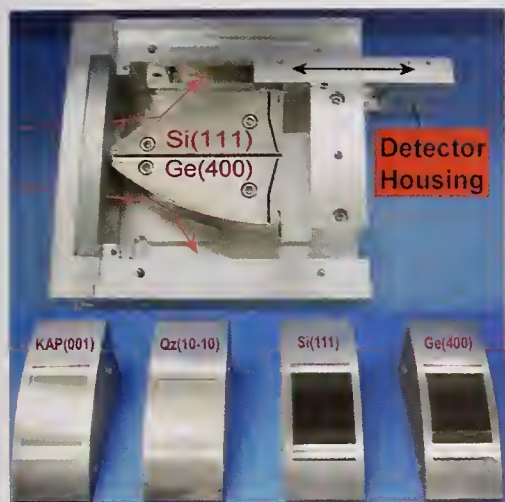


Figure 3. Reflection-geometry spectrometers constructed as a National Ignition Facility plasma diagnostic (top). Four convex, curved crystals (bent to five inches radius of curvature) together provide cascading high-resolution x-ray spectral coverage from 1 keV to 20 keV. The four crystals shown (bottom) are Potassium Acid Phthalate, Quartz, Silicon, and Germanium.

ACCOMPLISHMENTS

Optical Properties in Support of UV Lithography

Optical-lithography technology is growing to more rely upon deep- and vacuum-ultraviolet radiation in order to further extend the performance of advanced integrated circuits. This necessitates the use of crystalline fluoride materials for the refractive optics, though little was known of the optical properties of these materials at these short wavelengths.

In May 2001, we uncovered a very large, completely unexpected intrinsic birefringence in calcium fluoride at short wavelengths. Its index of refraction depends on the polarization of the incident light. Since then, the 157 nm lithography community has been struggling to find ways to design around this aberration.

The NIST team continues to work on developing a new crystalline material that does not exhibit birefringence at 157 nm as one approach to ameliorate this problem. This material is based on mixed solid solutions of CaF_2 and SrF_2 , which separately have opposite signs of the effect. Working with industrial partners for material growth, this new material is being grown and characterized.

To establish the properties of this and other UV materials, NIST has developed a unique phase-shifting interferometer that can measure the index homogeneity and birefringence at wavelengths ranging from the visible through 146 nm (in the vacuum ultraviolet). It has enabled a determination of the dispersion of these properties in this complete wavelength range.

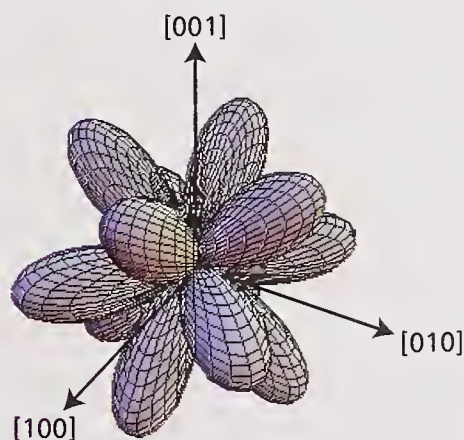


Figure 4. Directional dependence of the spatial-dispersion-induced birefringence in calcium fluoride and related cubic materials, first calculated and measured as part of this project. The figure shows the previously-unknown heptaxial behavior (seven nonbirefringent axes) for this cubic system.

An effort to characterize many materials and samples is being pursued to see if a scaling factor can be established which reliably provides the 157 nm values from the much more easily measured visible wavelength values.

CONTACT: Dr. John Burnett
(301) 975-2679
john.burnett@nist.gov

Ion-Gas Recombination Studies

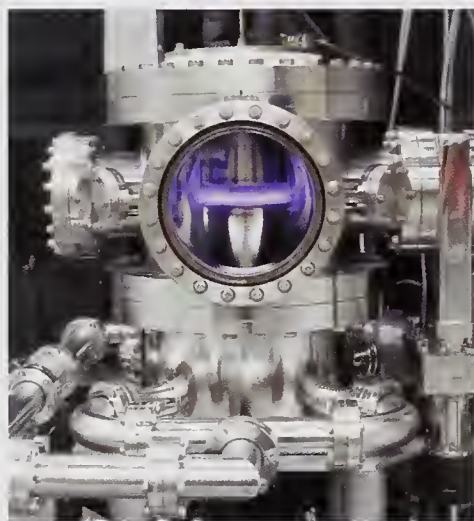
Motivated by a growing interest from the fusion-energy and astrophysics communities, we have expanded the NIST Electron Beam Ion Trap facility to allow ion-gas collision studies. We have installed a gas-jet target and additional detectors on our ion beamline to study the photons that are emitted as the ions traverse the target.

The new apparatus has yielded measurements on a sequence of charge states of krypton, starting at Kr^{27+} and extending through Kr^{36+} . The study reveals systematic changes in x-ray wavelength and intensity ratios as a function of ion charge state. Particularly dramatic is an abrupt increase, by a factor of two, in the $L\alpha/M$ ratio as the L-shell changes from single vacancy to multiple vacancy. A time-dependent collisional-radiative model of the excited-state population distribution confirms that the origin of this shift is the formation of metastable states.

CONTACT: Dr. John Gillaspay
(301) 975-3236
john.gillaspay@nist.gov

Detection of Chemical Contamination in a Semiconductor Plasma-Etching Reactor

High resolution, submillimeter wavelength, linear-absorption spectroscopy has been developed as a tool for monitoring chemical contamination in plasma-etching reactors. Contamination may arise from feed-gas impurities, vacuum-chamber leaks, and incomplete chamber cleaning. The submillimeter methods are particularly sensitive to contamination originating from water vapor, which has an intense rotational transition at 557 GHz.



© Robert Rathe

Figure 5. The GEC RF Reference Cell, a standardized plasma source designed to create plasmas similar to those found in commercial semiconductor etching reactors.

We have measured this rotational transition in a Gaseous Electronics Conference (GEC) reference cell, installed at a commercial company, under three different reactor conditions prior to initiating a fluorocarbon plasma. The apparatus has

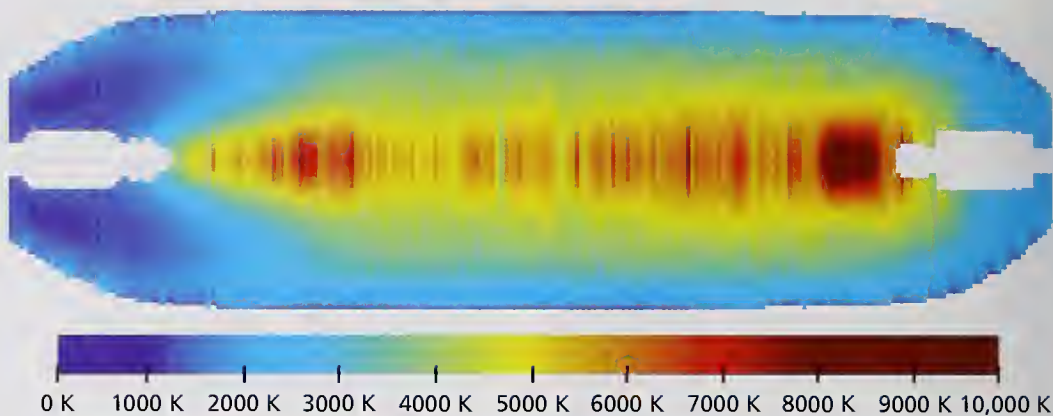


Figure 6. Temperature distribution in a high-pressure lighting discharge as revealed by x-ray absorption imaging.

demonstrated sensitivity levels less than 10 nmol/mol. Levels less than 1 nmol/mol should be possible.

CONTACT: Dr. Eric Benck
(301) 975-3697
eric.benck@nist.gov

A New Powerful Probe for High-Efficiency Lighting

There are an estimated one billion plasma light sources in service in the United States, consuming an estimated 2 exajoules (600 billion kilowatt-hours) of electrical energy annually. These sources are principally fluorescent lamps and metal-halide discharge lamps. In the past, metal-halide lamps were used mainly for high-intensity lighting of large spaces. Now, because of their high brightness and energy efficiency, they are also being developed for automobile headlights and interior lighting.

As a result, there is a growing interest in increasing their luminous efficiency through a better understanding of the processes that govern their operation.

These processes are so complex that they have defied attempts at predictive modeling or even the development of scalable design rules.

As part of a cooperative program with the Electric Power Research Institute, NIST researchers have used x rays from the Advanced Photon Source at Argonne National Laboratory to develop a new generation of diagnostic methods for metal-halide lamps. Both x-ray absorption and x-ray fluorescence were used to map the distribution of the temperature and the various elemental components in a production-style lamp.

The use of these techniques will enable lighting scientists and engineers to develop a more complete understanding of metal-halide arc lamps, leading to improved design rules, advanced production methods, and eventually, more energy-efficient lighting.

CONTACT: Dr. John Curry
(301) 975-2817
john.curry@nist.gov

The third strategic element is to advance measurement science at the atomic and nanometer scale, focusing on ultraprecise length-displacement measurements, x-ray and gamma-ray precision metrology, and nanooptics and nanosystems modeling.

Nanoscale and Quantum Metrology

INTENDED OUTCOME AND BACKGROUND

Optical and x-ray interferometry is being used to complete the intercomparison phase in displacement interferometry. We are measuring the effect of diffraction on interferometric measurements through comparison of Michelson and Fabry-Perot interferometry. We are evaluating a hybrid positioning system in which long-range positioning over 50 mm is provided by a high-quality commercial translation stage, and guiding errors are compensated by a fine positioning stage incorporating a multichannel closed-loop servo system. We are also working on the direct link of a displacement measurement to a cesium clock by means of a frequency comb. The goal is to provide the first measurement of a displacement directly related to the definition of the meter, without the intervention of a calibrated reference laser.

The wavelengths and energies of x- and gamma-ray transitions are determined for applications in crystallography and x-ray astronomy, for fundamental studies of the properties of matter, and for the fundamental constants. Crystal diffraction is the principal measurement tool, and the lattice spacings of nearly perfect crystals are determined by comparison to standard

crystals. Diffraction angles are measured interferometrically or with well-calibrated encoders. For lower-precision measurements, curved crystals are used with position-sensitive detectors.

ACCOMPLISHMENTS

Optical Fiber Tapering System for Supercontinuum Generation

The frequency comb produced by a mode-locked femtosecond laser has revolutionized optical-frequency metrology and is now being applied to displacement metrology. In order to relate the visible wavelengths used for interferometry with an infrared femtosecond laser, we shift the spectrum of the femtosecond laser by means of nonlinear optics in a fiber that is tapered to such a small diameter that the light propagates in the exterior of the cladding rather than the core.

We have constructed a facility to taper optical fibers to a well-controlled geometry. The facility consists of four stepper-motor-driven stages that simultaneously pull the fiber as it is being heated by a very small, traveling flame. By controlling the oscillatory motion of the flame as the fiber is pulled, we can force the fiber to adopt almost any arbitrary shape.

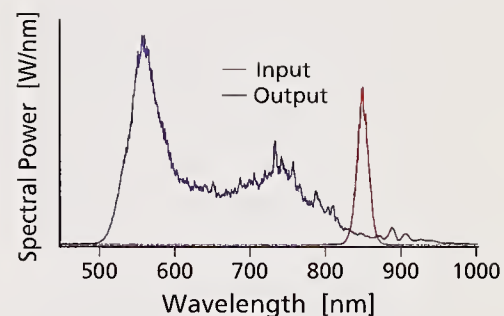


Figure 7. Tapered optical fiber shifts the frequency spectrum of mode-locked femtosecond laser output from 850 nm to cover most of the visible spectrum. The vertical scale is linear; the scales for input and output are different.

Figure 7 shows the spectrum from a fiber whose diameter had been reduced from 125 μm to 2.7 μm and which was pumped at 850 nm. We have successfully observed the beat from such a fiber and a helium-neon laser at 633 nm.

CONTACT: John Lawall
(301) 975-3226
john.lawall@nist.gov

Designing the Nanoworld: Atomic-Scale Simulations of Nanostructures and Nanodevices

Atomic-scale simulations of the electronic and optical properties of complex nanosystems at the meso/molecular interface are being carried out. These systems include nanocrystals, self-assembled dots (as shown in Fig. 8), nanodot arrays and solids, molecular electronics, biomolecules, and bio/nanohybrids.

Atomic-scale variations in geometry, size, shape, and composition critically impact the functionality of these nanosystems. For example, our simulations show that the optical response of arrays of nanodots can be turned on or off simply by changing the number of atoms between the dots. Our studies of doped fullerenes show that dopants exist for p- and n-type doping, that these doped fullerenes can be combined to form molecular rectifiers, and that their properties can be tailored as dopant atoms are added one-by-one.

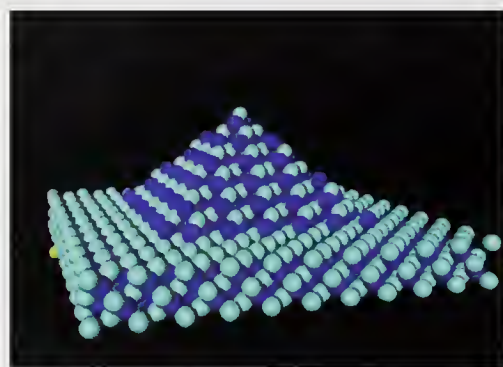


Figure 8. Schematic of a self-assembled pyramidal quantum dot. Atomic positions used in the modeling are indicated.

These simulations provide benchmarks for precision experimental tests of the atomic-scale sensitivity of nanosystems. The work is providing the foundation needed to build design tools for engineering nanolasers, detectors, biomarkers and sensors, quantum devices, and nanomaterials.

CONTACT: Dr. Garnet Bryant
(301) 975-2595
garnett.bryant@nist.gov

The fourth strategic element is to produce reference data on atomic structure and to critically compile reference data for scientific and technological applications.

Critically Evaluated Atomic Data

INTENDED OUTCOME AND BACKGROUND

The objective of this strategic element is to critically compile fundamental constants and atomic spectroscopy data from the far infrared to the x-ray regions. We disseminate these reference data on the Physics Laboratory website, produce high-quality data for urgent scientific or technological needs, and resolve discrepancies in the body of the data.

The NIST databases for atomic spectra and fundamental constants are recognized throughout the world. The Atomic Spectroscopic Database on our website now receives about 80,000 downloads per month, up from 60,000 only two years ago. The principal users are plasma physicists, crystallographers, astronomers, lighting engineers, and spectrochemists.

However, the databases are still far from complete, and the quality of the data available in the literature from which the databases are built is uneven. The current versions of our databases are not sufficiently reliable for some fields of science and technology, and needs for such reference data are continuously growing. Our scientists focus their resources on the most urgent needs of the user communities. When accurate, reliable data do not exist for high priority needs, specific measurements or calculations are undertaken to produce them.

ACCOMPLISHMENTS

New X-Ray Wavelength Table in Review of Modern Physics

Important experimental and theoretical developments in the field of x-ray transitions have made the mid-1960s database of these transitions obsolete. On the experimental side, x-ray wavelengths can now be more accurately linked to optical wavelengths and the SI definition of length, through combined x-ray and optical interferometry. In addition, a number of recent, accurate x-ray measurements, and updated values of the fundamental physical constants, are available to be included in the database. On the theoretical side, there has been continued development of better calculational procedures that produce results in excellent agreement with experiment. This good agreement creates the possibility that theoretical values can provide rather good estimates of missing or poorly measured experimental data.

In collaboration with theorists in France and Sweden, we have produced a new reference x-ray wavelength table that is being published in *Reviews of Modern Physics*. The new table is the culmination of a long-term NIST effort to produce an improved, comprehensive data resource for x-ray transition energies. It contains

K- and L- x-ray transition and absorption edge energies for all elements from neon to fermium. It includes carefully selected and evaluated experimental data robustly connected to the SI definition of length, and accurate, state-of-the-art theoretical estimates. The new x-ray wavelength table will soon be available also on the NIST Physics Laboratory website.

CONTACT: Dr. Ernest Kessler
(301) 975-4844
ernest.kessler@nist.gov

Handbook of Basic Atomic Spectroscopic Data

To meet increasing needs for reference spectral data for neutral and singly-ionized atoms, we completed a new database of wavelengths, energy levels, and transition probabilities for the most important transitions in all elements from hydrogen to einsteinium.

This Handbook of Basic Atomic Spectroscopic Data lists wavelengths and intensities for over 12,000 transitions. Energy levels and transition probabilities are given for about 2400 of the strongest lines, taken from over 400 references. Data for individual elements can be accessed by name, atomic number, or atomic symbol. A finding list is available to assist in identification of possible impurities in an observed spectrum.

This handbook will be published in standard paper format, in an e-book that combines ease of use and portability, and in an electronic version on the Physics Laboratory website.

CONTACT: Mrs. Jean Sansonetti
(301) 975-4725
jean.sansonetti@nist.gov

Precision Measurement of Laser Wavelengths for 157 nm Microlithography

The next generation of microlithography tools will be based on a molecular-fluorine laser operating at 157 nm. In order to design optical systems for focusing ultraviolet radiation from the laser onto the chip substrate, the index of refraction of the optical materials must be known to high accuracy. Since the index of refraction varies rapidly with wavelength, it is critical that the wavelength of the laser also be accurately known.

To obtain accurate wavelengths for the F₂ laser, we used the NIST 10 m vacuum spectrometer to measure the lasing lines from a commercial F₂ laser in the region of 157 nm. The experiment was conducted in collaboration with an excimer laser manufacturer, which supplied the laser. The spectra were calibrated by spectral lines from a platinum hollow-cathode lamp that had been measured by NIST and used to calibrate spectrometers

on the Hubble Space Telescope. The high accuracy of these measurements relied on a specially designed system to illuminate the spectrometer in such a way as to eliminate small shifts between the spectrum of the lasing lines and that of the calibration lamp.

Wavelengths of six lasing lines were measured to an uncertainty of ± 0.0001 nm. Three of the lines were newly observed lasing lines.

CONTACT: Dr. Craig Sansonetti
(301) 975-3223
craig.sansonetti@nist.gov

GOAL: TO PROVIDE THE FOUNDATION OF OPTICAL RADIATION MEASUREMENTS FOR OUR NATION.

OPTICAL TECHNOLOGY DIVISION

The strategy for meeting this goal is to develop and provide national measurement standards and services to advance optical technologies spanning the ultraviolet through the microwave spectral regions.

The first strategic element is to develop and provide optical radiation standards based on the SI units.

Optical Radiation Standards

INTENDED OUTCOME AND BACKGROUND

The Optical Technology Division plays a fundamental role in promoting the use of optical technology by undertaking research and development to advance the measurement science needed to maintain the Nation's primary SI standards for the candela and kelvin and associated photometric, colorimetric, pyrometric, and spectral radiometric quantities. These standards affect a host of industries, from aerospace to lighting, by ensuring the accuracy and agreement of measurements between and within organizations.

A significant part of the Division's activities includes participation in international comparisons of measurements with other national metrology institutes through the Consultative Committees on Temperature,

and on Photometry and Radiometry, of the International Committee of Weights and Measures. These comparisons provide an important assessment of measurement quality and help guarantee the international acceptability of our Nation's optical radiation measurements.

To ensure unsurpassed measurement accuracy, the Division's radiometric scales are increasingly being based on stable, low-noise, highly linear detectors, radiometers, and photometers. Their absolute responsivities are traceable to optical-power measurements performed using cryogenic radiometry and a state-of-the-art laser facility, SIRCUS (Spectral Irradiance and Radiance Calibrations with Uniform Sources). Cryogenic radiometry provides the most accurate optical-power measurements by directly comparing optical and electrical power. The Division's High-Accuracy Cryogenic Radiometer (HACR), the Nation's standard for optical

power, achieves a relative standard uncertainty of less than 0.02 %. This will be reduced to 0.01 % with the completion of HACR 2.

The improvements realized by tying the radiometric measurements to a cryogenic radiometer are significant. Recently the Division's spectral-irradiance scale, as disseminated by FEL lamps, was converted to a detector-based scale traceable to optical-power measurements performed by HACR. The improved detector-based scale has led to a reduction of the spectral-irradiance uncertainties by a factor of two for ultraviolet and visible radiation, and a more significant reduction for infrared radiation.

These activities in detector-based radiometry are complemented by new research in source-based radiometry, i.e., radiometry based on a source of radiation whose spectral output is absolutely known. This new research uses synchrotron radiation from an electron-storage ring, the recently upgraded NIST Synchrotron Ultraviolet Radiation Facility (SURF III), as a source of continuously tunable, intense ultraviolet radiation.

ACCOMPLISHMENTS

Detector-Based Radiance and Radiance-Temperature Scales

We have reduced the uncertainties of the present, source-based, spectral-radiance and radiance-temperature scales by converting to detector-based scales.

These scales are tied to an absolute imaging pyrometer (AP1). We calibrated its absolute radiance responsivity at the SIRCUS facility, using a tunable, laser-illuminated integrating sphere as the source of spectral radiance. The spectral radiance is traceable to silicon trap detectors calibrated for absolute power responsivity against HACR and a set of apertures of known area to define the geometry.

Measurements performed with AP1 of the freezing point of a high-emissivity blackbody cavity in contact with molten gold reveal a noise-equivalent temperature of 2 mK ($k = 2$) at 1337 K. The total uncertainty of the measurements, about 120 mK ($k = 2$) at this temperature, is due to the combined uncertainties arising from the radiance-responsivity calibrations, the size-of-source effect, and the long-term stability of the pyrometer.

In concert with the AP1 development, we have performed radiance-temperature measurements of a 2950 K high-temperature blackbody (HTBB), comparing both conventional source-based and newer detector-based measurement methods. The source-based approach uses measured radiance relative to a gold-point, fixed-temperature blackbody to assign the temperature to the HTBB as prescribed by the International Temperature Scale of 1990. The detector-based approach

uses a set of filter radiometers to assign a temperature to the HTBB. Their spectral-irradiance responsivities are traceable to the HACR optical-power scale through the Division's Spectral Comparator Facility. The spectral-irradiance responsivities are converted to spectral-radiance responsivities by an appropriate choice of precision apertures and measurement geometries. The aperture areas required in the analysis are determined using an optical coordinate-measuring machine.

The net result: we demonstrated a detector-based temperature uncertainty of 0.21 K ($k = 2$) at 3000 K, more than a factor of six better than the source-based approach.

CONTACT: Dr. Howard Yoon
(301) 975-2482
howard.yoon@nist.gov

SURF III as an Absolute Source of Spectral Irradiance

An experiment was undertaken to verify that the absolute spectral irradiance from the NIST Synchrotron Ultraviolet Radiation Facility (SURF III) can be predicted using the Schwinger relativistic electro-dynamical model for synchrotron radiation and knowledge of the electron-beam energy, current, and radius.

The study was performed on Beamline 3, recently developed for absolute, source-based, ultraviolet radiometry at SURF III. The measurements consisted of characterizing the angular spread of the radiation from SURF III in the direction perpendicular to the orbital plane of the electron beam. Because of the highly relativistic

speed of the electron beam, the angular spread is narrowly confined to within a fraction of a degree of the orbital plane. Narrow-band filtered radiometers, with spectral responsivities measured to 0.1 % relative uncertainty ($k = 2$) at the SIRCUS facility, were used to directly measure the radiation emitted from a tangential source point of the ring, from the near ultraviolet to the infrared.

The experiment demonstrated agreement with theory to within 0.5 %. Such excellent agreement not only confirms the Schwinger theory, but it also connects the detector-based spectral-irradiance scale, based on SIRCUS and cryogenic radiometry, to the source-based scale of SURF III. The study further validates Beamline 3 as a broadband standard of spectral irradiance for the absolute calibration of optical instruments and for the calibration of deuterium and FEL incandescent lamps as secondary or transfer standards.

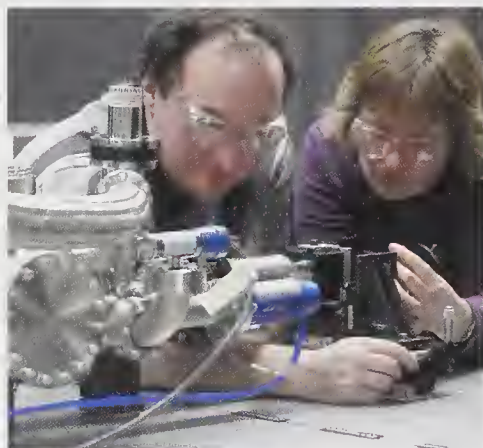
CONTACT: Dr. Ping Shaw
(301) 975-4416
shaw@nist.gov

Second-Generation High-Accuracy Cryogenic Radiometer (HACR 2)

A second-generation cryogenic radiometer is under development to further reduce the uncertainty in our optical-power measurements. The expected factor-of-two reduction in the power-measurement uncertainty will affect many of the radiometric and photometric scales maintained in the Division and presently tied to the first-generation HACR.

The new instrument is designed to have a greater dynamic range, from 1 μ W up to 70 mW in power, faster response time, lower noise figure, and improved modular construction. It will be installed in the SIRCUS facility, providing ready access to a variety of lasers. These lasers allow a broad range of wavelength and power levels to be selected for scale transfer to silicon trap detectors, further reducing the uncertainties in the measurement chain. Additionally, the modularity of the detector section permits new detector modules to be designed and built, optimized for specific wavelengths and power levels.

CONTACT: Dr. Joseph Rice
(301) 975-2133
joe.rice@nist.gov



© Robert Rathe

Figure 1. Jeanne Houston and Joe Rice preparing to calibrate a silicon-photodiode trap detector using our second-generation High Accuracy Cryogenic Radiometer, HACR 2.

The second strategic element is to develop novel optical measurement methods for solving problems in critical and emerging technology areas.

Optical Measurement Methods

INTENDED OUTCOME AND BACKGROUND

The Division strives to improve the accuracy, acceptability, and utility of optical measurements by conducting long-term, directed research in the NIST strategic focus areas of homeland security, nanotechnology, and health care, and in such promising technology growth areas as interface science, biophysics, semiconductor manufacturing, and quantum communication.

In the areas of nanotechnology and interface science, we are developing linear and non-linear laser and near-field techniques to characterize thin-films, surfaces, and interfaces important in molecular biology, polymer science, and nanotechnology.

In biophysics and health care, new optical methods based on surface-enhanced Raman spectroscopy and confocal, fluorescent, imaging microscopy are being developed for the investigation of single, biological molecules. This is part of a larger, inter-laboratory competence program in Single-Molecule Measurement and Manipulation, funded by the NIST Director.

The Division's activities in support of semiconductor manufacturing include research to improve the accuracy of temperature

measurements in rapid thermal processing, to develop optical-scattering metrology for the next-generation wafer inspection tools, and to develop chemical diagnostic methods for reactive, ion-etching plasmas using submillimeter spectroscopy. Ultraviolet-radiation metrology is being developed to ensure a measurement infrastructure for 157 nm and shorter-wavelength lithography, leveraging the unique ultraviolet-radiometry capabilities of SURF III to target needs in optical-materials properties, detector radiation-damage characterization, and laser-power measurements.

In response to recent events, our support of optical-radiation measurements for homeland security has increased, building on expertise developed through the NIST Director's competence program in THz Metrology. We are investigating femto-second-pulsed THz spectroscopy for the detection of biological-warfare agents in paper envelopes that are effectively transparent in the THz spectral region, and continuous-wave THz spectroscopy for the sensitive detection of chemical-warfare agents.

We are also using our unique expertise in correlated-photon radiometry to develop novel, single-photon-on-demand sources for secure quantum cryptography, in collaboration with other PL Divisions.

ACCOMPLISHMENTS

Optical Scattering by Nanoparticles on Si Wafers

Light-scattering methods were developed to allow accurate measurement of the diameters of standard reference particles bound to silicon substrates. This was in response to the semiconductor industry's need for improved metrology of particles and other defects on silicon wafers. The identification and quantification of such defects are required to facilitate the transfer of wafers from the factory to the chip manufacturers, and to locate and diagnose problems in the chip fabrication line.

To calibrate inspection tools, and thus to assure agreement between the wafer and chip manufacturers, the industry intentionally deposits accurately-sized, polystyrene spheres onto reference wafers. Because the deposition process can lead to changes in the size distribution of the particles, techniques are required to accurately determine the diameters of the deposited particles.

To address this need, we did a combined theoretical and experimental investigation of the optical properties of subwavelength-diameter spheres on surfaces. The Bobbert-Vlieger theory of light scattering by a spherical particle on a flat substrate was extended to account for films on both the substrate and the particle, and then validated by measurements on deposited, polystyrene and copper nanospheres. The copper spheres provided a particularly demanding test of the theory due to the presence of a strong near-field interaction between the conducting spheres and the silicon substrate.

To assess the measurement uncertainty of the diameter of the particles, the effects of non-sphericity, size distribution, and doublet formation were investigated. The modal diameter of the 100 nm polystyrene sphere standard (SRM[®] 1963) was determined to be 99.7 nm with an uncertainty of 1.7 nm ($k = 2$), in excellent agreement with aerosol measurements.

The technique is presently being incorporated into semiconductor industry standards.

CONTACT: Dr. Thomas Germer
(301) 975-2876
germer@nist.gov

Single-Molecule Optical Probe of Binding in Antibody-Antigen Force Measurements

As part of a NIST-wide competence program in Single-Molecule Measurement and Manipulation (SM³), we are developing sensitive, single-molecule, spectroscopic and imaging techniques for incorporation into MEMS-based, molecular-screening platforms.

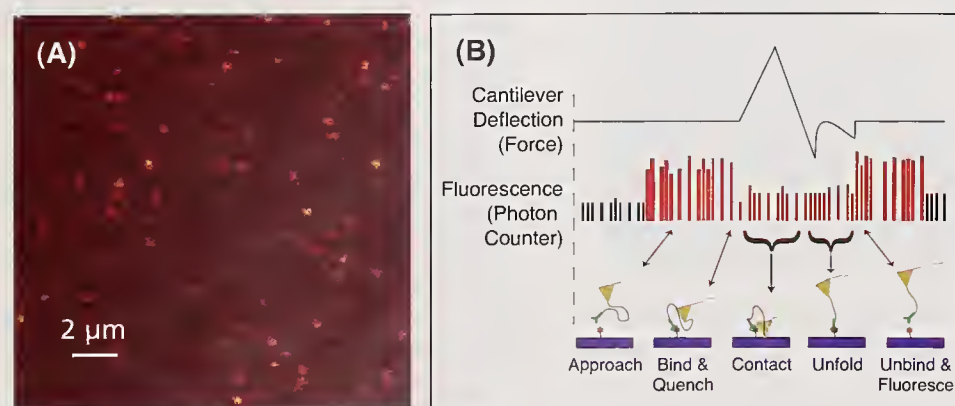
One technique recently developed uses single-molecule fluorescence spectroscopy to monitor atomic-force measurements. Individual Alexa-488 dye molecules are

tethered to a glass substrate in an aqueous buffer solution. The sharpened tip of a microfabricated cantilever, with Alexa-488 antibodies attached by 200 nm long polymer tethers, is positioned over the dye-prepared surface. As the tip is lowered onto the surface, the cantilever deflection and the laser-driven single-molecule fluorescence from the surface dye molecules are monitored (Fig. 2). At some time during an approach, an Alexa antibody may bind to an Alexa dye molecule, quenching its fluorescence. The shape of the force curve and the recovery of fluorescence verify binding as the cantilever is retracted and the bond is broken.

Force assays are widely used in biology to elucidate binding and folding dynamics of proteins and DNA or RNA. The addition of independent, optical verification of single-molecule binding helps distinguish true binding events from other interactions that commonly interfere with these assays.

CONTACT: Dr. Lori Goldner
(301) 975-3792
lori@nist.gov

Figure 2. (A) Fluorescence image of single Alexa dye molecules on glass. (B) Illustration of a simultaneous force and optical data sequence, showing how cantilever deflection changes as the tip approaches, binds, and retracts.



In situ Nonlinear Vibrational Spectroscopy for Biological Interfaces

In collaboration with CSTL, Doubly Resonant Sum Frequency Generation (DR-SFG) spectroscopy is being developed as a sensitive molecular probe of biological interfaces important for biosensors, DNA arrays, tissue-engineering research, and the understanding of cell-membrane structure and function.

The method relies on the enhanced nonlinear mixing of infrared and ultraviolet or visible laser beams at an interface when both lasers are resonant with molecular transitions, typically a vibrational transition for the infrared laser and an electronic transition for the visible or ultraviolet laser. Femtosecond laser technology and nonlinear optics are used to generate spectrally broad, infrared pulses between 2.5 μm and 12 μm , which are mixed with picosecond ultraviolet or visible laser pulses at the interface to generate an entire broadband DR-SFG spectrum at high signal-to-noise ratio.

The approach was used to measure the first ultraviolet (270 nm) DR-SFG spectra of DNA base dimers tethered to a gold-coated surface using thiol attachment chemistry. Figure 3 presents DR-SFG spectra of oligomers of the DNA bases adenine (A), cytosine (C), and guanosine (G), all of which have electronic transitions in the 260 nm to 270 nm range to enhance the SFG effect. The vibrational modes were identified by analogy to ultraviolet resonance-Raman spectra at the same 270 nm wavelength. For instance, the intense feature for adenine near 1600 cm^{-1} corresponds predominantly to the in-plane stretching motion of the

carbon atoms, C_4 and C_5 , linking the double ring of the purine.

The dependence of the amplitude of DR-SFG features on the polarization direction of the laser beams will permit the spatial orientation of the molecules to be deduced. The method is being extended further into the ultraviolet to 200 nm to allow the investigation of peptides and proteins.

CONTACT: Dr. Kimberly Briggman
(301) 975-2358
kbriggma@nist.gov

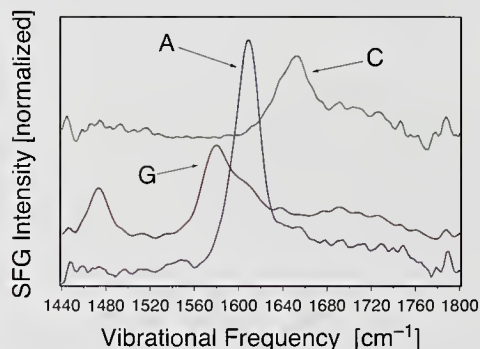


Figure 3. DR-SFG spectra of DNA bases A, C, and G tethered to the surface via a thiolate linkage: $\text{Au-S-(CH}_2)_6\text{-Base-Base}$.

Terahertz Spectroscopy of Biological Molecules

Novel THz spectroscopy and imaging methods are being developed and demonstrated as part of a NIST competence program on Advanced Terahertz Metrology. The methods are being applied to characterize the molecular structures, intramolecular force fields, low-frequency concerted motions, and conformational dynamics of biological molecules.

Continuous-wave and pulsed THz spectra were recorded for a large number of amino acids, peptides, sugars, carbohydrates, and vitamins at room temperature and at liquid-helium temperature. The complex spectra reveal distinct absorption features and patterns that provide information on the molecular conformations and the vibrational and intramolecular force fields.

A collaborative study with the NIST Center for Neutron Research and the Institut Laue-Langevin in Grenoble, France, is attempting to interpret these spectra, building on a previous, successful modeling of the neutron-scattering, vibrational spectrum of crystalline glucose.

The unique signatures of these biological molecules has led to an effort to use THz spectroscopy for identifying chemical- and biological-warfare agents in paper and plastic packaging that is transparent to THz radiation. We have measured the THz spectra of about one hundred common materials and biological samples and compiled a modest database for this purpose. This DARPA-funded project is being undertaken in collaboration with SPARTA, Inc.

CONTACT: Dr. Edward Heilweil
(301) 975-2370
ejh@nist.gov

Single-Photon-On-Demand Sources for Quantum Cryptography

The security of quantum cryptography and communication schemes depends on the use of single photons to carry information. Parametric down-conversion (PDC),

which produces photons in correlated pairs, is the basis for one type of single-photon source. Unfortunately, present single-photon sources are generally incapable of producing single photons on demand with high probability, while simultaneously suppressing the probability of yielding two or more photons. This compromises the overall security of the communication. One reason PDC-based schemes have this problem is because they employ photon-counting detectors which cannot discriminate whether just one or a burst of photons was detected.

In response to the need for an improved, on-demand, single-photon source, we have proposed a multiplexed version of the PDC scheme that allows independently adjustable probabilities for producing one and more than one photon. The system operates by collecting multiple pairs of correlated photons from the ring of correlated photon pairs azimuthally distributed around the PDC pump-laser propagation axis, as pictured in Fig. 4. The scheme allows a single, conventional, photon-counting detector to better approximate a true "photon-number" detector, which in turn allows the overall system to better approximate a true single-photon source.

A recent experimental test of this concept with four channels was successful.

CONTACT: Dr. Alan Migdall
(301) 975-2331
alan.migdall@nist.gov

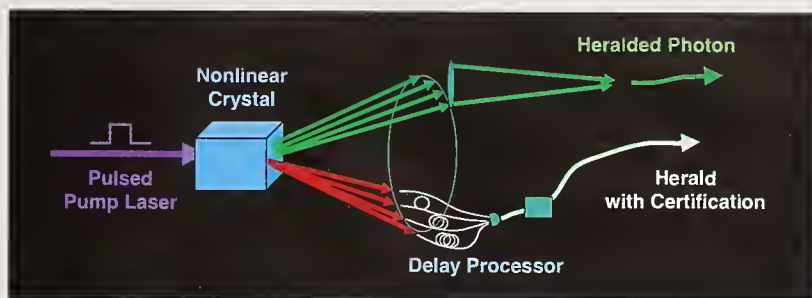


Figure 4. Multiplexed version of a parametric down-conversion scheme for producing single photons on demand.

The third strategic element is to disseminate optical radiation measurements and standards to industry, government, and academia.

Optical Measurement Services

INTENDED OUTCOME AND BACKGROUND

The Division builds and maintains world-class optical-radiation measurement facilities to meet the continued and emerging needs for standards and specialized measurements by government and industry. These facilities are available to government and industry customers through formal calibration services, special tests, and standard reference materials offered through NIST Technology Services or through collaborative research efforts.

We maintain facilities for optical-properties measurements of reflectance, transmittance, and gloss; for photometric measurements including luminous intensity and color temperature; and for radiometric measurements, including spectral radiance, spectral irradiance, spectral responsivity, and radiance temperature. The Division has highly specialized facilities for performing low-background radiometric measurements, for characterizing remote-

sensing instruments, for measuring the area of precision radiometric apertures, and for determining the absolute optical power, radiance, and irradiance spectral responsivities of instruments. New measurement facilities under development include reflected color, emittance, retroreflectance, and ultraviolet spectral irradiance.

The Division strives to ensure the quality of these programs by publishing our research and measurement methodologies



Figure 5. Charles Gibson preparing a black-body-radiation source for calibration of spectral irradiance.

© Robert Rathe

as NIST Special Publications or in outside peer-reviewed archival journals, by participating in measurement comparisons with other laboratories, and by maintaining a measurement-quality program. The Division also aids the dissemination of good optical-radiation measurement practice by publishing training documents and offering formal short-courses in Photometry, Spectroradiometry, and Radiation Temperature Measurements.

ACCOMPLISHMENTS

High-Accuracy, Deep-Ultraviolet, Index of Refraction Measurements at SURF III

A new beamline (BL-5) was completed at the NIST Synchrotron Ultraviolet Radiation Facility (SURF III), equipped with a high-resolution, deep-ultraviolet, Fourier-transform spectrometer (DUV-FTS) to measure the index of refraction of materials, with high accuracy. In contrast to the traditional, prism-goniometer measurement of the refracted angle, the DUV-FTS analyzes the fringe pattern in the transmittance spectrum of an etalon made from the sample material.

Using independent measurements of the sample thickness and fringe order, we determined the index of refraction with uncertainties ($\approx 10^{-5}$) similar to that of the classical prism method. The interferometer approach offers significant advantages over the prism method, including greater speed, continuous wavelength coverage, and the ability to measure thin samples such as absorbing fluids.

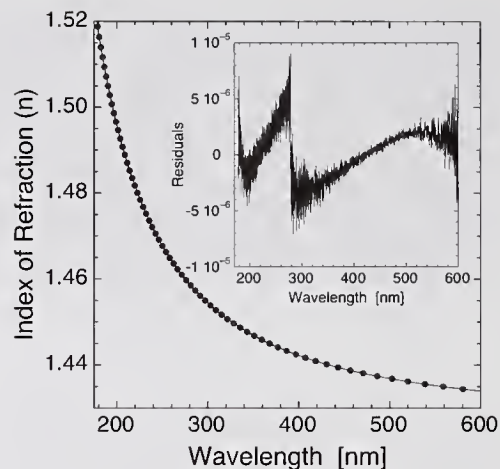


Figure 6. Index of refraction of CaF_2 measured with the DUV-FTS at SURF III. The solid circles show the measured values, and the solid line shows a three-term Sellmeier fit, whose residuals are shown in the inset.

Initial results at room temperature on a 1 mm thick CaF_2 sample at wavelengths between 175 nm and 600 nm are shown in Fig. 6. The solid circles indicate the measured index values, while the solid line is the result of a three-parameter Sellmeier fit. The residuals from the fit, shown in the inset, are approximately 5×10^{-6} . Comparison to our previous prism measurements on CaF_2 at 193 nm shows agreement within 1.3×10^{-5} , consistent with the estimated combined uncertainties in the two measurements.

Plans are underway to extend the range to below 157 nm for measuring optical materials important to the deep-ultraviolet photolithography industry. Measurements are also planned on deionized water at 193 nm, which is under consideration for immersion photolithography.

CONTACT: Dr. Keith Lykke
(301) 975-3216
keith.lykke@nist.gov

New Reference Colorimeter

We have constructed and are presently testing a new reference instrument for measuring the reflectance color of materials. This project was undertaken in response to industry and government demands for improved color measurements and standards, as articulated in the 6th and 7th Reports of the Council for Optical Radiation Measurements (CORM). Improved color standards are required to ensure better color matching of products manufactured at different sites. Because the color of a product often plays a major role in its acceptability, color measurements and standards are extremely important to industry.

Our new instrument performs measurements for all possible combinations of illumination and viewing angles, including the standard $0^\circ/45^\circ$ and $6^\circ/\text{diffuse}$ geometries, allowing the complete characterization of the reflectance properties of an object. The popular $0/45$ measurements are highly automated through a sample wheel with a capacity for 20 samples, as shown in Fig. 7.

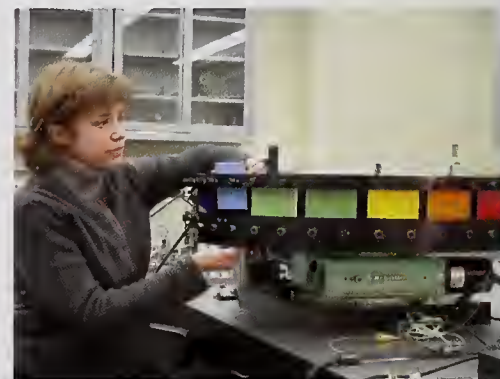


Figure 7. Maria Nadal prepares the NIST reference colorimeter.

We did a complete uncertainty analysis, considering wavelength accuracy, stray-light rejection, reproducibility of sample positioning, and signal noise. A critical aspect of the analysis was the inclusion of the statistical correlation between signals at the same wavelength and between reflectance factors at different wavelengths. The estimated measurement uncertainties are $\Delta E_{ab} < 0.4$, where $\Delta E_{ab} = 1$ is generally taken as the threshold for visual discrimination between two colors.

CONTACT: Dr. Maria Nadal
(301) 975-4632
maria.nadal@nist.gov

Thermal-Infrared Transfer Radiometer Verifies Radiance Scales Used in Earth Remote Sensing

To establish the traceability of radiometric measurements performed by the remote-sensing community to NIST's radiometric scales, and to perform on-site calibration verifications of critical remote-sensing instruments, we have developed the transportable Thermal-Infrared Transfer Radiometer (TXR). Such traceability helps ensure that the measurements undertaken by this community are of the highest accuracy and can be compared to similar measurements performed by other countries or at other times.

The TXR was deployed at the University of Miami's Rosenstiel School of Marine and Atmospheric Sciences, in collaboration with NASA-Goddard, to verify the radiance scales of several blackbody sources used by the sea-surface remote-

sensing community to calibrate ship-based radiometers. These, in turn, validate satellite measurements of sea-surface temperature. The radiometer was then sent to ITT Industries in Ft. Wayne, Indiana, to measure the radiance of two calibration targets used to verify the calibration of the NOAA Geostationary Operational Environmental Satellite (GOES) imagers. A third deployment was made to Los Alamos National Laboratory, to measure the radiance of blackbody sources in a cryogenic vacuum chamber previously used to calibrate a space-flight instrument for the Department of Energy.

The success of these deployments has led to new efforts to improve the calibration of the TXR and to extend its operational range to temperatures below 288 K by performing the measurements in a low-infrared-background, liquid-N₂-cooled, vacuum test chamber. To do these measurements, the NIST Medium-Background Infrared (MBIR) facility was used to calibrate the TXR against a high-accuracy cryogenic blackbody in conditions that simulate outer space. The facility allowed the extension of the TXR radiance scale down to 200 K and enabled the evaluation of measurement uncertainties due to room-temperature infrared background radiation and atmospheric infrared absorption and emission.

CONTACT: Dr. Joe Rice
(301) 975-2133
joe.rice@nist.gov

Wire-Contrast Measurement Standards

We developed a new facility to measure the contrast of ultraviolet-laser-written

markings on electrical wires used in aerospace and military vehicles, in response to a request by the Navy for improved standards in this area. Although the ultraviolet-laser-written markings are immune to fading with age, the gray color of the writing reduces the visual contrast relative to black-ink markings. A high contrast level is desirable for these markings to ensure the correct identity of a wire during installation, repair, or maintenance. Writing-contrast values of 60 % or higher are recommended by industry standards. However, the measured values for the same wire sample often vary by as much as 10 % to 20 %.

Our new reference instrument consists of a well-characterized luminance meter with a microscope to measure the luminance on a circular spot of 12 μm diameter or larger. The wire is illuminated by a fiber-optic source with a known spectral distribution. A three-axis translation stage under computer control automatically scans the wire surface. The computer also acquires and analyzes the data. The instrument characterization yields an expanded relative measurement uncertainty of better than 2 % for typical wire colors and sizes.

A formal calibration service is being established for both standard wires and contrast-measuring instruments.

CONTACT: Dr. Yoshi Ohno
(301) 975-2321
ohno@nist.gov

GOAL: TO PROVIDE THE
FOUNDATION OF IONIZING
RADIATION MEASUREMENTS
FOR OUR NATION

IONIZING RADIATION DIVISION

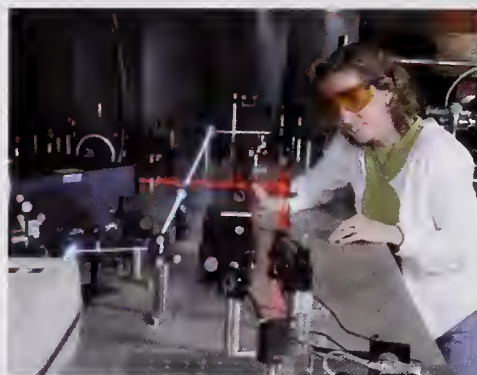
The strategy for meeting this goal is to develop, maintain, and disseminate the national standards for ionizing radiation and radioactivity to meet national needs for health care, U.S. industry, and homeland security.

The first strategic element is to develop and provide standards for radioactivity based on the SI unit, the becquerel, for homeland security, environmental, medical, and radiation protection applications.

Radioactivity Standards

INTENDED OUTCOME AND BACKGROUND

The Radioactivity Group is responsible for developing metrological techniques to standardize new radionuclides for research, and for exploring applications in health care, worker protection, environmental protection, and national defense. A vigorous program is underway to develop microcalorimetric methods to measure power from radioactive sources. This work is proceeding in parallel with liquid-scintillation detector methods based on triple-to-double-coincidence ratio (TDCR) counting. Accurate activity measurements over a broad dynamic range are obtained using these two complementary techniques. For ultra-low-level atom counting, we are continuing development of resonance ionization mass spectrometry (RIMS), which has applications in nuclear forensics as well as in environmental radioactivity.



© Robert Rathe

Figure 1. Dr. Leticia Pibida adjusting laser optics for resonance ionization mass spectrometry (RIMS).

The Radioactivity Group also provides leadership in a national program for radiopharmaceutical standards. We provide the national standards for radionuclides used in 13 million diagnostic procedures and 200,000 therapeutic nuclear medicine procedures annually in the U.S. This work has been expanded to include radioactivity

measurements of brachytherapy sources used to prevent restenosis following balloon angioplasty.

With heightened concern in the U.S. regarding terrorists' attacks using radiological or nuclear weapons, we are leading a national effort to develop standards and protocols for radiation instrumentation for first responders. Initial efforts are directed towards four areas:

- 1) equipment standards and test methods for hand-held detectors for first responders;
- 2) a testbed for cargo-container and truck inspections for radiological and nuclear materials;
- 3) radionuclidic forensic methods based on mass spectrometry; and
- 4) a national quality-assurance system that supports homeland security needs.

Many tens of thousands of low-level radiochemical measurements are made annually to support environmental remediation and occupational health programs. The credibility of these measurements has been based on participation in regulation-driven, performance evaluation programs of limited scope. The fundamental flaw

that the metrology community recognizes is that there is a lack of direct linkage to national radioactivity standards. This situation is being addressed in the publication of three ANSI standards. These consensus standards call for a traceability-testing program that links the quality of operational measurements to the national standards.

ACCOMPLISHMENTS

Cargo-Container Inspection System

The smuggling of materials or weapons in shipping containers represents a clear threat to the U.S. Major radioisotopes of concern are predominantly the plutonium and highly enriched (weapons grade) uranium isotopes, as well as some of their fission products, e.g., ^{90}Sr and ^{137}Cs . These are the key ingredients of nuclear fuel and nuclear warheads. The threat also includes radioisotopes primarily used in industrial and medical applications, such as ^{60}Co , ^{137}Cs , ^{170}Tm , ^{192}Ir , ^{125}I , $^{99\text{m}}\text{Tc}$, ^{241}Am , and ^{226}Ra .

We are developing a cargo-container inspection testbed to provide a means for calibrating detectors used for radioactivity measurements in the field. This testbed is outdoors to simulate actual operational conditions. Different kinds of standard radioactive sources will be placed inside a cargo container, so that different kinds of detectors can be tested and calibrated to optimally detect and measure the sources. Computer modeling will be used to confirm changes in effectiveness due to possible geometrical changes of the sources with respect to

the detection system, and to predict the shielding effect of other materials in the container.

The goal of this work is to develop a standard container and measurement protocol, so manufacturers can calibrate their detectors, and users can develop criteria, for radiological detection in ports of entry in the U.S.

CONTACT: Dr. Leticia Pibida
(301) 975-5538
leticia.pibida@nist.gov

Gamma-Ray Spectrometry System

Due to increased concerns about a possible terrorist attack using radioactive materials in dispersal devices, we have initiated new research in gamma-ray measurements. Information about the equipment required for these kinds of measurements is of great importance.

Two new CdZnTe detectors were tested, and their ability to detect gamma-ray emitting sources was compared with existing High-Purity Germanium and NaI(Tl) detectors. Because these detectors all can operate at room temperature, they are attractive candidates for field measurements. The detectors' efficiency, detection limits, and energy resolution were measured to determine their performance and the circumstances under which they could be used.

The measured energy resolution of the CdZnTe detector is better than that of the NaI(Tl) detector, but its efficiency is lower, mainly due to the smaller crystals that are presently available in the market. On the other hand, its small size can be an

advantage for measurements in confined and narrow places, and it has low power consumption. It may be the best choice for monitoring relatively high-level source movement or dispersal.

CONTACT: Dr. Leticia Pibida
(301) 975-5538
leticia.pibida@nist.gov

Microcalorimetry for Absolute Radioactivity Standardizations

A new, primary standardization capability has been established at NIST to provide standardizations for rather large, GBq-range, brachytherapy sources. In addition to the dual-compensated, cryogenic calorimeter operating at $\approx 8\text{ K}$, a commercial "isothermal microcalorimeter" has been adapted and evaluated for use in performing classical, calorimetric-based standardizations.

This dual-cell, near-isothermal (heat flow) calorimeter operates at near-ambient temperatures, utilizes specially-fabricated source-holder cells that are used to maximize the energy absorption of the ionizing radiation, and incorporates resistance heaters within these measurement cells to obtain very-accurately-determined, independent, power calibrations.

Evaluations were initially performed on two different types of intravascular brachytherapy sources containing nuclides that decay by pure β emission, viz., (1) a stainless-steel-jacketed ^{90}Sr - ^{90}Y source with a highly-refractory, ceramic-like, inner matrix, and (2) a "hot-wall" balloon-catheter source that consists of a thin film of ^{32}P enveloped between

polyethylene walls. The measured thermal power was related to source activities through the use of calculated average energies per decay, and was compared against known source activities determined from previous radioanalytical destructive assays. Monte Carlo calculations for the energy deposition in the measurement cells were used to correct for power losses due to escaping ionizing radiation.

This verification work clearly demonstrated, quantitatively, that the "isothermal" microcalorimeter was sufficient for performing primary calibrations.

CONTACT: Dr. Ronald Collé
(301) 975-5527
ronald.colle@nist.gov

New Technique for Absolute Standardization of Radionuclides

Beta-emitting radionuclides make up the majority of nuclides used in nuclear medicine. Because of its high detection efficiency, liquid scintillation counting (LSC) is the preferred method for calibrating these radionuclides. Traditional applications of LSC require the use of tracers, such as ^3H , and a calculational model to determine the detection efficiency for the nuclide under investigation. The Triple-to-Double Coincidence Ratio (TDCR) method is a new, quasi-absolute, LSC technique that can determine the counting efficiency for a radionuclide, without the use of an external tracing standard.

We have constructed a TDCR spectrometer with three phototubes and the electronics to process 2- and 3-fold coincidences of detected photons emitted from the liquid scintillator medium. We measured its operating characteristics using solutions of NIST SRMs for ^3H (tritiated water) and ^{63}Ni . The TDCR-measured activities agree with previously certified values to within 0.04 % and 0.2 %. We now can calibrate radionuclides encountered in nuclear medicine with shorter sample preparation times and with less, long-lived, radioactive waste.

CONTACT: Dr. Brian Zimmerman
(301) 975-5191
brian.zimmerman@nist.gov

Workshop on Standards for Important Radiotherapy Nuclide

The American Cancer Society estimates that there will be a total of 64,000 new cases of lymphoma in the U.S. this year, with an expected five-year survival rate (for non-Hodgkin's lymphoma) of 52 %. A new drug for treatment of this disease is Zevalin, which is a monoclonal antibody labeled with the radionuclide ^{90}Y . While ^{90}Y has many properties that make it suitable for use in radiotherapy, those same properties present a number of challenges regarding its measurement.

Anticipating imminent FDA approval of Zevalin and an exploding need for standards and measurement quality assurance for other radiopharmaceuticals using this nuclide, NIST held a workshop in December 2001 to address the measurement issues. Invited speakers included

representatives from NIH, radiopharmaceutical manufacturers, radiopharmacies, isotope producers, government regulators, and NIST.



© Robert Rathe

Figure 2. Michelle Millican preparing radioactive standards for a radiotherapy nuclide.

Among the concerns expressed by the 46 participants were the need for more frequent distribution of standards for ^{90}Y (currently once a year), a desire for NIST to issue ^{90}Y solution standards in clinically useful geometries instead of the standard NIST 5 mL glass ampoules, and the need to establish measurement traceability for an estimated 450 radiopharmacies. NIST is working with radiopharmacies, the FDA, the Society of Nuclear Medicine, the American Pharmaceutical Association, and others to organize and implement a program that meets these needs.

CONTACT: Dr. Brian Zimmerman
(301) 975-5191
brian.zimmerman@nist.gov

The second strategic element is to develop and provide neutron standards and measurements needed for worker protection, nuclear power, homeland security, and fundamental applications.

Neutron Standards and Measurements

INTENDED OUTCOME AND BACKGROUND

The Neutron Interactions and Dosimetry Group has initiated a homeland-security program to improve the ability to detect fissile materials in transit. Working with the Radioactivity Group, we are creating a cargo-container inspection testbed at NIST in order to improve our ability to test commercially developed, homeland-security neutron detectors. In addition to testing detectors, the group is developing a high-sensitivity neutron spectrometer for detecting fissile materials in transit.

Another project with homeland-security implications, as well as energy and environmental applications, involves imaging chemical processes in fuel cells. Compared to other forms of radiation, neutrons are highly efficient in probing complex structures. This is because of their tremendous penetration capability in almost all known materials and their unique ability to distinguish different materials with very similar physical properties. They are particularly effective in detecting hydrogenous materials and light elements.

A new, neutron-imaging facility has been constructed at the BT6, high-intensity, thermal neutron beamline at the NIST National Center for Neutron Research (NCNR) nuclear reactor. The primary use of this facility will be to non-destructively characterize water-transport mechanisms using real-time imaging of fuel cells.

Neutron lifetime and decay-asymmetry experiments improve our knowledge of the fundamental nucleon weak couplings and may ultimately lead to a significant test of the unitarity of the CKM matrix for three generations of quarks. If these measurements establish a violation of unitarity, then it will provide an important clue to the physics beyond the Standard Model of particle physics. The search for a time-reversal-violating asymmetry also probes physics beyond the Standard Model. We operate three beams at the NCNR to carry out such measurements. These include a 0.5 nm monochromatic beam, a 0.9 nm monochromatic beam dedicated to ultracold neutron production, and a high-intensity polychromatic beam.

The primary focus of our polarized ^3He program is the development of neutron spin filters and application of these devices to both neutron scattering and fundamental neutron physics. We are developing two optical-pumping methods, spin-exchange and metastability-exchange, for producing the polarized ^3He gas. We are pursuing applications at the NCNR, the Intense Pulsed Neutron Source at Argonne National Laboratory, and the Los Alamos Neutron Science Center.

The Neutron Interferometry and Optics Facility is a national user facility operated by the group. Radiography and tomography services and research involve academic and industrial customers and collaborators. During the past year, analysis of the n-H, n-D, and n- ^3He scattering-length data was completed and the time-dependent water distribution in an operating fuel cell was non-destructively imaged and quantified. The success of the fuel-cell imaging drove the development of the neutron-imaging facility described above.

Neutron cross-section standards for key, fundamental reactions are important since almost all neutron cross sections are measured relative to them. Any improvement in a cross-section standard leads to improvement in all measurements that have been or will be made relative to that standard. We have improved neutron cross-section standards through both data evaluation and experimental work, and are leading an effort that will result in a new international evaluation of neutron cross-section standards.

ACCOMPLISHMENTS

Detection of Nuclear Materials in Transport

Spent fuel from nuclear reactors, weapons-grade plutonium, and certain weapons-initiator materials emit large numbers of neutrons from spontaneous fission or (α , n) reactions. These are materials which terrorist groups could obtain fairly easily for constructing radiation-dispersal weapons or fission weapons. Because U.S. borders are easily crossed in many wilderness areas, and because these materials could be obtained from sites within the U.S., it is not sufficient to inspect baggage and cargo at points of entry.

Very sensitive neutron detectors coupled with surveillance cameras could be positioned at highway choke points on the outskirts of major cities or near other sensitive locations to detect neutrons from contraband nuclear components, and provide warnings to security personnel to try to prevent an attack. The major advantage of neutron detectors over beta and gamma detectors is that the background rates and incidences of false positives would be much lower. There is only a very low level of neutron background due to cosmic rays, much lower than the natural beta/gamma background.

We are developing a very-high-sensitivity neutron spectrometer that could be configured for unattended, remote-sensing duty. This spectrometer is based on photon emission from recoil protons in

a liquid scintillator followed by thermal neutron capture. It uses a segmented geometry to improve energy resolution. This spectrometer is based on a technique developed for detecting background neutrons in a neutrino-detection experiment and is expected to have sensitivity of 10 % or higher. The energy resolution will be optimized for detecting secondary fission neutrons from ^{235}U triggered by active portal monitors and released through the (γ , n) reaction or fast-neutron activation.

CONTACT: Dr. David Gilliam
(301) 975-6200
david.gilliam@nist.gov

Advances in Neutron Imaging of Fuel Cells

Neutron imaging is ideally suited for non-destructive, *in situ* visualization and quantification of water-transport phenomena in operating, polymer-electrolyte-membrane (PEM) fuel cells.

With a prototype facility we have demonstrated that the time-dependent water distribution in an operating fuel cell could be non-destructively imaged and quantified. A one-second time resolution was achieved. The total water content inside the fuel cell as a function of time was also quantified. The water content showed periodic behavior with time. From time-lapse images it appeared that the water drains only when it reaches a certain volume. The periodic drainage also appeared to be uncorrelated with the temperature fluctuations and hydrogen-flow variations (which were small and random, inconsistent with observed periodicity).

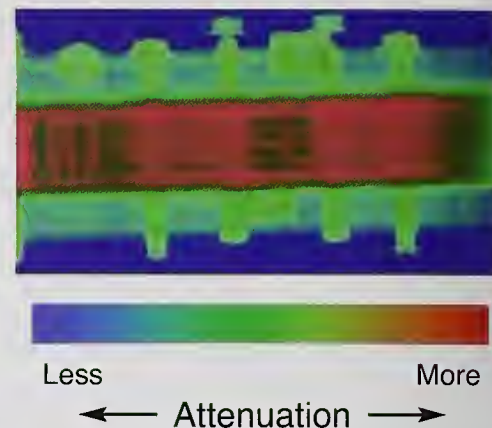


Figure 3. Image of water transport in an operating fuel cell obtained by neutron transmission radiography.

Because the quantification of time-dependent water distribution is a critical tool in theoretical modeling of fuel-cell water-transport characteristics, and because our capabilities are unique in the world, we have recently designed a new, state-of-the-art neutron-imaging facility for fuel-cell research. This facility will be used for critical water-transport studies in the membrane electrode assembly (MEA) and the flow channels, for the measurements of the hydrogen-diffusion coefficient across the MEA and water/vapor phase, and for evaluation of the integrity of various interfaces.

CONTACT: Dr. Muhammad Arif
(301) 975-6303
muhammad.arif@nist.gov

Prospects for an Improved Measurement of the Neutron Lifetime: Magnetic Trapping of Ultracold Neutrons

Recent success in magnetic confinement of ultracold neutrons in an Ioffe-type superconducting magnetic trap should lead to an improved measurement of the neutron lifetime τ_n .

The trap is loaded through inelastic scattering of 0.89 nm neutrons with phonons in superfluid ^4He . Trapped neutrons are detected when they beta decay. Energetic decay electrons ionize helium atoms in the superfluid, resulting in efficient conversion of electron kinetic energy into light (scintillation). The changing rate of neutron decays in the trap is proportional to the number of neutrons in the trap. To the extent that this population is changing only by the beta-decay of the trapped neutrons, the rate of detected neutron decays will decrease exponentially with a lifetime of τ_n .

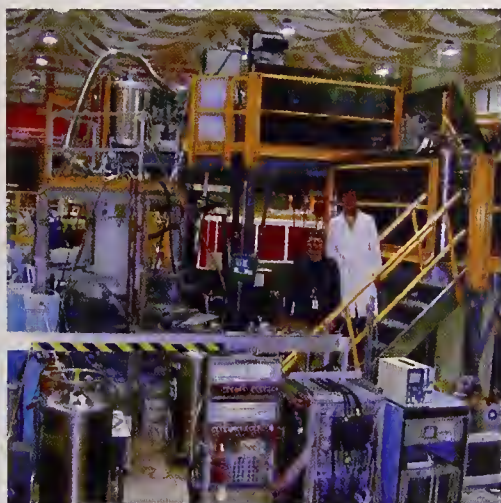


Figure 4. Students in Guide Hall at experiment station for magnetic trapping of ultracold neutrons.

The advantages of this technique over previous experiments are: continuous detection of scintillations from decay electrons, and the elimination of wall losses and betatron oscillations. Analysis indicates that systematic errors due to neutron losses should be controllable to $10^{-5} \tau_n$. A measurement of τ_n at the 10^{-3} level of statistical accuracy should be possible, given the flux available from the NG6 beamline at the NCNR.

CONTACT: Dr. Paul Huffman
(301) 975-6465
paul.huffman@nist.gov

Neutron Spin Filters Based on Polarized ^3He

Notable progress has been made in developing and applying neutron spin filters based on polarized ^3He gas. We continue to employ two optical-pumping methods, spin-exchange and metastability-exchange, to produce the polarized gas for applications in both neutron scattering and fundamental neutron physics.

Specular reflection tests using a polarized- ^3He spin filter on the NCNR NG1 reflectometer were performed to compare the use of a ^3He analyzer to that of a conventional supermirror analyzer. The ^3He cell was 6 cm in diameter, and the gas was polarized to 57 % using spin-exchange

techniques. The cell was polarized off-line and used on the beamline in the absence of optical pumping. The polarization lifetime of the cell is 550 h, which is close to the theoretical limit set by dipole-dipole relaxation. A compact, magnetically-shielded solenoid permitted a relaxation time of 350 h on the NG1 instrument in the presence of stray fields from a 0.6 T magnet at the sample position and guide field magnets.

The efficiency of ^3He spin filters depends strongly on the achievable ^3He polarization. We have reproduced a value of 70 % polarization that the University of Wisconsin had obtained with a unique, optical quality, long-lifetime cell provided by us. We have also duplicated the spectrally-narrowed, high-power diode laser developed at Wisconsin, which has particular relevance to the size and pressure ranges of neutron-spin-filter cells. In large spin-filter cells, we have obtained 55 % to 65 % ^3He polarization with both broadband lasers and the spectrally narrowed system, but the much higher efficiency of the narrowed system will permit further improvement with modest laser-power levels.

CONTACT: Dr. Alan Thompson
(301) 975-4666
alan.thompson@nist.gov

The third strategic element is to develop dosimetric standards for x rays, gamma rays, and electrons based on the SI unit, the gray, for homeland security, medical, radiation processing, and radiation protection applications.

Radiation Dosimetry Standards

INTENDED OUTCOME AND BACKGROUND

The Radiation Interactions and Dosimetry Group promotes accurate and meaningful measurements of dosimetric quantities pertaining to ionizing radiation: x rays, gamma rays, electrons, and energetic, positively charged particles. We maintain the national measurement standards for the System International (SI) unit for radiation dosimetry, the gray.

NIST is a world leader in the measurement of high levels of absorbed dose, as required in the industrial radiation processing of materials (e.g., sterilization of single-use medical devices, food irradiation, and destruction of biological weapons). Accurate transfer dosimetry is increasingly done on the basis of alanine/EPR dosimetry, rather than the radiochromic film dosimetry originally developed at NIST and offered here for many years as a calibration service. A new NIST system is near completion for on-demand, Internet-based e-calibrations for industry, based on alanine/EPR dosimetry.

Brachytherapy (treatment with sealed radioactive sources) has seen a tremendous increase in the use of low-energy,

photon-emitting seeds to treat prostate cancer and in the use of beta-particle- (and photon-) emitting sources to inhibit arterial restenosis (re-closing) following balloon angioplasty. In both cases, NIST has responded to the needs of the manufacturers, regulators, and clinical physicists. We develop new standards and measurement methods to calibrate the quantities needed to ensure accurate dosimetry for the wide variety of sources introduced, and we disseminate these standards through a network of secondary calibration laboratories.

More than 600,000 cancer patients per year are treated in the U.S. with radiation beams, mainly from high-energy electron accelerators (either directly with the electrons or by converting them to high-energy x rays). NIST maintains and disseminates the standards for air kerma (exposure) and for absorbed dose to water from ^{60}Co gamma-ray beams. These provide the basis for calibrating instruments used to measure the absorbed dose delivered in therapy beams. Standards for diagnostic radiology are developed and maintained at NIST in terms of air-kerma, for x-ray beams from 10 kVp to 300 kVp (x-ray source accelerating potential in kilovolts). These are disseminated to manufacturers and the medical physics community in North America through a network of secondary

calibration laboratories. NIST maintains more than 75 beam qualities for conventional, W-anode, x-ray beams, and 17 beam qualities for mammographic, Mo- and Rh-anode, x-ray beams.

The radiation-transport and Monte Carlo methods pioneered and developed at NIST to calculate the penetration of electrons and photons in matter are used in most of the major codes today. Monte Carlo simulation is increasingly applied to problems in radiation metrology, protection, therapy, and processing as an accurate tool for designing and optimizing radiation systems and for providing important insight into processes inaccessible to measurement.

ACCOMPLISHMENTS

Radiation-Sources for Medical and Industrial Applications

In addition to a dozen gamma-ray (^{60}Co and ^{137}Cs) sources and five x-ray ranges, NIST maintains the Medical Industrial Radiation Facility (MIRF), along with a 4 MeV Van de Graff and a 500 keV electrostatic accelerator. These are used in a variety of radiation applications, such as material modification, radiation-hardness testing, electron- and bremsstrahlung-beam dosimetry, and high-energy computed tomography development. Design and construction are underway on two new accelerator facilities. Installation is being completed of a 6 MeV to 20 MeV electron-beam (6 MV and 18 MV bremsstrahlung-beam) linear accelerator

to support the development of direct, therapy-level dosimetry calibrations. Planning is also underway for a 10 MeV, 17 kW electron linac to support the standards and calibrations program for industrial radiation processing and the study of radiation effects in materials.

CONTACT: Dr. Fred Bateman
(301) 975-5580
fred.bateman@nist.gov

Assistance to U.S. Postal Service in Decontamination of Mail

After anthrax-laced mail was delivered to media and government offices, resulting in five deaths, numerous illnesses, and enormous disruption and economic loss, we responded rapidly to identify industrial irradiation of the mail as an effective and readily-available process to kill anthrax spores. Leading a task force established by the White House Office of Science and Technology Policy, we worked with the Armed Forces Radiobiology Research Institute, the U.S. Postal Service (USPS),

and industrial irradiation facilities to provide critical dosimetry measurements and to validate the process.

Based on an extensive program of Monte Carlo radiation-transport calculations and accurate dosimetry measurements in a variety of mail configurations, NIST provided advice for optimizing the process parameters and developing a national strategy to effectively handle the highly-variable mail and parcel stream.



Figure 5. NIST test packages to validate radiation doses needed to decontaminate parcels for U.S. Postal Service.

This collaboration continues, expanded to include qualitative measurements of radiolytic products produced in the mail during the irradiation, quantitative measurements of the effects on the archival properties of paper due to irradiation, and the design of a dedicated USPS mail-irradiation facility.

CONTACT: Mr. Stephen Seltzer
(301) 975-5552
stephen.seltzer@nist.gov

High-Energy Computed Tomography (HECT) Facility

The 7 MeV to 32 MeV Saggataire linac in the NIST Medical Industrial Radiation Facility (MIRF) offers unique possibilities as an x-ray source for a high-energy computed tomography facility. A beam-line and camera are under development at MIRF to study the x-ray inspection of cargo containers, trucks, and other large objects. We are also carrying out theoretical and experimental investigations into neutron production in high-energy x-ray beams. It may prove possible to also use photoneutrons, produced at high photon energies, as an active probe to interrogate containers and screen for explosives and other terrorist materials.

CONTACT: Mr. Julian Sparrow
(301) 975-5578
julian.sparrow@nist.gov

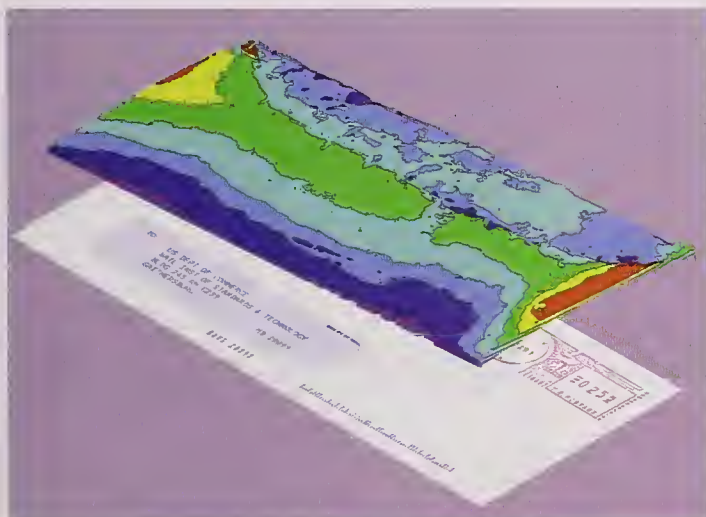



Figure 6. Dose distribution of sample of irradiated mail.



GOAL: TO PROVIDE
THE FOUNDATION OF
FREQUENCY MEASUREMENT
AND CIVIL TIMEKEEPING
FOR OUR NATION.

TIME AND FREQUENCY DIVISION

The strategy of the Time and Frequency Division is to advance measurement science and to provide time and frequency standards and measurement services to commerce and industry.

The first strategic focus is to develop the standards that serve as reference for time-and-frequency services and research on advanced measurement systems.

Time and Frequency Standards

INTENDED OUTCOME AND BACKGROUND

The intended outcome of this program is the continuous operation of frequency and time standards with the accuracy and stability essential for supporting U.S. commerce and trade. This includes coordinating our activities with those of other national standards laboratories.

The NIST time scale provides accurate time-and-frequency reference for our services and for research on new standards and measurement methods. It is an ensemble of commercial cesium-beam standards and hydrogen masers, combined

under computer control. We are advancing the performance of the time scale by acquiring more stable clocks and improving the electronic systems that read the clock outputs. Such improvements are critical to the successful evaluation and use of the next generation of primary frequency standards.

The accuracy of the NIST time scale is derived from the current primary frequency standard, NIST-F1, a cesium-fountain standard with a relative frequency uncertainty of 1 fHz/Hz. The Division plans to build an improved cesium-fountain frequency standard in the near future, designed so as to simplify the process of accuracy evaluation.

Since the accuracy of frequency standards has improved by more than an order-of-magnitude every decade since

1950, and practical applications have historically always followed these advances, an aggressive program of research and development in this area is easily justifiable. The Division is developing frequency standards based on optical transitions that have dramatically higher Q factors. These optical standards already provide much higher stability and promise orders of magnitude improvement in accuracy. They would not have been practical choices, however, without the recent development of extremely stable laser oscillators and the means for directly connecting their optical outputs to microwave frequencies.

Since the world operates on a unified time system, Coordinated Universal Time (UTC), highly accurate time transfer (to coordinate time internationally) is a critical ingredient in standards operations. To achieve this coordination, the Division is developing and using several satellite-transfer techniques.

ACCOMPLISHMENTS

Improved Steering of UTC(NIST) to UTC

The process of running a national time scale involves periodically steering it to the international average, that is, to UTC. Since UTC is formed by averaging clock data submitted by many institutions, this BIPM-generated paper average, delivered on a monthly schedule to all laboratories, represents the performance of the time scale at past times. In fact, for a given monthly report, the most recent BIPM data are at least two weeks old. Each laboratory must have a strategy for accomplishing this steering.

Until recently, NIST opted to place maximum emphasis on frequency stability. BIPM data arriving mid-month were analyzed, and a fixed steering rate was determined for the following month. For example, the decision might have been made to add (or to subtract) 1 ns per day to (from) the scale for the following month. A decade ago, the noise on UTC(NIST) and UTC made it difficult to steer more carefully than this.



Figure 1. Judah Levine and Tom Parker discussing strategies for time-scale steering.

Stimulated by the acquisition of five hydrogen masers over the last decade and the development of a more accurate primary frequency standard, NIST-F1, we investigated other steering algorithms. Using old clock data, we found that improved time-offset performance could be achieved by increasing the number of steers to two each month and by modifying the objectives of the steering. The philosophy for steering was changed from an emphasis on frequency stability only to one in which frequency stability could be degraded slightly to achieve smaller time offsets.

The result is that UTC(NIST) now typically deviates from UTC by no more than 20 ns, an improvement of better than a factor of two.

CONTACT: Dr. Judah Levine
(303) 497-3903
jlevine@boulder.nist.gov

Reproducibility of Optical Frequency

The mercury-ion optical-frequency standard has the potential for an accuracy surpassing that of the cesium-fountain standard by two or more orders of magnitude. With a Q factor greater than 10^{14} and a transition that is relatively insensitive to environmental factors, the potential uncertainty for the standard is as small as 1 aHz/Hz (0.001 fHz/Hz).

The reproducibility of this standard relative to the present cesium standard (NIST-F1) was studied over a two-year period. Measurements were referenced to NIST-F1

through the intermediary of a hydrogen maser. The short-term stability of the mercury standard is superior to that of NIST-F1, so the maser played a key role in the comparisons.

The variation in the frequency of the S-D optical transition relative to NIST-F1 was found to be less than ± 10 fHz/Hz over the two years.

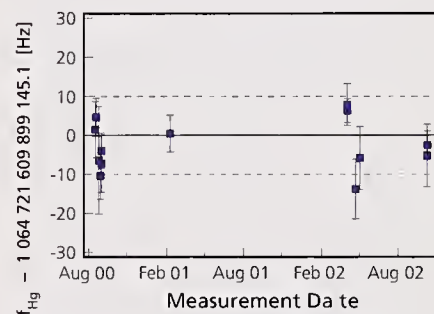


Figure 2. Measurements over two years of the frequency of the mercury optical standard relative to the cesium primary frequency standard.

The uncertainty of the absolute measurement (at this same level) is the most accurate measurement ever made of an optical frequency and a very encouraging result, since no significant effort had been made to control systematic frequency shifts. The largest of these shifts is expected to be the atomic quadrupole shift, which depends on the orientation of the applied magnetic field relative to ambient, static electric-field gradients. Concepts for determining and controlling this and other smaller shifts have been developed, but further studies are needed to test them.

CONTACT: Dr. James Bergquist
(303) 497-5459
berky@boulder.nist.gov

Improved Calcium Frequency Standard

Because the Doppler-cooling limit for calcium is 2 mK, the uncertainty in frequency measurements of the 657 nm transition are limited at about 10 Hz by the residual motions of the atoms. Thus, second-stage cooling is needed to improve this as an optical-frequency standard.

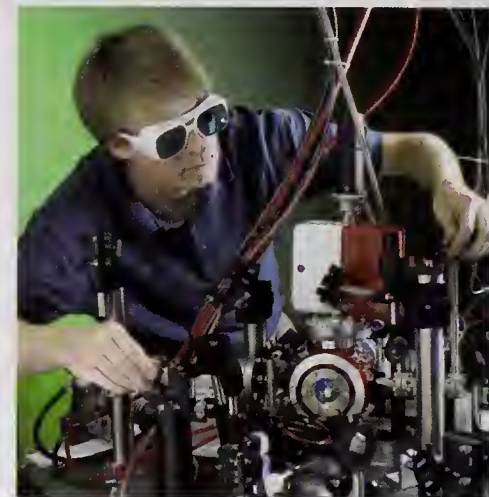
Last year, we reported a concept for achieving sub-Doppler cooling, called quenched narrow-line laser cooling (QNLC), and demonstrated it in one dimension. This year, we extended our system to three dimensions.

The three-dimensional cooling relies on the same basic principal, but uses simultaneous rather than sequential excitation for the three-level system (clock and quenching transitions). A frequency-doubled diode-laser system generates the light at 423 nm used for Doppler cooling. The second-stage cooling requires an additional beam at 552 nm for the quenching transitions.

With these methods we reduced the average atom velocity by a factor of 15 and lowered the atom temperature to 10 μ K. At this temperature, the frequency shifts due to motional effects are < 1 Hz at the clock transition, 456 THz. Further improvements should reduce the frequency uncertainty due to motions to < 0.4 Hz, which corresponds to a relative uncertainty of less than 1 fHz/Hz.

Having achieved 10 μ K, we turned off the three-dimensional cooling lasers and reapplied a pulsed version of one-dimensional QNLC cooling to the already-cooled atoms. This reduced the temperature even lower, to 300 nK. This suggests that even further cooling is possible and that the calcium optical-frequency standard has much greater potential than previously recognized.

CONTACT: Dr. Chris Oates
(303) 497-7654
oates@boulder.nist.gov



© Geoffrey Wheeler

Figure 3. The calcium optical-frequency standard being adjusted by Chris Oates.

The second strategic focus is to develop and operate the frequency and time services essential for synchronizing important industrial/commercial operations and supporting trade and commerce.

Time and Frequency Services

INTENDED OUTCOME AND BACKGROUND

The intended outcome of this program is the reliable delivery of frequency-reference and time-reference signals to the United States to support industry, trade, science, and the general public. The telephone system, the Internet, radio broadcasts, and satellites are all used to deliver these signals. We serve a broad range of systems in business, telecommunications, science, transportation, and radio/TV broadcasting.

The Division provides timing broadcasts from stations WWV and WWVB in Fort Collins, Colorado, and from WWVH in Hawaii. WWVB has a broadcast power of 50 kW. It is substantially more useful for mobile and consumer applications because the antenna/receiver cost and size are very small.

We also operate telephone-based and Internet-based time services. We provide a telephone audio service and a modem-based Automated Computer Time Service (ACTS). On the Internet, our 14 servers at 11 sites respond to all three common transaction protocols. Usage now exceeds one billion transactions daily.

Industrial calibration laboratories are served by the Division's Frequency Measurement Service, a system that provides these laboratories with continuous assurance of the accuracy of their frequency measurements. The most demanding applications are served by the Division's Global Time Service, which uses GPS common-view time transfer to deliver to the user's site a timing reference close in accuracy to that of the NIST time scale.

To enhance U.S. expertise in this field, the Division offers a variety of training courses. A 3½ day metrology seminar is offered annually, and we co-sponsor an annual workshop on synchronization in telecommunications systems. Additionally, NIST staff members teach courses at conferences.

ACCOMPLISHMENTS

NIST Internet Time Service

This service continues to grow rapidly and is approaching a usage level of 1 billion hits per day. Downloads of the instruction files for setting up a users' computer are averaging 100,000 per month. Conservative estimates of the total number of users range as high as 50 million.

Efforts continue toward finding ways in which this service might be operated commercially. However, the lack of a means for efficiently collecting service fees for delivery of a few bytes of transmission serves as a stumbling block.

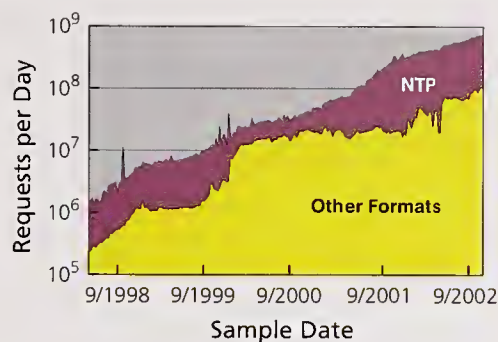


Figure 4. Growth in use of the NIST Internet Time Service.

To deal with this continued growth, we initiated two new projects this year. The first involves the use of switches (routers) that will be used to load-balance among the 14 time servers, since some servers are near saturation while others are experiencing only modest use. Four switches were purchased and successfully tested. They will be installed soon.

The second project, which is only now getting started, is to implement an encrypted time-delivery system through one or more of the servers, using a concept we developed and patented. The objective is to provide the means for secure delivery of time signals to systems operated by industry.

The hope is that there will be a gradual growth of commercial delivery of time signals by companies that are targeting specific market sectors. At this point, we are working with several companies that are interested in delivering time services to financial traders.

CONTACT: Dr. Judah Levine
(303) 497-3903
jlevine@boulder.nist.gov

WWVB Time Broadcasts

Recognizing that there has been a tremendous expansion in the number of consumer products based on the WWVB time broadcasts, we made a variety of improvements to the broadcast systems during the last year. These were made as part of a long-term plan to assure continuity of operation of this service.

New insulators were installed at the ground level of all of the guy wires supporting the eight antenna towers. These insulators are designed to be fail-safe and retain their mechanical integrity even if the insulator should break. This will prevent the sort of tower damage experienced several years ago when one of the guy-wire supports failed completely due to an insulator failure. These caused substantial damage to the tower.

A secure climbing line was added to each of the 120 m towers to comply with OSHA tower-safety requirements. Not only will this assure climbing safety, but it will also speed maintenance and repair activities.

The old tower beacons were replaced with new FAA-approved beacons to improve the visibility of the beacons to low-flying aircraft. We plan to repaint the towers in the FAA-approved manner to assure good visibility to aircraft during daylight hours.



Figure 5. An aerial view of the WWVB antenna systems.

Finally, we designed a field-strength meter for the 60 kHz signal and contracted to have a number of these produced for field monitoring purposes. These will be placed at various locations around the country to continuously monitor signal strength. The field-strength information will be fed periodically to the station website for use by WWVB product manufacturers and their their customers.

CONTACT: Mr. John Lowe
(303) 497-5453
lowe@boulder.nist.gov

The third strategic focus is to develop new measurement systems and methods in support of emerging technologies.

New Measurement Systems and Methods

INTENDED OUTCOME AND BACKGROUND

Through this program, the Division prepares for the future of time-and-frequency measurements and calibrations. Through interactions and discussions with NIST constituents, we identify important, emerging industrial requirements and technologies, and develop measurement systems and methods designed to meet their needs.

NIST has a long history of metrology expertise and leadership in such areas as: the non-stationary statistics of clocks and oscillators; optical-frequency measurement systems; atomic and optical oscillators; time-and-frequency transfer through satellites; low-phase-noise electronics; and network synchronization. The ultimate goal is to apply our expertise to carefully selected projects so as to assure continuity in providing the highest-performance time-and-frequency services to U.S. industry, science, and the general public.

The synthesis and measurement of optical frequencies have become a central focus in this program. The new optical-frequency combs generated by femtosecond lasers have provided the means for measuring optical frequencies at uncertainty levels orders-of-magnitude better than

could be done previously. Such measurements will clearly have impact on wavelength standards for fiber communications systems and on absolute length metrology. These same combs are being used to generate microwave outputs from optical-frequency standards, essentially providing the basis for a whole new generation of atomic standards. Now that the accuracy of these measurement systems has been established, work involves simplification and noise reduction.

Another component of this program is the measurement of close-to-carrier noise in oscillators and other electronic components. A closely related effort involves improving statistical metrics for analyzing such noise. Projects in this area will have impact not only on improvements in characterization of clocks and oscillators, but also in telecommunications systems, advanced radars, and other narrow-band electronic systems.

Finally, smaller, less-accurate oscillators play a major role in a variety of measurement instruments and electronic systems. We have often contributed to developing and improving such oscillators. The newest program in this area, stimulated in large part by some of our fundamental research, is a DARPA-funded program to develop a chip-scale atomic clock, a program involving NIST, several universities, and a number of companies.

ACCOMPLISHMENTS

Improved Frequency-Comb Generator

One of the key stability/reliability issues with the usual frequency-comb generator involves the microstructure optical fiber used to broaden the output of the femtosecond laser to a full octave. The very high power density required to achieve this broadening causes damage to the fiber. It must be adjusted and replaced periodically.

We recently collaborated with the Institut für Halbleitertechnik (Germany) to demonstrate a phase-coherent link from optical to microwave frequencies in a system that does not require a microstructure fiber for spectrum broadening. This success is based on the use of a 1 GHz repetition-rate, mode-locked laser and the application of a scheme that requires coverage of only $\frac{2}{3}$ of an octave. In this self-referencing scheme, the 2nd and 3rd harmonics of the optical signal of interest are heterodyned with elements of the frequency comb to ultimately lock the 1 GHz repetition rate of the mode-locked laser to the optical signal. While our new 1 GHz femtosecond laser just generates a full octave, further development will be needed to allow reliable locking using only the fundamental and 2nd harmonic of the optical signal.

The immediate consequence of this development is to increase the uninterrupted, microwave-frequency output, self-referenced to an optical transition, from tens of minutes to about a day. Such improvement in reliability is essential to the future of optical-frequency standards, since, ultimately, such standards will have to operate unattended for long periods. In the

experiments on this new system, the microwave output frequency from a comb that was phase-locked to a calcium optical-frequency standard (456 THz) was shown to have a short-term frequency stability 100 times better than that of a hydrogen maser. The long-term performance of the device will depend on how well systematic effects in the optical standard are controlled.

CONTACT: Dr. Scott Diddams
(303) 497-7459
sdiddams@boulder.nist.gov

Statistical Measure for Long-Term Stability

The measurement of the long-term stability of clocks and oscillators has been a long-standing problem for science and industry. The Allan deviation and another statistic, total deviation, both require data acquisition over twice the period of the desired averaging interval. For example, to determine the stability at 1 month would require a two-month-long data run.

Recently, we developed a new statistic that yields a measure of stability at the end-point of the data series. The most significant effect of this advance is to cut required measurement times in half, thus substantially cutting the cost of acquiring the most expensive data point.

Moreover, the statistic not only retains all of the desirable features of the Allan deviation, it has fewer intrinsic biases and much narrower confidence limits. We found that a more complex combination of frequency sums and differences could yield an Allan-like statistic clear out to the interval of the data run itself.

As a test, the statistic was used over the past two years for measuring the performance of the NIST time scale and the primary cesium-fountain frequency standard, NIST-F1.

The results clearly demonstrated the efficiency of the statistic. It served to improve the performance of the time scale and to reduce the time required to evaluate the accuracy of NIST-F1.

CONTACT: Dr. David Howe
(303) 497-3277
dhowe@boulder.nist.gov

Broadly Tunable Microwave Reference Oscillator

The measurement of phase-modulation (PM) noise and amplitude-modulation (AM) noise of clocks and oscillators presumes the availability of stable reference oscillators at the desired measurement frequencies. However, it is too expensive and cumbersome to maintain dedicated reference oscillators for each measurement frequency. To date, methods for synthesizing offsets from stable, fixed-frequency oscillators have been extremely complex. The problem is that frequency-offset synthesis generally creates unacceptable levels of noise.

We recently developed a simple reference-oscillator system with broad tunability, but without much of a noise penalty. In the traditional approach, a synthesized offset is added to a stabilized oscillator. Therefore, the noises of these two signals are independent and additive.

The innovation of the new system is in the placement of the offset synthesizer inside a servo control loop used to stabilize a high-Q microwave cavity. The frequencies of two oscillators, the reference signal and the offset, must add up to the fixed resonance frequency of the cavity. Therefore, the reference-signal frequency will be changed in a direction opposite to changes in the synthesized offset frequency. The system suppresses the total noise on the reference signal.



Figure 6. David Howe and Craig Nelson with the microwave cavity used to suppress noise in their new reference oscillator.

The concept was experimentally demonstrated using a high-Q microwave cavity with a resonance frequency of 10.6 GHz, a dielectric resonant oscillator, and a digital offset-frequency synthesizer. The results demonstrated the addition of tunability without substantially adding to the noise. This development advances the art of PM and AM noise measurement.

CONTACT: Dr. David Howe
(303) 497-3277
dhowe@boulder.nist.gov

Chip-Scale Atomic Clock

Earlier fundamental research at NIST on a very small atomic clock, based on the concept of coherent population trapping, has served to focus broader interest on the subject of miniaturization. In fact, a new DARPA-funded program was stimulated by a NIST-hosted workshop held 1½ years ago in Boulder. The advantage of the coherent-population-trapping concept is that the traditional microwave cavity is eliminated. The need for a microwave cavity has long been an impediment to miniaturization below the few-centimeter level.

We are now collaborating with a group of eight companies and universities, also funded by DARPA, on developing a chip-scale atomic clock. Because of our expertise in miniaturizing atomic clocks, we will study basic aspects of miniature atomic clocks to help guide developments on this aspect of the program. Success in this endeavor could have impact on military

systems, particularly GPS, and civilian technology such as wireless telephony.

We are focusing on several projects. The first involves characterizing miniature vapor cells, both wall-coated and buffer-gas-filled cells. One of the objectives will be to experimentally establish the scaling (size) laws, thus defining the limits for miniaturization. We are also supporting studies at the University of Colorado of the cell-wall coatings deemed to be essential to miniaturization to the sub-millimeter level. An auxiliary study, being performed collaboratively with NIST EEEL staff, is to examine the potential of direct interaction between magnetically coated MEMS oscillators and atoms. Success in this experiment could provide a dramatically simpler approach to miniaturizing atomic clocks and atomic magnetometers.

CONTACT: Dr. John Kitching
(303) 497-4083
kitching@boulder.nist.gov

The fourth strategic focus is to develop quantum-logic components and quantum-information systems based on trapped ions, in support of new atomic frequency standards and a national program aimed at advancing computation and communication.

Quantum-Information Processing Using Trapped Ions

INTENDED OUTCOME AND BACKGROUND

The intended outcome of this program is the development and demonstration of prototype logic circuits that can serve

as the basis for quantum computation, quantum measurement, and noise reduction in atomic clocks.

The current program grew out of a NIST competence project to reduce fundamental, quantum-projection noise in multi-ion atomic clocks. The realization that the same trapped-ion systems could also be used for quantum information processing

generated substantial outside interest. As a result, the ion program expanded and its success stimulated the development of other quantum-computation and quantum-communication programs at NIST. Today, the ion quantum-information project represents only a portion of a NIST centrally coordinated effort that now has fairly broad objectives.

There are several strong motivations for this work. From a national perspective, developing a quantum computer, while an extremely challenging undertaking, would have a major impact. This arises from the fact that a quantum computer should be able to perform certain functions exponentially faster than even the largest array of conventional computers. As examples, a quantum computer could much more efficiently factor large numbers, a process that is at the heart of decryption, and it could greatly speed database searches.

The second broad motivation is the expected impact on measurement science. The ability to produce and manipulate arbitrary states of single atoms and collections of atoms has clear implications for measurement science and for atomic clocks in particular. Last year, we demonstrated noise reduction below the standard quantum limit for two entangled ions, and implied that these methods can be extended to many ions, providing for increased performance in atomic clocks. More generally, the ability to engineer quantum states at the single- and few-atom level has implications for metrology in nanoscale systems.

ACCOMPLISHMENTS

Geometrical-Phase Quantum-Logic Gate

The recent demonstration of a novel, two-qubit, geometrical-phase quantum-logic gate significantly advances prospects for quantum computation. This new gate appears to have features that overcome a number of difficulties identified earlier.

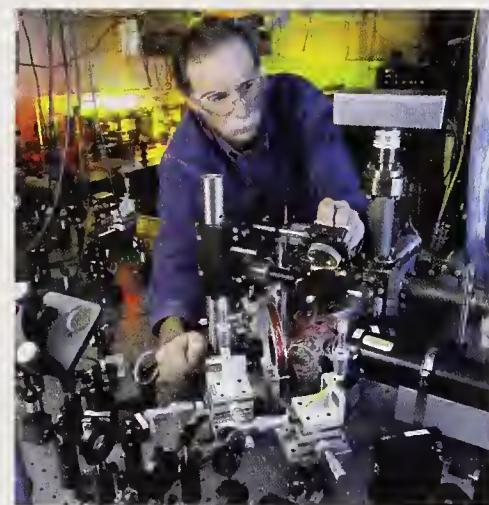
In this device, rather than manipulating the direction of the spin states, we control the phases of the spin states using optical dipole forces. The greatest advantage of this change is that the requirements on control of the phase of the probe laser are dramatically reduced. For gates of the sort we demonstrated and reported two years ago in *Nature*, the laser phase had to be kept constant throughout the full, coherent sequence of operations on the entire set of qubits involved in the system. For the new gate, the laser phase has to be well controlled only during a single-gate operation. This is dramatically easier to do.

The geometrical-phase gate also shares many of the positive attributes of the earlier gate. It is a one-step gate. All of the qubits involved can be placed into proper states at the same time. Also, individual-ion addressing is not required. In fact, the ions are best illuminated simultaneously. This means that careful laser focusing is not needed. Finally, motional eigenstates are not required as long as the ions are tightly contained and within the Lamb-Dicke limit.

The new gate is particularly well suited to application in multiplexed trap systems, a design approach that will provide for


scaling to larger logic systems. For example, there is no requirement for maintaining equal laser couplings to each ion as in the previous, two-qubit gate. This means that sympathetic cooling can be used in more complex systems without introducing difficulties in maintaining specific laser-beam couplings to the ions. In addition, in contrast with the practical realization of other gates, the phases imposed on qubits can be generated with co-propagating Raman laser beams. This means that the qubit phases will be highly immune from displacement between the ions and the laser beams. Thus, motions (vibrations) of the trap relative to the laser beams will cause fewer problems.

CONTACT: Dr. David Wineland
(303) 497-5286
wineland@boulder.nist.gov



© Geoffrey Wheeler

Figure 7. David Wineland adjusting one of the systems used for studying quantum-logic gates.



GOAL: TO PROVIDE FUNDAMENTAL UNDERSTANDINGS OF NANO-, BIO-, AND QUANTUM OPTICAL SYSTEMS IN PARTNERSHIP WITH THE UNIVERSITY OF COLORADO AT JILA.

QUANTUM PHYSICS DIVISION

The strategy of the Quantum Physics Division is to help produce a new generation of scientists and to investigate new ways of directing and controlling atoms and molecules, measuring chemical and biological processes and their interactions with nanostructures, and exploiting interactions of ultrashort light pulses with matter.

The first strategic element is to develop the laser as a precise measurement tool.

Laser Research

INTENDED OUTCOME AND BACKGROUND

Laser capabilities today are used for a wide variety of industrial and scientific purposes, ranging from providing the length scale for mechanical measurements to providing a means to directly connect the optical- and microwave-frequency domains. The Quantum Physics Division continues a leadership role in these fields, developing new techniques *vis-à-vis* precision lasers and their applications.

In laser research, various schemes are explored for stabilizing lasers and for using them as frequency standards. Recent work of the Division addresses the creation, utilization, and study of ultrafast laser pulses, which can be applied both to produce and control wave packets and to study nonlinear optical-wave interactions. The evanescent-wave property of light has

been exploited to guide atoms through hollow fibers and prevent them from touching the sides. The Division has a rapidly developing research program in ultrafast phase-control and frequency measurements, which are applied to control atomic and molecular dynamics, as well as to access wholly new types of frequency and length standards.

One of our senior scientists, Jan Hall (one of JILA's original scientists), is widely acknowledged to be the "father" of much of the laser stabilization and associated precision-measurement methods that are used today by NIST, the international standards community, and leading universities throughout the world. Our recent hires serve to further strengthen this activity and to assure NIST of a continuing world-leadership position in this critical standards and measurement domain.

ACCOMPLISHMENTS

Precision Spectroscopy of Cold Atoms and Molecules

We have extended the coverage of iodine-based, optical-frequency standards toward the shorter wavelength region, from 532 nm to 500 nm. Owing to the attractive properties of newly discovered resonances, namely narrow linewidth and high signal-to-noise ratio, we are developing a new generation of cell-based optical-frequency standards with instability less than 10 fHz/Hz at 1 s averaging time. We have made absolute frequency measurements on several of these transitions using the JILA-developed, femtosecond, frequency-comb technology. We have also discovered new and interesting changes in the hyperfine interactions of the iodine molecules when the transitions approach the dissociation limit in the excited state.

Broadband, femtosecond lasers and ultra-high-resolution spectroscopy have been linked in experiments on laser-cooled rubidium (Rb) atoms. A phase-coherent, wide-bandwidth optical comb was used to induce multi-path quantum interference for the resonantly enhanced, two-

photon transition in cold Rb atoms. We have also demonstrated the possibility of using cold atoms to control both degrees of freedom for the femtosecond-laser system, namely the comb spacing and the carrier-offset frequency.

Working with the trap dynamics of laser-cooled, alkaline earth, ^{88}Sr atoms, we have established the first rigorous test of Doppler-cooling theory in a strictly two-level atomic system. We have also, for the first time, magnetically trapped the ^{88}Sr atoms in their long-lived, metastable states, paving the way for a possible evaporative-cooling route toward quantum degeneracy of the alkaline-earth atoms. Furthermore, we demonstrated the existence of a sub-Doppler cooling mechanism for the fermionic isotope ^{87}Sr using its nuclear magnetic substructure. ^{87}Sr has been identified as the best candidate for an ultimate optical-frequency standard based on cold neutral atoms, due to the existence of an electromagnetic-field-insensitive, narrow, forbidden transition from $^1\text{S}_0$ to $^3\text{P}_0$.

Our cold molecule "machine" has started to produce results. The goal of this project is to explore control techniques on molecules similar to those applied to atoms. We have successfully produced rotation- and vibration-cooled OH radicals from a pulsed, supersonic beam source. These polar molecules can then be guided downstream using high-voltage, electrostatic fields that can be switched to slow down the translation velocity. We will eventually trap the cold molecules in an electrostatic trap and perform the first

OH cold collisions with a controlled magnetic field. We believe these kinds of experiments will mark a new era in physical chemistry.

CONTACT: Dr. Jun Ye
(303) 735-3171
ye@jila.colorado.edu

Precision Frequency Metrology and Ultrafast Science

By achieving the first experimental demonstration of tight synchronization and controlled phase coherence between independent femtosecond (fs) lasers, we have opened up a new sub-field in ultrafast science. The following is a list of novel experiments performed in the laboratory in the past year.

(1) Sub-femtosecond ultrafast laser synchronization. The ultimate goal of this research is to develop an arbitrary lightwave generator. To do this, one must have a timing jitter below the optical-carrier period. For 800 nm, this is 2.7 fs. We implemented a wide-bandwidth servo loop to synchronize two independent mode-locked lasers on a *sub-femtosecond time scale*, with 1 ms averaging. Even with a detection bandwidth above 2 MHz, we still see a timing jitter of under 2 fs. This is the lowest timing jitter ever reported using an active-synchronization scheme, and even passive techniques have not been shown to be any better.

There are many benefits of using active synchronization (as opposed to passive). For example, we can arbitrarily set the time delay between the two pulse trains to any value we choose, with femtosec-

ond-level precision. We have already demonstrated all-electronic, precision switching between two time delays, with high speed and no hysteresis. In principle, our active-synchronization technique could lock together as many different lasers with different gain media as desired.

(2) Nonlinear imaging for biological applications. We have reported another significant breakthrough in ultrafast technology that has potentially a wide range of applications. We apply our synchronization technique to coherent anti-Stokes Raman scattering (CARS) spectroscopy, one of the most powerful methods for acquiring chemically-selective maps of biological samples. With the availability of tight synchronization, we can now utilize two independent picosecond (ps) lasers, with great flexibility of wavelength tuning and pump-power manipulation. We have shown that technical noise associated with timing jitter can be completely eliminated from the CARS signal, and we have recorded CARS vibrational images of living cells and polymer beads with significantly improved quality. This new technical capability will be of great interest to chemists, materials scientists, and biophysicists.

(3) Arbitrary wavelength/spectrum generation. We have demonstrated a new experimental approach for flexible femtosecond pulse generation in the mid-IR, using difference-frequency-generation from independent Ti:sapphire (Ti:S) lasers. This work represents a significant step towards realizing an ideal light source for coherent control of molecular vibrations in the mid-IR region.

The resultant mid-IR pulse train can be easily tuned, with an adjustable repetition frequency up to 100 MHz. Arbitrary, rapid switching of the generated wavelength and programmable amplitude modulation are achieved via precision setting of the time delay between two original pulses. The average power of the pulses exceeds 15 μ W, which to our knowledge represents the highest power in the $> 7.5 \mu\text{m}$ spectral range obtained from direct difference-frequency-generation of Ti:S pulses.

(4) Optical frequency metrology.

Having demonstrated last year the first optical atomic clock, we have now improved its simplicity and reliability. The optical atomic clock offers unprecedented short-term stability and will provide better long-term stability as well. We note that our progress has been acknowledged with a large MURI contract from the Office of Naval Research, with JILA as the center of this multi-university research project.

Comparison and dissemination of the optical-frequency standards and atomic-clock signals have now become an urgent need. We have carried out work in transmitting and comparing highly stable rf- and optical-frequency standards using two dark fibers already installed in the Boulder Research and Administrative Network (BRAN). The optical link between our labs at JILA and NIST Boulder is 6.9 km long, roundtrip. A hydrogen-maser-based rf standard with an instability of ≈ 240

fHz/Hz at 1 s is transferred from NIST to JILA via this link. This maser-based rf reference, about ten times more stable than our commercial, cesium atomic clock, is used as the time base for femtosecond-laser-based optical combs used for absolute optical-frequency measurements. The maser-based signal is also used to make direct comparisons against the output of an optical clock, i.e., the repetition frequency of the femtosecond comb stabilized by an optical transition. This optical-frequency standard is based on an iodine-stabilized Nd:YAG laser at 1064 nm with an instability of ≈ 40 fHz/Hz at 1 s, which is transferred from JILA to NIST using the second fiber. With independent femtosecond frequency combs operating in both laboratories, the absolute optical frequency can be measured simultaneously with reference to the common maser-based rf standard.

A direct optical-frequency comparison enabled by the fiber link was also carried out, with results that are clearly superior to the rf-based measurements. We measured the degradation of the optical and rf standards due to the instability in the transmission channel and developed methods for active frequency-noise cancellation over the 6.9 km roundtrip distance. Optical-frequency transfer instability between JILA and NIST through the BRAN fiber is now about 3 fHz/Hz at 1 s after noise cancellation. A unique aspect of the optical phase-noise compensation is that the transit time of the optical link is comparable to the coherence time of the laser, leading to interesting coherence effects.

CONTACT: Dr. Jun Ye
(303) 735-3171
ye@jila.colorado.edu

Progress In Cell-Based Optical-Frequency Standards

With the recent breakthrough in optical-frequency measurements using fs-laser comb technology, it is clear that optically based frequency standards will play a decisive role in future frequency standards and applications. Right now, the NIST program in ion-trap systems is the world leader. However, gas-cell approaches appear capable of providing comparable stability at vastly less cost and in more compact space, although with somewhat less accuracy potential.

Accordingly, we have developed a full theory of the limits achievable with compact, gas-cell-based, optical-frequency standards. This shows that another factor-of-ten improvement should be possible on our iodine-based system, which has already been shown to be more stable than other available frequency sources—including the NIST H-maser—for times less than a few hundred seconds. Use of a still more favorable transition should provide another five-fold gain. Another major advance likely to improve the long-term stability is in the technology of distortion-free modulation, where we recently demonstrated that fringing fields in the Electro-Optic Modulator (EOM) could be controlled.

CONTACT: Dr. John L. Hall
(303) 492-3126
jhall@jila.colorado.edu

Phase Control of Ultrashort Optical Pulses

During the last few years, there has been a remarkable convergence between the technology of ultrafast lasers and that used to stabilize single-frequency cw lasers. This has led to significant advances in the fields of optical-frequency metrology and optical atomic clocks. It also promises to have a large impact on ultrafast science by making it possible to control the carrier-envelope phase of ultrashort pulses.

Control of the carrier-envelope phase will allow arbitrary electronic waveforms (as opposed to intensity waveforms) to be synthesized at optical frequencies. Such electronic-waveform synthesis will be useful in signal-processing applications, in coherent control of quantum processes, and in extremely nonlinear optics.

Before these avenues can be explored, a train of optical pulses with identical carrier-envelope phase must be generated, i.e., the carrier-envelope phase coherence must be preserved for times longer than it takes to perform an experiment. The carrier-envelope phase evolution in the pulse train emitted by a mode-locked laser is manifest as an offset frequency, f_0 , in its spectral comb, with carrier-envelope phase fluctuations causing the spectrum of f_0 to broaden.

Recent results show that, with optimization of the stabilization, the linewidth of f_0 can be below 1 MHz, corresponding to a carrier-envelope phase coherence time of hundreds of seconds.

CONTACT: Dr. Steven Cundiff
(303) 492-7858
cundiffs@jila.colorado.edu

Spin Coherence in *N*-Doped Semiconductors.

The possibility of using the spin degree-of-freedom of electrons for encoding information has recently attracted significant attention. Proposed implementations include devices analogous to traditional microelectronic devices and those based on quantum-information concepts. Optical techniques are currently the best way to prepare and probe spin-coherent states, as true "spintronic" devices are still very primitive. In addition, optical preparation and probing is likely to be useful for quantum-information applications.

The observation at the University of California (Santa Barbara) of very long spin-coherence times in *n*-doped, bulk GaAs provided significant impetus for our research. We use the technique of Faraday rotation to probe the spin coherence of such systems and to study how it depends on the density of optically excited electrons, which are initially spin polarized.

We have shown that the spin-coherence time decreases at high excitation density and that the electron *g*-factor changes subtly. The decreased spin-coherence time is attributed to an increase in spin-spin scattering amongst the electrons. The variation in the *g*-factor is presumably due to its *k*-dependence, coupled with the change in the average *k* of the electrons as the excitation density is changed. This is being tested by examining several samples with different doping densities. Measurement of the *k*-dependence of the *g*-factor is important since it effectively broadens the electron-spin precession, thereby decreasing the observed spin-coherence time.

CONTACT: Dr. Steven Cundiff
(303) 492-7858
cundiffs@jila.colorado.edu

Complete Measurement of Exciton Scattering in Quantum Wells

Many-body interactions among carriers influence the performance of optoelectronic devices, such as laser diodes and semiconductor optical amplifiers. Ultrafast measurements of coherent processes in semiconductors, using techniques such as transient four-wave-mixing (TFWM), have proven to be very sensitive to many-body interactions. The results of these measurements test the fundamental theories used to model devices.

We are using a 3-pulse implementation of TFWM to study excitonic scattering processes in GaAs/AlGaAs multiple quantum wells. By using a 3-pulse configuration, we can measure decay of the Raman-like coherence between the heavy-hole and light-hole excitons. In the same experiment, it is also possible to observe coherences between the heavy-hole exciton and the ground state, and between the light-hole exciton and the ground state. By studying these simultaneously, insight is gained into how coherence is lost during scattering events. The relative dependence of the scattering rates on the excitation density and sample temperature helps distinguish carrier-carrier scattering and phonon-carrier scattering.

CONTACT: Dr. Steven Cundiff
(303) 492-7858
cundiffs@jila.colorado.edu

The second strategic element is to exploit Bose-Einstein condensation and quantum-degenerate Fermi gases for metrology and ultralow-temperature physics.

Bose-Einstein and Fermi-Dirac Gases

INTENDED OUTCOME AND BACKGROUND

The Quantum Physics Division and JILA are today a world focal point for studies of Bose-Einstein condensates and quantum-degenerate Fermi gases. The mutual advantage to NIST and the University of Colorado in collaborating at JILA was best exemplified when Eric Cornell (NIST) and Carl Wieman (CU) together achieved for the first time a Bose-Einstein condensate, and for that accomplishment were awarded the 2001 Nobel Prize in Physics. Coupled with the creation of the first quantum-degenerate Fermi gas by Deborah Jin (NIST) and one of her CU graduate students, Brian DeMarco, this places the Quantum Physics Division and JILA at the forefront of studies of macroscopic—and therefore easily studied—quantum-mechanical systems.

A better understanding of these systems is critical today because the miniaturization of electronic components is pushing into the size region where quantum-mechanical effects play a significant role in their operation. We plan to continue to explore and exploit the new quantum-mechanical systems that these discoveries have made accessible, and maintain our leadership position.

Additionally, a program to use current-carrying wires as “pipes” to both guide and “split” cold atoms for atom interferometry is being aggressively pursued.

ACCOMPLISHMENTS

Frequency Shift Metrology

We are in the midst of a series of studies to understand the microwave transition in ultracold rubidium. Ultracold temperatures and magnetic-trapping technology make possible interrogation times extending to 2 s, which leads to very narrow line widths and correspondingly higher precision.

Residual interactions between the atoms cause shifts in the transition frequency that must be accounted for. We can track these small shifts with great accuracy since the extended interrogation time makes it possible to follow the frequency shifts as the cloud heats, cools, decoheres, and even undergoes a phase transition into or out of a Bose-condensed state.

Many of the observed effects are quite counterintuitive, and therefore help us reshape our understanding of what it means for a sample of gas to lose its internal coherence.

CONTACT: Dr. Eric Cornell
(303) 492-6281
cornell@jila.colorado.edu

BEC on a Chip

In other cold-boson work, we have succeeded in injecting a condensate into a lithographically patterned microstructure, an “atom chip.” The long-term technological goal of this work is to develop super-precise inertial sensors, i.e., gyroscopes and gravity gradiometers. The condensate will travel through the chip and be coherently split and recombined. The resulting interference signal will be exquisitely sensitive to minute inertial effects.

For now, our very preliminary condensate-in-chip studies have demonstrated that minute imperfections in the wire can have deleterious effects on the condensate’s coherence. Our new generation chips will be constructed with considerably more attention to this issue.

CONTACT: Dr. Eric Cornell
(303) 492-6281
cornell@jila.colorado.edu



© Geoffrey Wheeler

Figure 1. Eric Cornell, co-discoverer (together with Carl Wieman) of Bose-Einstein condensation in dilute atomic vapors.

"Destroying" BEC

Ironically, one of the more important scientific advances in our ultracold research this year is progress not towards creating a Bose-Einstein condensate but towards destroying it. As a ball of Bose-condensed gas starts to rotate, it becomes pierced by progressively more, tiny tornadoes known as quantized vortices. When the rotation rate is very high, these vortices organize themselves into a tightly packed, triangular array. At the highest level of rotation, the size of each vortex becomes large compared to the spacing between the vortices.

Theory predicts there will be a reordering transition in which the condensate is destroyed, to be replaced by a highly correlated gas reminiscent of the quantum Hall state in solids. Achieving and characterizing this transition in the lab is a prime scientific goal, because we anticipate it will generate important insights into analogous transitions in technologically important, condensed-matter systems, including the giant-magneto-resistance phenomenon that is so vital to progress in disk-drive read-sensor technology. During the year we advanced the figure-of-merit for producing the transition a factor of 20 closer to the goal.

CONTACT: Dr. Eric Cornell
(303) 492-6281
cornell@jila.colorado.edu

Cold Fermions

We successfully implemented a number of new experimental capabilities that enhance our research opportunities in exploring Fermi gases of cold atoms. We developed a far-off-resonance, optical-dipole trap for confining fermionic atoms in any combination of hyperfine spin-states. This trap will be used to search for a new superfluid phase driven by resonant interactions in the gas.

To this end, we made the first measurement of a magnetic-field-tunable, Feshbach scattering resonance for fermionic atoms. This resonance allows us to control interaction strengths and is a key ingredient for realizing resonance superfluidity as predicted by Holland and co-workers. We have also measured the first p -wave Feshbach resonance for fermionic atoms. This resonance occurs in the scattering of atoms in the same spin-state and could provide a mechanism for realizing superfluidity with p -wave Cooper pairs.

In another experiment, we demonstrated simultaneous cooling and trapping of Bose and Fermi gases in the quantum regime. Bose-Einstein condensates are produced using ^{87}Rb atoms. Simultaneously trapped, fermionic ^{40}K atoms are cooled sympathetically and reach roughly a quarter of the Fermi temperature. Work is proceeding in characterizing this new system.

CONTACT: Dr. Deborah Jin
(303) 492-0256
jin@jila1.colorado.edu



© Geoffrey Wheeler

Figure 2. Deborah Jin aligns an infrared laser for a magneto-optical trap. The trap is used to collect 1 billion rubidium atoms under ultra-high vacuum. The atoms are then sent to a second trap under even higher vacuum and cooled to 100 nanokelvin. The result is a so called "Bose Einstein condensate" in which a large number of atoms behave coherently.

The third strategic element is to investigate biological systems at the single-molecule level. With a new thrust in biophysics, the Quantum Physics Division aims to investigate critically important biological systems at the single-molecule level, drawing upon our measurement expertise and experience with atomic and quantum systems.

Biophysics

INTENDED OUTCOME AND BACKGROUND

As JILA and the Quantum Physics Division look to the future, it is clear that an important scientific revolution is presently taking place in the area of biophysics. Accordingly, we are evolving a part of our research program in this direction to help NIST contribute to and be a meaningful part of this scientific future.

Our strengths—namely, our ability to build institutional bridges to university departments that are already strong in this area, a superlative infrastructure that serves to extend the quickness of our eyes and the reach of our hands, our experience in manipulating and measuring similarly sized atomic and quantum-mechanical systems, and a reputation that allows us to attract and successfully hire the best and brightest of today's young scientists—all suggest that we can hope to become a significant contributor to this scientific revolution. We have therefore embarked on a program in biophysics that is to be carried out in close collaboration with the University of Colorado, in particular with the Department of Molecular,

Cellular, and Developmental Biology, and with the Biochemistry Division of the Chemistry Department.

We expect that bridging JILA to additional departments will enhance the very productive, interdisciplinary character of JILA. Most importantly, we expect to be able to find a niche where, by capitalizing on our existing expertise, we will be able to bring this program to the same very high stature as we have for our other programs.

This year, three research projects were initiated, with NIST and other-agency support. They build on our fundamental laser skills and chemical-physics experience, and contribute as well to the rapidly evolving NIST research programs in nanotechnology and single-molecule biophysics.

ACCOMPLISHMENTS

Fluorescence Microscopy Studies of Biomolecular Conformational Dynamics

This biometrology project is based on ultrasensitive time-, color-, and polarization-resolved fluorescence detection of single biomolecules (specifically, dye-labeled DNA and RNA oligomers) in a high-numerical-aperture confocal microscope.

The operation of this apparatus is as follows. A pulse train from a mode-locked laser (532 nm, doubled Nd:YAG, 80 MHz repetition rate) is focused into an aqueous sample with a water-immersion microscope objective (NA = 1.3), thereby illuminating ≈ 0.1 femtoliter of solution. For sufficiently dilute samples of labeled DNA/RNA, this corresponds to less than single-molecule occupancy in the detection region, which permits laser-induced fluorescence from single molecules to be unambiguously monitored.

The resulting weak fluorescence is collimated, separated from the $\approx 10^8$ fold stronger, incident laser with high-rejection dichroic filters, sorted by both polarization and color, and finally imaged on single-photon-counting avalanche photodiodes. The individual photon events are then efficiently sorted by color and polarization and stored as a function of time—after the incident laser pulse. The fluorescence dynamics of the biopolymers are then extracted via time-correlated, single-photon counting. This permits measurement of fluorescence decay rates of the labeled DNA/RNA species, or fluorescence-resonant-energy-transfer (FRET), between donor and acceptor dyes on a single DNA strand.

In a complementary thrust, we are developing methods for immobilizing dye-labeled biomolecules in aqueous gels to allow us to measure fluorescence and to image single molecules by raster-scanning of the laser over the sample with a precision, PZT, servo-controlled stage.

The combination of FRET, immobilized labeled biomolecules, and ultrasensitive single-molecule detection methods offers new opportunities for directly probing the extremely important conformational dynamics of biomolecules in real time, e.g., folding and unfolding. This class of information is of crucial relevance to issues concerning RNA-based enzymes, so-called ribozymes.

CONTACT: Dr. David Nesbitt
(303) 492-8857
djn@jila.colorado.edu

Single-Biomolecule Electrophoresis

A second new biometrology project is single-molecule electrophoresis. The apparatus for these studies is based on wide-field microscopy through a thin gel-electrophoresis cell, in which weak electric fields (1 V/cm to 5 V/cm) are used to coax single DNA molecules through a $\approx 20 \mu\text{m} \times 20 \mu\text{m}$ field of view. The DNA molecular motion can be studied by labeling with highly fluorescent dyes that are illuminated with cw 488 nm laser excitation and detected by imaging on an intensified, CCD camera. The sensitivity of the method is sufficient to image at a 10 Hz frame-repetition rate. This permits monitoring of single DNA electrophoretic dynamics in real time.

These sorts of studies permit detailed tests of "reptation" models of electrophoresis and can begin to address issues in improving separation efficiency in the limit of

high biomolecular strand lengths. Also of interest are kinetics/dynamics of protein-DNA/RNA binding, which are relevant to cell regulatory processes and would now be amenable to detection at the single-molecule level.

CONTACT: Dr. David J. Nesbitt
(303) 492-8857
djn@jila.colorado.edu

Single-Molecule Measurement with Nanometer Resolution

The biochemical cycle of mechano-enzymes generates a force and a displacement that can be measured at the single-molecule level. The third new project aims to determine how motor proteins transduce chemical energy into physical motion.

This research focuses on developing assays and precision instrumentation to measure the properties of single DNA-based molecular motors. The enabling technology is optical tweezers, a focused laser beam that can manipulate micrometer-sized beads in solution, allowing measurements of position and force in the nanometer and piconewton ranges.

Measurement of steps and stall forces provide fundamental information on the mechanics of motion. For many enzymes, different proposed mechanisms of motion predict different step sizes. Steps have been seen for myosin along actin (5.5 nm) and for kinesin along microtubules (8 nm).

Enzymatic motion along the DNA is measured by anchoring the enzyme to a surface and monitoring the position of an optically

trapped bead attached to the DNA's distal end. To date, unitary steps of DNA-based molecular motors have been too small to resolve. Their presumed step sizes are 1.4 nm or smaller, but such steps may be attenuated by the compliance of DNA.

Building on our demonstration that 0.3 nm steps of a stuck bead can be resolved, we are building a microscope for measuring 1 nm motion along DNA. The electronics for this microscope are a high bandwidth (250 kHz) quadrant photodetector connected to a differential normalizing amplifier. These detectors do not exhibit wavelength-dependent reduction in bandwidth as seen in earlier designs. By incorporating PZT mirrors instead of acousto-optic deflectors, we eliminate the nanometer-sized, artifactual steps observed to arise from standing waves inside the AO crystal.

CONTACT: Dr. Thomas T. Perkins
(303) 492-8186
tperkins@jila.colorado.edu



© Geoffrey Wheeler

Figure 3. Using a modified microscope, Tom Perkins measures the motion generated by a single enzyme moving along DNA.

GOAL: TO COORDINATE
AND FACILITATE THE
ELECTRONIC DISSEMINA-
TION OF INFORMATION
VIA THE INTERNET.

OFFICE OF ELECTRONIC COMMERCE IN SCIENTIFIC AND ENGINEERING DATA

The strategy for meeting this goal is to publish Physics Laboratory information on the World Wide Web, to develop web-accessible databases of physical reference data, and to evolve protocols to ensure interoperability in the exchange of scientific and engineering data.

WWW Dissemination of Information

INTENDED OUTCOME AND BACKGROUND

The Office of Electronic Commerce in Scientific and Engineering Data (ECSED) is responsible for the Physics Laboratory (PL) world wide web (WWW) pages at *physics.nist.gov*. We produce material for WWW publication, encourage and support the production of material by others, and ensure the high quality of disseminated information. We are also engaged with PL Divisions and the NIST Standard Reference Data Program in developing physical reference databases for WWW dissemination. We design and develop effective WWW database interfaces to facilitate access to the data.

Since June 1994, we have provided a wide array of information ranging from physical reference data, technical activities, research and calibration facilities, technical contacts, publication lists, general

interest, and news items. In a recent month (October 2002), there were nearly one million requests for web pages from the Gaithersburg server (nearly half from our ≈ 25 online databases), and nearly 8.8 million requests for web pages from all PL web servers (including *time.gov* and *tf.nist.gov*).

There are many new web databases currently under development, including:

- 1) Handbook of Basic Atomic Spectroscopic Data,
- 2) Spectral Data for the Chandra X-ray Observatory,
- 3) X-ray Transition Energies Database,
- 4) Chemical Agents Database,
- 5) Potentials of Alkaline-Earth Dimers,
- 6) Amorphous Metals Database, and
- 7) Hydrogen and Deuterium Energies and Transition Frequencies (an interactive website).

ACCOMPLISHMENTS

Units Markup Language

We have continued a collaboration with Lawrence Berkeley National Laboratory and NIST's Electronics and Electrical Engineering Laboratory to develop an XML (eXtensible Markup Language) schema for encoding scientific measurement units. Adoption of this schema will allow for the unambiguous exchange of numerical data over the Internet.

We are in the process of creating an international working group to examine and discuss the completed first draft of the UnitsML schema. In addition, we have begun collaborating with the NIST Information Technology Laboratory to establish a NIST registry containing SI and non-SI unit information and to create an XML registry containing the UnitsML schema. We anticipate this registry will be used by our customers to download industry-specific dictionaries of scientific units.

CONTACT: Dr. Robert Dragoset
(301) 975-3718
robert.dragoset@nist.gov

Molecular Spectroscopy Tutorials On-Line

We collaborated with the Optical Technology Division to make available on the WWW two popular tutorials in molecular spectroscopy. The original documents were converted to HTML, and the equations were formatted as both images and LaTeX to ensure their wide accessibility.

The first of these documents is the extensively cited NBS Monograph 115, *The Calculation of Rotational Energy Levels and Rotational Line Intensities in Diatomic Molecules*, <http://physics.nist.gov/DiatomicCalculations>. It played a major role in standardizing the complex conventions and nomenclature used to describe the quantum-mechanical behavior of diatomic molecules.

The document describes the derivation of the intensities of the spectral lines, and contains a clear discussion of the rotational Hamiltonian and its symmetry properties, necessary for calculating molecular energy levels. This pedagogical monograph is of interest to the wide community of scientists dependent on molecular spectroscopy for their success, including atmospheric and planetary scientists, astronomers, plasma physicists, and analytical chemists. It is the accepted, more rigorous companion to the popular textbook, *Spectra of Diatomic Molecules*, written by the late Nobel Laureate Gerhard Herzberg.

The second tutorial newly offered on-line is *Methane Symmetry Operations*, <http://physics.nist.gov/Methane>. It was initially written in response to the needs

of chemists and physicists for conventions and guidance in working with the complex mathematics involved in calculating the rotational energies and intensities of tetrahedral molecules, such as methane and carbon tetrachloride. Scientists interested in atmospheric sensing, combustion diagnostics, and climate change will benefit from ready access to this document.

CONTACT: Mrs. Gloria Wiersma
(301) 975-5547
gloria.wiersma@nist.gov

Molecular Databases On-Line

We collaborated with the Optical Technology Division to make available on the WWW three linked databases of the microwave and RF spectra of diatomic, triatomic, and hydrocarbon molecules. Originally published as spectral tables in the Journal of Physical and Chemical Reference Data, the on-line version includes additional molecules and allows advanced browsing and searching of the data—by molecular species, type, or frequency.

Rotational spectral lines for 121 diatomic molecules, 55 triatomic molecules, and 91 hydrocarbon molecules are included. The isotopic molecular species, assigned

quantum numbers, observed frequency, estimated measurement uncertainty, and reference are given for each transition. The spectral lines for many molecules and normal isotopic species have been refit to produce a comprehensive and consistent analysis of all the data obtained from many sources. The derived molecular properties, such as rotational and centrifugal distortion constants, hyperfine structure constants, electric dipole moments, rotational *g*-factors, and internuclear distances (for diatomic molecules) are listed with one-standard-deviation uncertainties for all species.

The Diatomic, Triatomic, and Hydrocarbon Spectral Databases can be accessed on the WWW at <http://physics.nist.gov/MWtables>. Further information on additional molecular spectroscopic databases developed by the Office of ECSED is available at <http://physics.nist.gov/data>.

Development of these databases was supported in part by NIST's Standard Reference Data (SRD) Group and by NIST's Systems Integration for Manufacturing Applications (SIMA) program.

CONTACT: Mrs. Karen Olsen
(301) 975-3286
karen.olsen@nist.gov

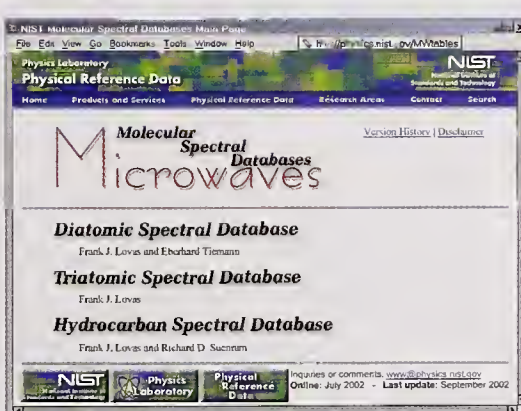


Figure 1. Screen capture of a browser window for the "Molecular Spectral Databases" main web page.

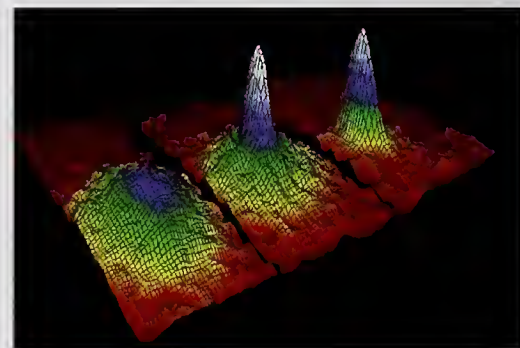
HONORS AND AWARDS

2001 Nobel Prize in Physics



Eric Cornell (l) receives the 2001 Nobel Prize in Physics from King Carl XVI Gustaf of Sweden (r).

Eric A. Cornell, Quantum Physics Division/JILA, received the 2001 Nobel Prize in Physics, jointly with his JILA colleague, **Carl E. Wieman**, University of Colorado, and **Wolfgang Ketterle**, Massachusetts Institute of Technology, for “the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates.” Announced on October 9, 2001, by the Royal Swedish Academy of Sciences, it is the second Nobel Prize awarded to NIST Physics Laboratory scientists. In 1997, William D. Phillips received the Nobel Prize for pioneering research on cooling and trapping atoms with laser light. The Bose-Einstein condensate, or BEC, is essentially a new form of matter that allows scientists to study the strange and extremely small world of quantum physics. Its creation in 1995 by Cornell and Wieman established a new branch of atomic physics that has provided a treasure-trove of scientific discoveries, including the atom laser, first demonstrated by Ketterle, quantum whirlpools, atom waveguides, and other coherent atom-optical phenomena.



The Bose-Einstein condensate, first demonstrated by NIST and University of Colorado scientists at JILA, was Science magazine’s 1995 Molecule of the Year. A new state of matter, the BEC “superatom,” forms as rubidium atoms trapped in a magnetic field are cooled to a temperature close to absolute zero. The graphic shows three-dimensional, successive snapshots in time during which the atoms are cooled to less than 170 billionths of a degree.

Max Born Award



John L. Hall
Quantum Physics
Division, was pre-
sented the Optical
Society of America's
Max Born Award
"for pioneering the

field of stable lasers, including their applications in fundamental physics and, most recently, in the stabilization of femtosecond lasers to provide dramatic advances in optical frequency metrology." Jan is one of the "fathers" of today's laser-generated optical combs that have allowed us to directly connect the optical and microwave frequency regimes.

Presidential Rank Award

John L. Hall also received a 2002 Presidential Rank Award from the U.S. Office of Personnel Management for exceptional technical accomplishments spanning four decades of research in the Quantum Physics Division at JILA. Dr. Hall was one of the first scientists to join JILA when it was established in 1962 as a unique, interdisciplinary partnership between NBS and the University of Colorado.

William O. Baker Award



Deborah S. Jin,
Quantum Physics
Division, was award-
ed the National
Academy of Science
Award for Initiatives
in Research, "for her

experimental realization and characterization of a new quantum system, the vapor-phase degenerate Fermi gas." Known as "the Baker Prize," the award recognizes innovative young scientists for research likely to lead towards new capabilities for human benefit.

Maria Goeppert-Mayer Award

Deborah S. Jin was also awarded the Maria Goeppert-Mayer Award of the American Physical Society, "for her innovative realization and exploration of a novel quantum system, the degenerate Fermi atomic gas, and the scientific promise portended by her pioneering work." This award recognizes the wide-ranging future implications of work in ultra-cold gases.



Archie Mahan Prize of the Optical Society of America

(r to l) **Edward W. Hagley**, **Charles W. Clark**, and **Lu Deng**, Electron and Optical Physics Division, **William D. Phillips**, Atomic Physics Division, and **Keith Burnett**, Oxford University, were awarded the Archie Mahan Prize of the Optical Society of America, "for authorship of *The Atom Laser*, a focused and well-organized article that succinctly connects recent observations in the field of phase coherent matter waves with early 20th century research on Bose-Einstein condensation."

Presidential Early Career Award for Scientists and Engineers



Jun Ye, Quantum Physics Division, received a 2002 Presidential Early Career Award for Scientists and Engineers (PECASE),

“for pioneering research on laser interactions with atoms and molecules and their applications to precision control and measurement of light fields, matter waves, and optical frequencies.” This Presidential Award is the highest honor bestowed by the United States Government on scientists and engineers beginning their independent careers. Sixty awards were given nationally and presented by President George W. Bush in a White House ceremony.

100 Top Young Innovators

Jun Ye was also chosen as one of the world’s “100 Top Young Innovators” by Technology Review, published by the Massachusetts Institute of Technology. The TR100, all individuals under 35 years of age, are recognized for their contributions to technology. Dr. Ye’s work is in the fields of ultrasensitive high-resolution laser spectroscopy, cold atoms, continuous-wave and ultrafast-pulse laser stabilization, and optical frequency standards.

Arthur S. Flemming Awards



Leonard M. Hanssen, Optical Technology Division, received a 2002 Arthur S. Flemming Award, “for developing and establishing innovative infrared technology for measuring optical properties of materials.” These achievements have established NIST as the world leader in infrared measurement science and standards and have played a critical role in the success of U.S. defense and remote-sensing satellite systems dependent on state-of-the-art infrared technology.



Steven L. Rolston, Atomic Physics Division, received a 2002 Arthur S. Flemming Award, “for innovative leadership in the study of new physical phenomena in ultra-cold atomic gases, including the first creation of ultra-cold plasmas and strongly-coupled plasmas.” Dr. Rolston’s research is part of the Laboratory’s program to develop new laser cooling and trapping techniques and applications.



John H. Burnett, Atomic Physics Division, received a 2002 Arthur S. Flemming Award, “for developing and applying world-class measurement systems critically needed for the design of advanced photolithography manufacturing tools.” Dr. Burnett measured a refractive effect called “intrinsic birefringence,” showed that it was sufficiently large in candidate lens materials to prevent photolithography tools from focusing properly at the targeted wavelength of 157 nm, and proposed methods for overcoming the problem.

Service to America Medal



Katharine B. Gebbie, Director of the Physics Laboratory, received the 2002 Service to America Medal, “for career achievement,” cosponsored by the Atlantic Media Company (Government Executive Magazine, National Journal, and The Atlantic Monthly) and the Partnership for Public Service. She was cited for being the founding director of the award-winning NIST Physics Laboratory, pioneering the practical application of emerging technologies, enhancing scientific career opportunities for women and minorities, and fostering a culture of excellence that has made NIST one of the world’s preeminent research institutions.

William F. Meggars Award



James C. Bergquist, Time and Frequency Division, was recognized with the William F. Meggars Award of the Optical Society of America

(OSA). The award is "for seminal contributions to high-resolution, high-accuracy laser spectroscopy with applications to fundamental metrology and clocks."

Dr. Bergquist developed the world's most stable laser and used it as the local oscillator for an optical atomic clock based on a single mercury ion. This work is central to the most accurate optical-frequency measurement ever made, and the first optical-frequency standard with a microwave-frequency output.

American Physical Society's Outstanding Thesis Award



Brian DeMarco was awarded the 2002 Outstanding Doctoral Thesis Award by the American Physical Society's Division of Atomic, Molecular, and Optical Physics (DAMOP). This award recognizes thesis research of outstanding quality and achievement. Dr. DeMarco's thesis, entitled "Quantum Behavior of an Atomic Fermi Gas," concerned the extension of the magnetic-trapping and evaporative-cooling techniques used to produce atomic Bose-Einstein condensation to create

the first quantum-degenerate Fermi gas of atoms. His work included measurements of the atomic-collision mechanisms by which such gases reach thermal equilibrium. This work was carried out at JILA, in collaboration with Dr. Deborah Jin of the Quantum Physics Division. Dr. DeMarco now has a postdoctoral appointment in the Ion Storage Group of the Laboratory's Time and Frequency Division.

Fellowship of the American Physical Society



Zachary H. Levine, Electron and Optical Physics Division, was elected a Fellow of the American Physical Society, "for leadership in demonstrating x-ray tomography of integrated circuit interconnects with submicron resolution." Dr. Levine has made both theoretical and experimental contributions to the field of high-resolution x-ray imaging and was recently awarded a patent, "Parallel X-Ray Tomography," for the measurement techniques he pioneered.



Carl J. Williams, Atomic Physics Division, was elected an APS Fellow, "for definitive calculations of atomic collision processes, which have improved our understanding of photoassociation spectroscopy, dynamics of Bose-Einstein condensates, and effects of radiation retardation on atomic collisions." Dr. Williams' work relates to the NIST experimental program in laser cooling and trapping and is foundational for the quantitative understanding of cold-atom collisions.

Sigma Xi (NIST Chapter) Award for Support to Scientists



Anita K. Sweigert, Physics Laboratory Office, received the NIST Chapter of Sigma Xi Award, "for outstanding support to NIST scientists."

Ms. Sweigert serves as central coordinator of the NIST Summer Undergraduate Research Fellowship program (SURF), an enormously successful, educational outreach program aimed at providing research opportunities to college and university students. The class of '02 had 102 students, selected from 195 applications. The students were placed in all seven NIST Measurement Laboratories.

Sigma Xi (NIST Chapter) Young Scientist Award



Eric L. Shirley, Optical Technology Division, was recognized with a 2002 Sigma Xi Young Scientist Award, "for sustained excellence

in his contributions to the quantitative theory of condensed-matter electronic structure." This award highlights his work in condensed-matter (solid-state) theory, which includes studies of x-ray absorption by crystals. His calculations, based on the electronic band structure of the crystals and including electron-(core) hole interactions, have proven to be the best in the world.

Women of Color Research Leadership Award



Maria E. Nadal, Optical Technology Division, received the 2002 Women of Color Research Leadership Award. The award, given to

elite women in government and defense, honors Dr. Nadal, "for innovative research and scientific leadership in optical properties measurements in support of industry and government." The award is presented by Career Communications Group, Inc. (CCG), publisher of U.S. Black Engineer & Information Technology, and Hispanic Engineer & Information Technology magazines. Dr. Nadal has developed new standards for reflectance and new measurement services for such hard-to-characterize properties as gloss, luster, and sheen, which strongly influence the appearance of materials.

Gold Medal (DoC)

The Gold Medal is the highest honor award conferred upon an employee by the Department of Commerce, for "distinguished performance characterized by extraordinary, notable, or prestigious contributions that impact the mission of the Department of Commerce and/or operating unit and which reflect favorably on the Department."

Bert M. Coursey, Ionizing Radiation Division, received the Department of Commerce Gold Medal, "for leadership in helping solve the problem of anthrax-contaminated mail, detecting nuclear and radiological threats, and ensuring public safety."



Dr. Coursey is recognized for his leadership in helping to protect first responders and the American public from terrorist attacks. An expert in radiation measurement technology, he worked with the U.S. Postal Service, the Armed Forces Radiobiology Research Institute, and industry to develop a system for decontaminating more than 20 million letters and 200,000 parcels, and is leading the development of a national measurement system for combating nuclear smuggling and radiological threats. He is shown here to the right of his colleagues from the U.S. Postal Service and the Armed Forces Radiobiology Research Institute, hurrying to an irradiation facility in Lima, Ohio, to validate the process using an instrumented box of mail.



Katharine B. Gebbie and **William R. Ott** received the Gold Medal, "for leading NIST's Physics Laboratory (PL) and creating an atmosphere in which innovative scientific research flourishes in support of NIST's mission." Drs. Gebbie and Ott have led the Physics Laboratory since its inception 13 years ago.

Their strong and enduring support of research directed at important measurement challenges, such as developing the world's most accurate clock, providing measurement support for protecting the U.S. mail from bioterrorism, probing the limits of quantum-based measurements, and improving medical treatments and diagnosis with optical and ionizing radiation technologies, has resulted in numerous awards and recognition for the Laboratory's scientists and programs, including the Nobel Prize in 1997 and 2001.

Silver Medal (DoC)

The Silver Medal is the second highest honor awarded by the Department of Commerce, for "exceptional performance characterized by noteworthy or superlative contributions that have a direct and lasting impact."

(l to r) **Eric L. Shirley**, Optical Technology Division, **John H. Burnett**, Atomic Physics Division, and **Zachary H. Levine**, Electron and Optical Physics Division, received the Silver Medal, "for advancing next-generation semiconductor lithography by the discovery of deep ultraviolet birefringence in calcium fluoride."

Through a combination of theoretical work and laboratory measurements, the team developed a precise understanding of the effect, and devised conceptual methods for engineering around it. By providing an early warning to the semiconductor industry about a critical, previously neglected problem, the three scientists smoothed the way for the timely introduction of the next generation of microlithography.



Bronze Medal (NIST)

The Bronze Medal is the highest honorary recognition available for Institute presentation. The award recognizes work that has resulted in more effective and efficient management systems, as well as the demonstration of unusual initiative or creative ability in the development and improvement of methods and procedures. It is also given for significant contributions affecting major programs, scientific accomplishment within the Institute, and superior performance of assigned tasks for at least five consecutive years.



Karen J. Combs, Physics Laboratory Office, received the Bronze Medal, "for improving NIST-wide administrative and technical support." Mrs. Combs led a NIST-wide administrative working group that promoted efficiencies in administrative policies and procedures, improved NIST-wide communication among and between administrative disciplines, encouraged collaboration and cooperation, and improved training and career development.

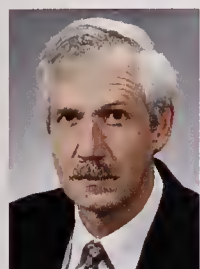
Brian E. Zimmerman, Ionizing Radiation Division, received the Bronze Medal, "for his leadership of the NIST program for radiopharmaceutical standards." Dr. Zimmerman and his colleagues provide the national standards for radionuclides used in diagnostic and therapeutic nuclear medicine. To develop, maintain, and disseminate the national standards for radiopharmaceuticals, Dr. Zimmerman carries out a vigorous research program focused



on radionuclides used for therapy and administers a collaborative program with industry to deliver radiopharmaceutical standard reference materials. He is also collaborating with NIH and developing radioactivity standards for cancer imaging and therapy applications.

Allen V. Astin Measurement Science Award (NIST)

The Astin Award recognizes outstanding achievement in the advancement of measurement science or in the delivery of measurement services.



Bert M. Coursey, Ionizing Radiation Division, received the Astin Measurement Science Award, "for his leadership in devel-

oping and providing modern radiation standards and measurement services for health care providers." Dr. Coursey's leadership in measurement science has improved health care for millions of Americans. He developed the NIST Medical-Industrial Radiation Facility (MIRF) to provide standards for high-energy radiation therapy. He improved dose standards used in all 11,000 mammography facilities in the Nation (26 million mammograms/year). He led the development of radiation standards for brachytherapy used to prevent the closing of arteries following angioplasty and to treat prostate cancer (40,000 treatments/year). He initiated new measurement services for nuclear medicine applications for imaging of tumors, infection, cardiac, or brain function (36,000 procedures/day), and for radioimmunotherapy and bone palliation (200,000 therapeutic procedures/year).

Edward Uhler Condon Award (NIST)

The Condon Award recognizes distinguished achievement in written exposition in science or technology.

(r to l) **Edward W. Hagley**, **Charles W. Clark**, and **Lu Deng**, Electron and Optical Physics Division, **William D. Phillips**, Atomic Physics Division, and **Keith Burnett**, Oxford University, were awarded the Condon Award, "for authorship of *The Atom Laser*, Optics and Photonics News (May 2001), a broadly-accessible account of coherent matter-wave physics."



Edward Bennett Rosa Award (NIST)

The Rosa Award recognizes outstanding achievements in the development of meaningful and significant standards of practice in the measurement field.



B. Carol Johnson, Optical Technology Division, received the Rosa Award, "for research and leadership in developing measurement standards for ensuring the accuracy of remote-sensing instruments monitoring climate change." Dr. Johnson has developed novel optical radiation measurement instruments, standards, and methods for ensuring the accuracy and reliability of satellite and ground-based instruments monitoring climate change. Her world-leading research program further supports the remote sensing community by offering training and education through formal courses, lectures, and publications, and by providing instrument measurement validation through laboratory comparisons. Her efforts have accelerated the advancement of the fundamental metrology of optical radiation measurements, leading to the development of unique NIST facilities for calibrating remote-sensing instruments.

Equal Employment Opportunity/Diversity Award (NIST)

The Equal Employment Opportunity/Diversity Award recognizes significant EEO/Diversity contributions that have been performed in an outstanding manner.

Robert A. Dragoset, Office of Electronic Commerce in Scientific and Engineering Data, and **Chiara F. Ferraris**, Building and Fire Research Laboratory, received the EEO/Diversity Award, "for organizing *Science: Get Psyched*, an annual program of hands-on demonstrations for hundreds of girl scouts aimed at increasing interest in science." In small groups, the girls visit successive rooms and interact with NIST scientists providing lively science demonstrations and supervising the girls' participation. The scouts also attend panel discussions where they can ask female scientists what it is like to be a scientist. The volunteer program, now in its ninth year, aims to increase the pipeline of young scientists.



Safety Award (NIST)



The Safety Award for Superior Accomplishment recognizes unusually significant contributions to the NIST Occupational Safety and Health program activities.

(l to r) **Timothy F. Mengers**, Occupational Health and Safety Division, **Michael P. Unterweger** and **Bert M. Coursey**, Ionizing Radiation Division, **Zachary H. Levine**, Electron and Optical Physics Division, **Stephen M. Seltzer**, Ionizing Radiation Division, **Thomas G. Hobbs**, Occupational Health and Safety Division, and **Charles W. Clark**, Electron and Optical Physics Division, were awarded the NIST Safety Award, "for prompt action to enhance the security of NIST radiation sources and radioactive materials in the aftermath of the terror attacks of September 11, 2001." This group demonstrated exceptional initiative in organizing a team to identify ways to improve security of NIST facilities where radiation sources are used and stored. A phased plan of action was developed; some steps were taken immediately, and others were presented to NIST Administration for rapid implementation as part of NIST-wide security efforts.

PHYSICS LABORATORY RESOURCES

Key to Table

Abbreviations:

STRS – Congressionally appropriated funds for NIST’s Scientific and Technical Research and Services

ATP – Intramural research funds provided to support the goals of the NIST Advanced Technology Program

OA – Funds provided by other agencies in support of research that they request

Other – Other sources of funding, including calibration fees

Federal Agencies Supporting Physics Laboratory Research

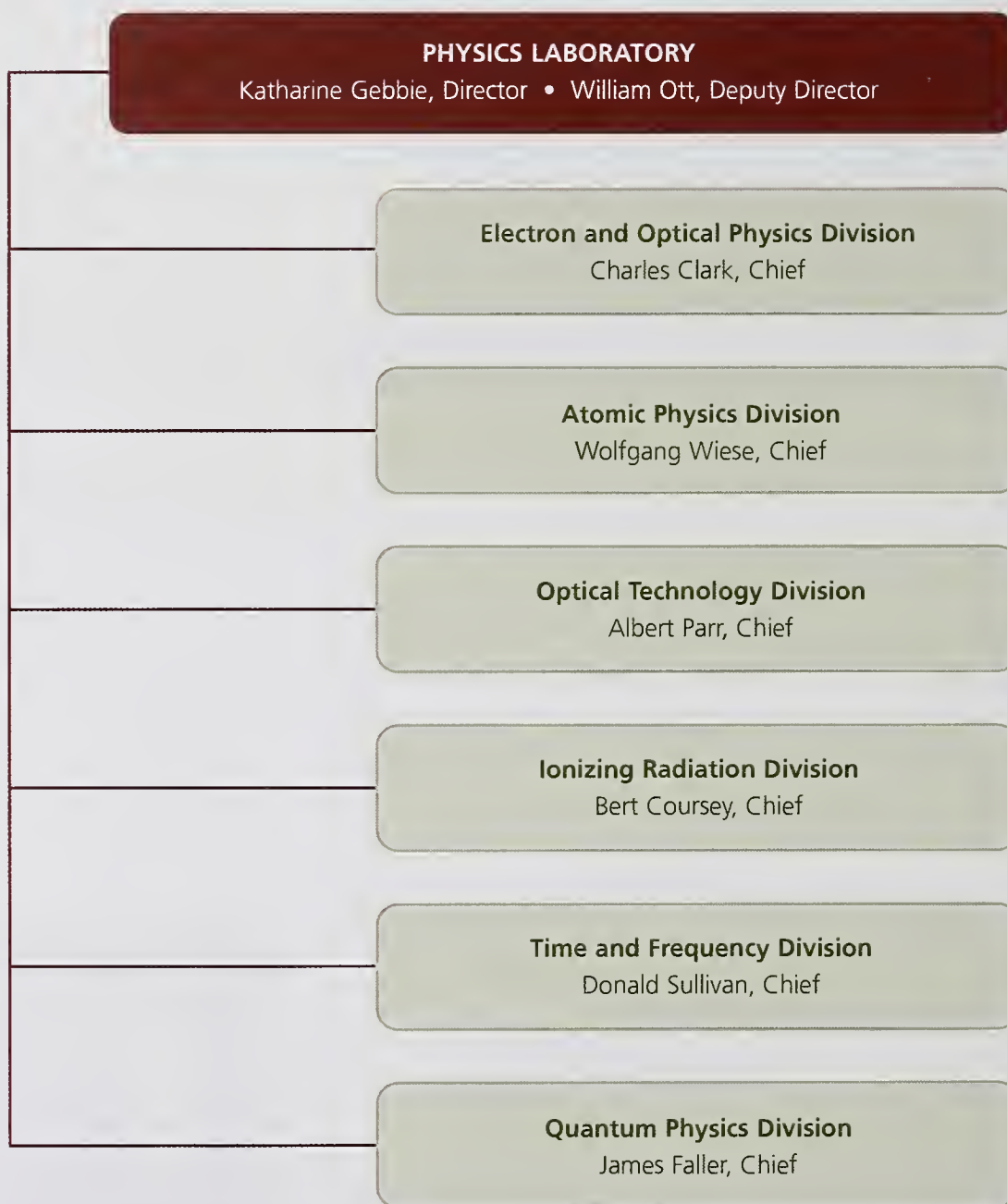
- Department of Defense
- National Aeronautics and Space Administration
- Department of Energy
- Department of Commerce
- Department of Health and Human Services
- National Science Foundation
- Environmental Protection Agency
- Department of Justice

| PHYSICS LABORATORY RESOURCES 1998 - 2002 (\$ MILLIONS) | | | | | |
|---|-------------|-------------|-------------|-------------|-------------|
| | 1998 | 1999 | 2000 | 2001 | 2002 |
| STRS | 33.1 | 34.7 | 34.8 | 37.1 | 39.9 |
| ATP | 1.8 | 1.8 | 1.8 | 2.1 | 2.9 |
| OA | 9.5 | 10.2 | 10.6 | 11.9 | 13.6 |
| Other | 3.8 | 3.7 | 4.4 | 4.5 | 5.0 |
| TOTAL | 48.2 | 50.4 | 51.6 | 55.6 | 61.4 |

Representative Private Sector Collaborators

- American Association of Physicists in Medicine
- American National Standards Institute
- American Physical Society
- American Society for Testing and Materials
- Commission Internationale de l’Éclairage
- Council for Optical Radiation Measurements
- Council on Ionizing Radiation Measurements and Standards
- Electric Power Research Institute
- EUV LLC
- Illuminating Engineering Society of North America
- Institute of Electrical and Electronics Engineers
- International Electrotechnical Commission
- International Organization for Standardization
- National Council on Radiation Protection and Measurements
- NCSL International
- Nuclear Energy Institute
- Optical Society of America
- Optoelectronics Industry Development Association
- International SEMATECH
- SAE International
- SPIE—The International Society for Optical Engineering

ORGANIZATIONAL CHART





EDITORS:

Jonathan E. Hardis, William R. Ott,
and Gloria G. Wiersma

Physics Laboratory, National Institute
of Standards and Technology


U.S. Department of Commerce
Donald L. Evans, Secretary

Technology Administration
Phillip J. Bond, Under Secretary for Technology

National Institute of Standards and Technology
Arden L. Bement, Jr., Director

NIST SP 994
February 2003

Disclaimer: any mention of commercial products is for information only; it does not imply NIST recommendation or endorsement, nor does it imply that the products mentioned are necessarily the best available for the purpose.



NIST PHYSICS LABORATORY
100 Bureau Drive, Stop 8400
Gaithersburg, MD 20899-8400

[www@physics.nist.gov](http://www.physics.nist.gov)